DEVELOPMENTS IN ENVIRONMENTAL MODELLING 21

FUNDAMENTALS OF ECOLOGICAL MODELLING

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S.E. Jørgensen and
G. Bendoricchio

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Preface, Third Edition

It is intended that this book be suitable for a variety of engineers and ecologists, who may wish to gain an introduction to the rapidly growing field of ecological and environmental modelling. An understanding of the fundamentals of environmental problems and ecology, as presented for instance in the textbook *Principles of Environmental Science and Technology* is assumed. Furthermore, it is assumed that the reader has either a fundamental knowledge of differential equations and matrix calculations or has read the Appendix, which gives a brief introduction to these topics.

Only a very few books have been published that give an introduction to ecological modelling. Although some cover particular aspects of the subject—population dynamics, for instance—a book covering the entire spectrum of ecological modelling is very difficult to find. There seems to be a need, therefore, for a book that is applicable to courses in this subject. Although many books have been published on the topic they usually require the reader to already have an understanding of the field or at least to have had some experience in the development of ecological models. This book aims to bridge the gap.

It has been the authors' aim to give an overview of the field which, on the one hand, includes the latest developments and, on the other, teaches the reader to develop his or her own models. An attempt has been made to meet these objectives by including the following:

1. A detailed discussion of the modelling procedure with a step-by-step presentation of the development of the model. The advantages and shortcomings of each step are discussed and simple examples illustrate all the steps. The volume contains many illustrations and examples; the illustrations are models explained in sufficient detail to allow the reader to construct the models, while the examples are modelling itself. Further exercises in the form of problems can be found at the end of most chapters.

2. A presentation of most model types which includes the theory, overview tables on applications, complexity, examples and illustrations.

3. A detailed presentation of both simple and complex models as illustrations of how to develop a model in practice. All the considerations behind the selection of the final model, particularly its complexity, are covered to ensure that the reader understands all the steps of modelling in detail. The previous edition of this book gave information about more models, but today such an extensive overview is hardly possible: the field has grown so rapidly in last 5–10 years that the literature contains probably twice as many models today as it did in 1994 when the second edition was published.

Emphasis has been placed on understanding the nature of models. Models are very useful tools in ecology and environmental management, but if developed and used carelessly, they can do more harm than good. Modelling is not just a mathematical exercise, it requires a profound knowledge of the system to be modelled. This is illustrated several times throughout the book.

After an introductory chapter, Chapter 2 deals with the modelling procedure in all phases. The author attempts to provide a complete answer to the question of how to model a biological system.

Chapter 3 gives an overview of applicable submodels or unit processes, i.e., elements in models. This chapter has been expanded considerably for this edition. Professor Bendoricchio, who is co-author of this third edition, used the second edition of the book in his course on environmental and ecological modelling at Padova University, but found that a more comprehensive presentation of most of the basic equations applied in modelling was needed. This textbook has certainly gained in value by this expansion of the overview of the applied mathematical expression. In addition, as a mathematician, Professor Bendoricchio has presented the mathematical considerations behind the submodels in a more correct form.

Chapter 4 reviews different methods of model conceptualization. As different modellers prefer different methods, it is important to present all the available methods.

The ambitious modeller would go for a dynamic model, but often the problem, system and/or the data might require that a simpler static model be applied. **In many contexts, a static model is completely satisfactory.** Chapter 5 presents various types of static models and gives detailed information about one model which serves as a good illustration of the development, usefulness and practical application of static models.

In principle, there is no difference between population models and other models, but they have a different history and are used to solve different problems. Chapter 6 gives an overview of population models: a more comprehensive treatment of this subject must however be found in books focusing entirely on this type of model. Ecological models in their broadest sense also comprise population dynamic models and ecological applications of such models are therefore included in this chapter.

Chapter 7 covers dynamic biogeochemical models. Eutrophication models and wetland models are used as illustrations.

Models of toxic substances in the environment and in the organism are covered in Chapter 8. This type of model has recently found a very wide use in environmental risk assessment. It was therefore considered important to give a comprehensive treatment of the development and application of ecotoxicological models.

Finally, Chapter 9 describes a recent development in ecological modelling: how to give models the properties of softness and flexibility which we know that ecosystems have. Different approaches to this question are presented and discussed. The application of chaos and catastrophe theory in modelling are also included, and the last section of the chapter describes four recently developed modelling techniques, including the use of machine learning and neural networks in ecological modelling.

The volume is completed by three appendices and a subject index. To help the reader to locate index terms in the text, all words included in the subject index are italicised in the text.

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CHAPTER 1

Introduction

1.1 Physical and Mathematical Models

Mankind has always used models as tools to solve problems as they give a simplified picture of reality. The model will, of course, never contain *all* the features of the real system, because then it would be the real system itself, but it is important that the model contains the characteristic features that are essential in the context of the problem to be solved or described.

The philosophy behind the use of models might best be illustrated by an example. For many years we have used physical models of ships to determine the profile that gives a ship the smallest resistance in water. Such a model will have the shape and the relative main dimensions of the real ship, but will not contain all the details such as, e.g., the instrumentation, the lay-out of the cabins, etc. These details are, of course, irrelevant to the objectives of that model. Other models of the ship will serve other aims: blue prints of the electrical wiring, lay-out of the various cabins, drawings of pipes, etc.

Correspondingly, an ecological model must contain the features that are of interest for the management or scientific problem we wish to solve. An ecosystem is a much more complex system than a ship, and it is therefore far more complicated to capture the main features of importance for an ecological problem. However, intense research in recent decades has made it possible today to set up workable ecological models.

Ecological models may also be compared with geographical maps (which themselves are models). Different types of maps serve different purposes: there are maps for aeroplanes, for ships, for cars, for railways, for geologists and archaeologists and so on. They are all different because they focus on different objects. They are also available in different scales according to the application of the map and to the underlying knowledge. Furthermore, a map never contains all the details of a particular geographical area because they would be irrelevant and distract from the

main purpose of the map. If, for instance, a map were to contain details of the positions of all cars at any given moment, the map would be invalidated very rapidly as the cars would have moved to new positions. A map therefore contains only the knowledge that is relevant for the user of the map.

In the same way, an ecological model focuses only on the objects of interest for the problem under consideration—too many irrelevant details would cloud the main objectives of a model. There are, therefore, many different ecological models of the same ecosystem, the appropriate version being selected according to the model's goals.

The model might be physical, such as the ship model used for the resistance measurements, which may be called micro cosmos or it might be a mathematical model describing the main characteristics of the ecosystem and the related problems in mathematical terms.

Physical models will only be touched on very briefly in this book, which will focus entirely on the construction of mathematical models. The field of ecological modelling has developed rapidly during the last two decades due essentially to three factors:

1. the development of computer technology, which has enabled us to handle very complex mathematical systems;
2. a general understanding of pollution problems, including the knowledge that a complete elimination of pollution is not feasible ("*zero discharge*"), but that proper pollution control with the limited economical resources available requires serious consideration of the influence of pollution impacts on ecosystems;
3. our knowledge of environmental and ecological problems has increased significantly; in particular, we have gained more knowledge of quantitative relationships in the ecosystems and between ecological properties and environmental factors.

Models may be considered to be a synthesis of what we know about the ecosystem with reference to the considered problem, as opposed to a statistical analysis, which will only reveal the relationships between the data. A model is able to encompass our entire knowledge about the system:

- which components interact with which others, i.e., zooplankton grazes on phytoplankton,
- the processes often formulated as mathematical equations which have been proved valid generally, and
- the importance of the processes with reference to the problem,

to mention a few examples of knowledge which may often be incorporated in an ecological model. This implies that a model can offer a deeper understanding of the system than a statistical analysis and can thereby yield a much better management plan for how to solve the focal environmental problem. This does not, of course, imply that statistical analytical results are ignored in modelling. On the contrary,

models are built on all available tools simultaneously including statistical analyses of data, physical–chemical–ecological knowledge, the laws of nature, common sense, and so on. This is the advantage of modelling.

1.2 Models as a Management Tool

The idea behind the use of ecological management models is demonstrated in Fig. 1.1. Urbanization and technological development have had an increasing impact on the environment. Energy and pollutants are released into ecosystems, where they may cause more rapid growth of algae or bacteria, may damage species, or alter the entire ecological structure. An ecosystem is extremely complex and so it is an overwhelming task to predict the environmental effects that such emissions will have. It is here that the model comes into the picture. With sound ecological knowledge, it is possible to extract the features of the ecosystem that are involved in the pollution problem under consideration in order to form the basis of the ecological model (see also the discussion in Chapter 2). As indicated in Fig. 1.1, the resulting model can be used to select the environmental technology best suited to the solution of specific environmental problems, or to legislation for reducing or eliminating the emission set up.

Figure 1.1 represents the ideas behind the introduction of ecological modelling as a management tool in around 1970. Today, environmental management is more complex and must *apply environmental technology*, *cleaner technology* as an alternative to the present technology and ecological engineering or *ecotechnology*. This latter technology is applied to solving problems of non-point or *diffuse pollution*, mainly originating from agriculture. The importance of *non-point pollution* was barely acknowledged before around 1980. Furthermore, global environmental problems play a more important role today than they did twenty years ago. The abatement of the *greenhouse effect* and the *depletion of the ozone layer* are widely

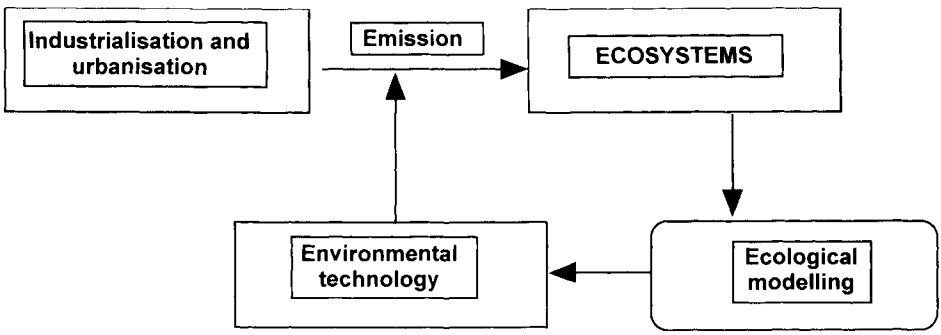

Fig. 1.1. Relationships between environmental science, ecology, ecological modelling and environmental management and technology.

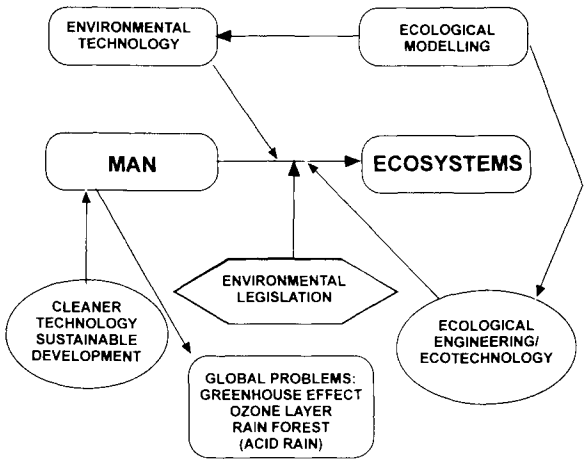

Fig. 1.2. The idea behind the use of environmental models in environmental management. Today, environmental management is very complex and must apply environmental technology, alternative technology and ecological engineering or ecotechnology. In addition, global environmental problems play an increasing role. Environmental models are used to select environmental technology, environmental legislation and ecological engineering.

discussed and several international conferences at governmental level have taken the first steps toward the use of international standards to solve these crucial problems. Figure 1.2 attempts to illustrate the more complex picture of environmental management today.

1.3 Models as a Scientific Tool

Models are widely used instruments in science. The scientist often uses physical models to carry out experiments *in situ* or in the laboratory to eliminate disturbance from processes irrelevant to his investigation. Chemostats are used, e.g., to measure algal growth as a function of nutrient concentrations. Sediment cores are examined in the laboratory to investigate sediment–water interactions without disturbance from other ecosystems components. Reaction chambers are used to find reaction rates for chemical processes etc.

However, mathematical models are also widely applied in science. Newton's laws are relatively simple mathematical models of the influence of gravity on bodies, but they do not account for frictional forces, influence of wind, etc. Ecological models do not differ essentially from other scientific models, not even by their complexity, as many models used in nuclear physics during the last decades might be even more complex than ecological models. The application of models in ecology is almost compulsory if we want to understand the function of such a complex system as an ecosystem. It is simply not possible to survey the many components of and their

reactions in an ecosystem without the use of a model as a synthesis tool. The reactions of the system might not necessarily be the sum of all the individual reactions; this implies that the properties of the ecosystem as a system cannot be revealed without the use of a model of the entire system.

It is therefore not surprising that ecological modelling has been used increasingly in ecology as an instrument to understand the properties of ecosystems. This application has clearly revealed the advantages of models as a useful tool in ecology, which can be summarized in the following points:

1. Models are useful instruments in the ***survey*** of complex systems.
2. Models can be used to reveal ***system properties***.
3. Models reveal the weakness in our knowledge and can therefore be used to set up research priorities.
4. Models are useful in tests of ***scientific hypotheses*** as the model can simulate ecosystem reactions, which can be compared with observations.

As will be illustrated several times throughout this book, we can use models to test the hypothesis of ecosystem behaviour, such as for instance, the principle of maximum power presented by H.T. Odum (1983), the concepts of ascendancy presented by Ulanowicz (1986), the various proposed thermodynamic principles of ecosystems and the many tests of *ecosystem stability concepts*.

The certainty of the hypothesis test using models is, however, not on the same level as the tests used in the more reductionistic science. Here, if a relationship is found between two or more variables by, for instance, the use of statistics on available data, the relationship is tested afterwards on several additional cases to increase the scientific certainty. If the results are accepted, the relationship is ready to be used to make predictions, and these predictions are again examined to see if they are wrong or right in a new context. If the relationship still holds, we are satisfied and a wider scientific use of the relationship is made possible.

When we are using models as scientific tools to test hypotheses, we have a 'double doubt'. We anticipate that the model is correct in the problem context, but the model is a hypothesis of its own. We therefore have four cases instead of two (acceptance/non-acceptance):

1. The model is correct in the problem context, and the hypothesis is correct.
2. The model is not correct, but the hypothesis is correct.
3. The model is correct, but the hypothesis is not correct.
4. The model is not correct and the hypothesis is not correct.

In order to omit cases 2 and 4, only very well examined and well accepted models should be used to test hypotheses on system properties, but our experience in modelling ecosystems today is unfortunately limited. We do have some well examined models, but we are not completely certain that they are correct in the problem

context and we would generally need a wider range of models. A wider experience in modelling may therefore be a prerequisite for further development in ecosystem research.

The use of a models as scientific tools in the sense described above is not only found in ecology: other sciences use the same technique when complex problems and complex systems are under investigation. There are simply no other possibilities when we are dealing with irreducible systems (Wolfram, 1984a; 1984b). Nuclear physics has used this procedure to find several new nuclear particles. The behaviour of protons and neutrons has given inspiration to models of their composition of smaller particles, the so-called quarks. These models have been used to make predictions of the results of planned cyclotron experiments, which have often given inspiration to further changes of the model.

The idea behind the use of models as scientific tools, may be described as an iterative development of a pattern. Each time we can conclude that case 1 (see above for the four cases) is valid, i.e., both the model and the hypothesis are correct, we can add another 'piece to the pattern'. And that of course provokes a question which signifies an additional test of the hypothesis: does the piece fit into the general pattern? If not, we can go back and change the model and/or the hypothesis, or we may be forced to change the pattern, which of course will require more comprehensive investigations. If the answer is 'yes', we can use the piece at least temporarily in the pattern, which is then used to explain other observations, improve our models

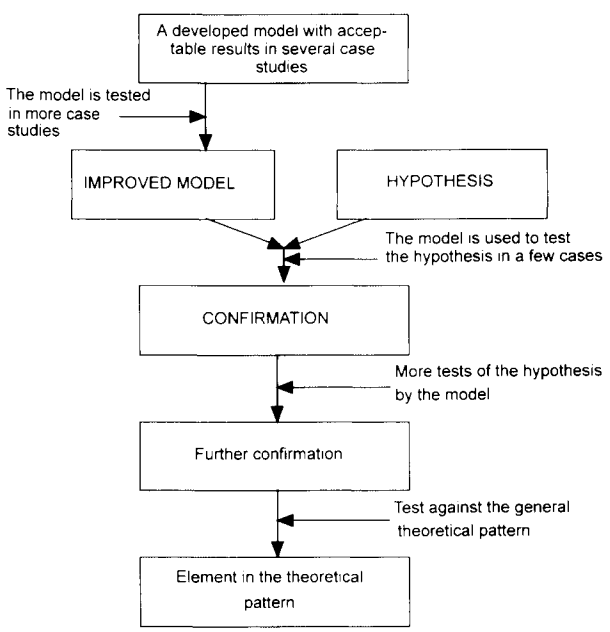

Fig. 1.3. Diagram showing how several test steps are necessary for a model to be used to test a hypothesis about ecosystems, as a model may be considered a hypothesis of its own.

and make other predictions, which are then tested. This procedure is used repeatedly to proceed step-wise towards a better understanding of nature on the system level. Figure 1.3 illustrates the procedure in a conceptual diagram.

We are not very far advanced in the application of this procedure today in ecosystem theory. As already mentioned, we need much more modelling experience. We also need a more comprehensive application of our ecological models in this direction and context.

1.4 Models and Holism

Biology (ecology) and physics developed in different directions until 30–50 years ago. There have since been several indications of a more parallel development that has been observed during the last decades: one which has its roots in the more general trends in science.

The basic philosophy or thinking in the sciences is currently changing with other facets of our culture such as the arts and fashion. During the last two to three decades, we have observed such a shift. The driving forces behind such developments are often very complex and are difficult to explain in detail, but we will attempted to show here at least some of developmental tendencies:

1. Scientists have realized that the world is more complex than we thought some decades ago. In nuclear physics we have found several new particles and, faced with environmental problems, we have realized how complex nature is and how much more difficult it is to cope with problems in nature than in laboratories. Computations in sciences were often based on the assumption of so many simplifications that they became unrealistic.

2. Ecosystem–ecology, which we may call the science of (the very complex) ecosystems, has developed very rapidly during recent decades and has revealed the need for systems sciences and also for interpretations, understanding and implications of the results obtained in other sciences, including physics.

3. It has been realized in the sciences that many systems are so complex that it may never be possible to know all the details. In nuclear physics there is always an uncertainty in our observations, expressed by *Heisenberg's uncertainty relations*. The uncertainty is caused by the influence of our observations on nuclear particles. We have similar uncertainty relationships in ecology and environmental sciences caused by the complexity of the systems. A further presentation of these ideas is given in Chapter 2, where the complexity of ecosystems is discussed in more detail. In addition, many relatively simple physical systems such as the atmosphere show chaotic behaviour which makes long-term predictions impossible (see Chapter 9). The conclusion is unambiguous: we cannot and will never be able to, know the world with complete accuracy. We have to acknowledge that these are the conditions for modern sciences.

4. It has been realized that many systems in nature are irreducible systems (Wolfram, 1984a and 1984b), i.e., it is not possible to reduce observations of system behaviour to a law of nature, because the system has so many interacting elements that the reaction of the system cannot be surveyed without use of models. For such systems other experimental methods must be applied. It is necessary to construct a model and compare the reactions of the model with our observations in order to test its reliability and gain ideas for its improvement, then construct an improved model, compare its reactions with our observations and again gain new ideas for further improvements, and so forth. By such an iterative method we may be able to develop a satisfactory model that can describe our observations properly. The observations do not result in a new law of nature but in a new model of a piece of nature; but as seen by description of the details in the model development, the model should be constructed based on causalities which inherit basic laws.

5. Modelling as a tool in science and research has developed as a result of the tendencies 1–4 above. Ecological or environmental modelling has become a scientific discipline in its own right—a discipline that has experienced rapid growth during the last decade. Developments in computer science and ecology have of course favoured this rapid growth in modelling as they are the components on which modelling is founded.

6. The scientific analytical method has always been a very powerful tool in research, yet there has been an increasing need for scientific synthesis, i.e., for putting the analytical results together to form a holistic picture of natural systems. Due to the extremely high complexity of natural systems it is not possible to obtain a complete and comprehensive picture of natural systems by analysis alone, but it is necessary to synthesize important analytical results to get system properties. The synthesis and the analysis must work hand in hand. The synthesis (i.e., in the form of a model) will show that analytical results are needed to improve the synthesis and new analytical results will then be used as components in the synthesis. There has been a clear tendency in sciences to give the synthesis a higher priority than previously. This does not imply that the analysis should be given a lower priority. Analytical results are needed to provide components for the synthesis, and the synthesis must be used to give priorities for the necessary analytical results. No science exists without observa-

Table 1.1. Matrix approach and pathways to integration

	Reductionistic/analytical	*Holistic*/integrative
In-depth single case	Parts and processes, linear causalities, etc.	Dynamic modelling, etc.
Comparative cross-sectional	Loading-trophic state; general plankton model, etc.	Trophic topology and metabolic types, homeostasis, ecosystem behaviour.

tions, but neither can science be developed without digesting and assimilating the observations to form a picture or pattern of nature. Analysis and synthesis should be considered as two sides of the same coin. Vollenweider (1990) exemplifies these underlying ideas in limnological research by using a matrix approach that combines in a realistic way reductionism and holism, and single case and cross-sectional methodologies. The matrix is reproduced from Vollenweider (1990) in Table 1.1 and it is demonstrated here that all four classes of research and their integration are needed to gain a wider understanding of, in this case, lakes as ecosystems.

7. A few decades ago the sciences were more optimistic than they are today in the sense that it was expected that a complete description of nature would soon be a reality. Einstein even talked about a "world equation", which should be the basis for all physics of nature. Today it is realized that it is not that easy and that nature is far more complex. Complex systems are non-linear and may sometimes react chaotically (see also Chapter 9 in which the applications of chaos theory and catastrophe theory in modelling are be presented). Sciences have a long way to go and it is not expected that the secret of nature can be revealed by a few equations. It may work in laboratories, where the results can usually be described by using simple equations, but when we turn to natural systems, it will be necessary to apply many and complex models to describe our observations.

1.5 The Ecosystem as an Object for Research

Ecologists generally recognize ecosystems as a specific level of organization, but the open question is the appropriate selection of time and space scales. Any size area could be selected, but in the context of this book, the following definition presented by Morowitz (1968) will be used: "An ecosystem sustains life under present-day conditions, which is considered a property of ecosystems rather than a single organism or species." This means that a few square metres may seem adequate for microbiologists, while 100 square kilometres may be insufficient if large carnivores are considered (Hutchinson, 1978).

Population–community ecologists tend to view ecosystems as networks of interacting organisms and populations. Tansley (1935) found that an ecosystem includes both organisms and chemical–physical components and this inspired Lindeman (1942) to use the following definition: "An ecosystem composes of physical–chemical–biological processes active within a space–time unit." E.P. Odum (1953) followed these lines and is largely responsible for developing the process–functional approach which has dominated the last few decades.

This does not mean that different views cannot be a point of entry. Hutchinson (1948) used a cyclic causal approach, which is often invisible in population–community problems. Measurement of inputs and outputs of total landscape units has been the emphasis in the functional approaches by Bormann and Likens (1967).

O'Neill (1976) has emphasized energy capture, nutrient retention and rate regulations. H.T. Odum (1957) has underlined the importance of energy transfer rates. Quilin (1975) has argued that cybernetic views of ecosystems are appropriate and Prigogine (1947), Mauersberger (1983) and Jørgensen (1981) have all emphasized the need for a thermodynamic approach to the proper description of ecosystems.

For some ecologists, ecosystems are either biotic assemblages or functional systems: the two views are separated. It is, however, important in the context of ecosystem theory to adopt both views and to integrate them. Because an ecosystem cannot be described in detail, it cannot be defined according to Morowitz's definition, before the objectives of our study are presented. Therefore the definition of an ecosystem used in the context of ecosystem theory as presented in this volume, becomes:

- ***An ecosystem is a biotic and functional system or unit, which is able to sustain life and includes all biological and non-biological variables in that unit. Spatial and temporal scales are not specified* a priori, *but are entirely based upon the objectives of the ecosystem study.***

Currently there are several approaches (Likens, 1985) to the study of ecosystems:

1. *Empirical studies* where bits of information are collected and an attempt is made to integrate and assemble these into a complete picture.
2. *Comparative studies* where a few structural and a few functional components are compared for a range of ecosystem types.
3. Experimental studies where manipulation of a whole ecosystem is used to identify and elucidate mechanisms.
4. Modelling or computer simulation studies.

The motivation in all of these approaches (Likens, 1983; 1985) is to achieve an understanding of the entire ecosystem, giving more insight than the sum of knowledge about its parts relative to the structure, metabolism and biogeochemistry of the *landscape*.

Likens (1985) has presented an excellent ecosystem approach to Mirror Lake and its environment. The study contains all the above-mentioned studies, although the modelling part is rather weak. The study demonstrates clearly that it is necessary to use *all* four approaches to achieve a good picture of the system properties of an ecosystem. An ecosystem is so complex that you cannot capture all the system properties by one approach.

Ecosystem studies widely use the notions of order, complexity, randomness and organization; they are used interchangeably in the literature, which causes much confusion. As the terms are used in relation to ecosystems throughout this book, it is necessary to give a clear definition of these concepts in this introductory chapter.

According to Wicken (1979, p. 357), randomness and order are each other's antithesis and may be considered as relative terms. Randomness measures the amount of information required to describe a system. The more information is required to describe the system, the more random it is.

Organized systems are to be carefully distinguished from ordered systems. Neither kinds of system is random, but whereas ordered systems are generated according to simple algorithms, and may therefore lack complexity, organized systems must be assembled element by element according to an external wiring diagram with a high level of information. Organization is functional complexity and carries functional information. It is non-random by design or by selection, rather than *a priori* by necessity.

Saunder and Ho (1981) claim that complexity is a relative concept dependent on the observer. We will adopt Kay's definition (Kay, 1984, p. 57), which distinguishes between *structural complexity*, defined as the number of interconnections between components in the system and *functional complexity*, defined as the number of distinct functions carried out by the system.

1.6 Outline of the Book

The third edition of this book presented a few models in all details while a number of models were just mentioned briefly. An overview of existing models was included in several chapters. During the last decade, the number of models has increased considerably as can be seen from the increasing number of pages published annually in the journal *Ecological Modelling*. It is therefore hardly possible today, within the framework of a textbook, to give an overview of all existing models. Consequently, it has been decided to write this modelling textbook around a few detailed illustrative examples for each of those model types that are most applied, with the aim of enabling the reader to learn to develop a range of useful models of different types. Those interested in a survey of existing models are referred to Jørgensen et al. (1995), where more than 400 models have been reviewed.

Chapter 2 presents a step-wise procedure to develop models, from the problem to the final test (validation) of a prognosis, based on the developed model. Particular emphasis is given to the following crucial steps: sensitivity analysis, parameter estimation included calibration, validation, selection of model complexity and model type, and model constraints. Selection of computer language is not covered because every modeller has his/her own preference. An illustration in Chapter 2 will, however, demonstrate the use of three different languages for one model.

Chapter 3 is a comprehensive presentation of a number of useful process descriptions by mathematical equations. The most relevant physical (Part A), chemical (Part B) and biological (ecological) (Part C), including ecotoxicological processes are covered in this chapter. These are the building blocks of ecological models. A useful ecological model consists of the right combination of buildings blocks.

Conceptualization of the model is an important step in model development. The ideas about how the ecosystem functions and is influenced by the various impacts on the system are illustrated and conceptualized in a diagram showing the components of the system and how they are interrelated. The methods most applied to conceptualize the model are presented in Chapter 4. Chapters 2–4 give details of the

general modelling tools: details about the step-wise development of ecological models, mathematical formulation of the processes and conceptualization of the ideas and thoughts behind the model.

Chapters 5–9 focus on specific type of models. The following issues are touched on for each type: characteristics, applicability, a brief overview of the application of the model type and one or a few illustrative, detailed examples or case studies, in which considerations of the step-wise development of the model are discussed.

Chapter 5 looks into *static models*. After the characteristic traits by this model type are presented, an illustrative detailed example is discussed. It is a model of the Lagoon of Venice by application of the steady-state software ECOPATH. Response models are also presented. The Vollenweider model for temperate lakes is used as an illustration of this type of model.

Chapter 6 covers population dynamic models. After a short presentation of a few simple classical models, some illustrative examples are presented, including an example with age distribution based on a matrix representation.

Chapter 7 is devoted to dynamic, *biogeochemical models* based on coupled differential equations. Development of *eutrophication* models and *wetland models* are used as typical, illustrative examples of biogeochemical models. Eutrophication is one of the most modelled environmental problems (see also next section). A wide spectrum of models of differing complexity has been developed. The general and important discussion on "which model to select or which model complexity to select" is therefore neatly illustrated by eutrophication models. Consequently, models of differing complexity from the simple so-called Vollenweider plot (presented in Chapter 5 as it is a *static model*) to very complex models with many variables and where they have found most application are discussed. Details of a model of medium-to-high complexity are also given to illustrate all the considerations that must be made to develop a model step by step, from discussion of process equations and *submodels* to prognosis validation and the general applicability of the model.

Chapter 8 focuses on ecotoxicological models. These are different from other type of models, as will be demonstrated; they are often relatively simple, as already illustrated by the steady-state example in Chapter 5. Parameter estimation of ecotoxicological parameters is particularly demanding and a number of methods are available which are briefly discussed in this chapter. Early in the chapter, it is discussed how to perform an Environmental Risk Assessment (ERA). The open question is how to find the Predicted Environmental Concentration (PEC), in what should be a realistic, but worst case. The use of toxic substance models has rapidly increased during the last decade due to a wider application of ERA. It is, therefore, natural to include an overview of this specific use of *ecotoxicological models* in this chapter.

Some examples are included in the chapter:

- An ecotoxicological ecosystem model of a specific case, namely chromium pollution in a Danish fjord. This model is very simple due to chromium's chemical properties and a relatively simple hydrodynamics. It is a proper case study to

apply to enable a discussion of which processes and additional variables we need to include in other case studies with a more complex chemistry and a more complex hydrodynamic situation. Furthermore, a mercury model of a bay is used to illustrate such a more complex model. The chapter also presents an example of lead and cadmium contamination of soil and crops.

- A *McKay-type model* which is mostly applied to gain an overview of the consequences of using a specific chemical, as the distribution of the chemical in the spheres is obtained as model result. The model is used for an entire region and therefore gives only first estimations, which are, however, very useful for comparing the environmental consequences of two alternative chemicals.

Chapter 9 covers the following recently developed model types:

- *fuzzy models* which are mostly used in a data-poor situation
- models showing *chaotic behaviour*
- catastrophe models which can be described as a relatively rapid shift in structure under certain sometimes well defined circumstances
- *structurally dynamic models* which consider one of the core properties of ecosystems: adaptation by change of the properties of the biological components or by a shift to other better-fitted species. This development is considered of utmost importance, because the aim of the application of models in environmental management is to be able to predict the effect of a given change in the impact on the ecosystem under consideration. In other words, we change the conditions of the system which inevitably implies that the properties of the biological ecosystem components are changed. The properties found under the previous conditions are therefore no longer valid, and the prognosis will be wrong if the model does not take into account the changes in properties resulting from a change in the prevailing conditions.

The application of objective and individual modelling are relatively recent ideas offering some advantages. These will be discussed in this last chapter, but are also briefly mentioned in Chapter 2 in the section on "Selection of Model Type". The application of expert knowledge and artificial intelligence in models offers, under certain circumstances, significant advantages. These advantages are reviewed in Chapter 9.

To summarize, this volume describes in complete detail how to build an ecological model, including all considerations that must be taken into account in the step-wise applied procedure. This topic is covered in Chapters 2–4. Chapters 5–9 give illustrative, very detailed examples for the model types most applied, which will enable readers to develop similar models for their own combination of ecosystem and problem. The types are: steady-state models, population dynamic models, dynamic *biogeochemical models*, *ecotoxicological models* which have their own

particular traits, fuzzy models, catastrophe models, individual models, objective models, application of expert knowledge and artificial intelligence in modelling and structurally dynamic models.

1.7 The Development of Ecological and Environmental Models

This section attempts to present briefly the history of ecological and environmental modelling. From history, we can learn why it is essential to draw upon previously gained experience and what can go wrong when we do not follow the recommendations that we have been able to set up to avoid previous flaws.

Figure 1.4 gives an overview of the development in ecological modelling. The non-linear time axis gives approximate information on the year in which the various

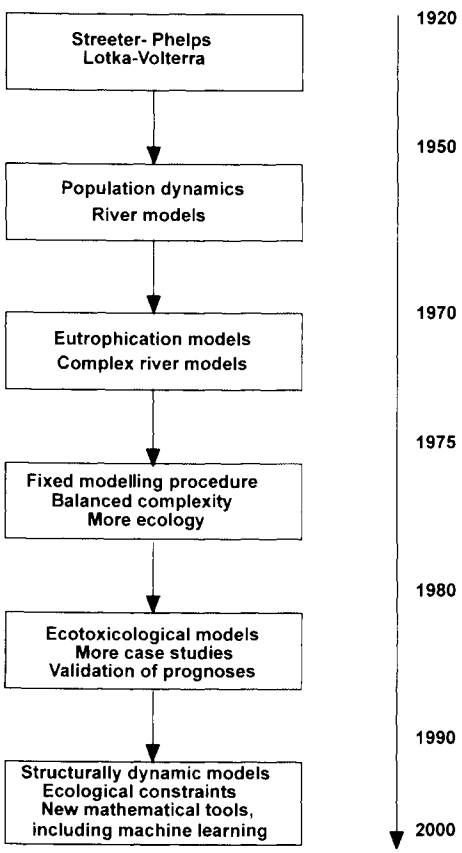

Fig. 1.4. The development of ecological and environmental models is shown schematically.

development steps took place. The first models of the oxygen balance in a stream (the *Streeter–Phelps model*, presented in Chapter 3) and of the prey–predator relationship (the *Lotka–Volterra model*, presented in Chapter 6) were developed in the early 1920s. In the 1950s and 60s further development of population dynamic models took place. More complex river models were also developed in the 60s. These developments could be called the second generation of models.

The wide use of ecological models in environmental management started around the year 1970, when the first *eutrophication* models emerged and very complex river models were developed. These models may be called the third generation of models. They are characterized by often being too complex, because it was so easy to write computer programs to handle rather complex models. To a certain extent, it was the revolution in computer technology that created this model generation. It became clear, however, in the mid-1970s that the limitations in modelling were not the computer and the mathematics, but the data and our knowledge about ecosystems and ecological processes. The modellers therefore became more critical in their acceptance of models; they realized that a profound knowledge of the ecosystem, the problem and the ecological components were the necessary basis for the development of sound ecological models. A result of this period is all the recommendations given in the next chapter:

- follow strictly all the steps of the procedure, i.e., conceptualization, selection of parameters, verification, calibration, examination of sensitivity, validation, etc.;
- find a complexity of the model which considers a balance between data, problem, ecosystem and knowledge;
- a wide use of sensitivity analyses is recommended in the selection of model components and model complexity;
- make *parameter estimations* by using all the methods, i.e., literature review, determination by measurement in laboratory or *in situ*, use of intensive measurements, calibration of *submodels* and the entire model, theoretical system ecological considerations and various estimation methods based on *allometric principles* and chemical structure of the considered chemical compounds.

Parallel to this development, ecologists became more quantitative in their approach to environmental and ecological problems, probably because of the needs formulated by environmental management. The quantitative research results of ecology from the late 1960s until today have been of enormous importance for the quality of the ecological models. They are probably just as important as the development in computer technology.

The models from this period, from the mid-1970s to the mid-1980s, could be called the fourth generation of models. The models from this period are characterized by having a relatively sound ecological basis, with emphasis on realism and simplicity. Many models were validated in this period with an acceptable result and for a few it was even possible to validate the prognosis.

The conclusions from this period may be summarized as follows:

1. Provided that the recommendations given above were followed and the underlying database was of good quality, it was possible to develop models, that could be used as prognostic tools.
2. Models based on a database of not completely acceptable quality should probably not be used as a prognostic tool, but they could give an insight into the mechanisms behind the environmental management problem, which is valuable in most cases. Simple models are often of particular value in this context.
3. Ecologically sound models, i.e., models based upon ecological knowledge, are powerful tools in understanding ecosystem behaviour and as tools for setting up research priorities. The understanding may be qualitative or semi-quantitative, but has in any case proved to be of importance for ecosystem theories and better environmental management.

1.8 State of the Art in the Application of Models

The shortcomings of modelling were, however, also revealed. It became clear that the models were rigid in comparison with the enormous flexibility, which was characteristic of ecosystems. The hierarchy of feedback mechanisms that ecosystems possess was not accounted for in the models, which made the models incapable of predicting adaptation and structural dynamic changes. Since the mid-1980s, modellers have proposed many new approaches, such as (1) *fuzzy modelling*, (2) examination of catastrophic and chaotic behaviour of models, and (3) application of goal functions to account for adaptation and structural changes. Application of objective and individual modelling, expert knowledge and artificial intelligence offers some new additional advantages in modelling. Chapter 9 discusses when it is advantageous to apply these approaches and what can be gained by their application. All these recent developments may be called the fifth generation of modelling.

Table 1.2 reviews types of ecosystems that have been modelled by *biogeochemical models* up to the year 2000. An attempt has been made to indicate the modelling effort by using a scale from 0 to 5 (see the table for an explanation of the scale).

Table 1.3 similarly reviews the environmental problems which have been modelled until today. The same scale is applied to show the modelling effort as in Table 1.2. Besides *biogeochemical models*, Table 1.3 also covers models used for the management of population dynamics in national parks and steady-state models applied as ecological indicators (see Section 6.4). It is advantageous to apply goal functions in conjunction with a steady-state model to obtain a good ecological indication, as proposed by Christensen (1991: 1992). This is touched on in Chapter 9, where various goal functions and their application are presented.

Table 1.2. Biogeochemical models of ecosystems

Ecosystem	Modelling effort (on a scale of 0 to 5)*
Rivers	5
Lakes, reservoirs, ponds	5
Estuaries	5
Coastal zone	4
Open sea	3
Wetlands	4–5
Grassland	4
Desert	1
Forests	4
Agricultural land	5
Savanna	2
Mountain lands (above timberline)	0
Arctic ecosystems	1

*Scale:
5: Very intense modelling effort, more than 50 different modelling approaches can be found in the literature.
4: Intense modelling effort, 20–50 different modelling approaches can be found in the literature;
4–5: May be translated to class 4 but on the edge of an upgrading to class 5:
3: Some modelling effort, 6–19 different modelling approaches are published;
2: Few (2–5) different models that have been fairly well studied have been published:
1: One good study and/or a few not sufficiently well calibrated and validated models;
0: Almost no modelling efforts have been published and not even one well studied model.
Note that the classification is based on the number of different models, not on the number of case studies where the models have been applied; in most cases the same models have been used in several case studies.

Table 1.3. Models of environmental problems

Problem	Modelling effort (on a scale of 0 to 5)*
Oxygen balance	5
Eutrophication	5
Heavy metal pollution, all types of ecosystems	4
Pesticide pollution of terrestrial ecosystems	4–5
Other toxic compounds include ERA	5
Regional distribution of toxic compounds	5
Protection of national parks	3
Management of populations in national parks	3
Endangered species (includes population dynamic models)	3
Ground water pollution	5
Carbon dioxide/greenhouse effect	5
Acid rain	5
Total or regional distribution of air pollutants	5
Change in microclimate	3
As ecological indicator	4
Decomposition of the ozone layer	4
Health–pollution relationships	2

*See Table 1.2 for explanation of scale.

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CHAPTER 2

Concepts of Modelling

2.1 Introduction

This chapter covers the topic of modelling theory and its application in the development of models. After the definitions of model components and modelling steps have been presented, a tentative modelling procedure is given and the steps discussed in detail. In addition, the chapter focuses on model selection, i.e., the selection of model components, processes and, in particular, model complexity. Various methods for selecting "close to the right" complexity of the model are given. The conceptual diagram is the first presentation of the model, but due to the great number of possibilities, this step is mentioned only briefly in this chapter, being covered in detail in Chapter 4. The following steps, however, are discussed in detail in this chapter: selection of model type and model complexity, verification, parameter estimation and validation. Illustrations are included to show the reader how these steps are carried out in practical model building.

Several model formulations are always available and the ability to choose among them requires that sound scientific constraints are imposed on the model. Possible constraints are introduced and discussed. A mathematical model will usually require the use of a computer and therefore a computer language. Although the selection of a computer language is not discussed, because there are many possibilities and new languages emerge from time to time, a brief overview of some of the languages most applied in ecological modelling will be given.

2.2 Modelling Elements

In its mathematical formulation, a model in environmental sciences has five components.

1. **Forcing functions, or external variables**, which are functions or variables of an external nature that influence the state of the ecosystem. In a management context the problem to be solved can often be reformulated as follows: if certain forcing functions are varied, how will this influence the state of the ecosystem? The model is used to predict what will change in the ecosystem when forcing functions are varied with time. The forcing functions under our control are often called **control functions.** The control functions in ecotoxicological models are, for instance, inputs of toxic substances to the ecosystems and in eutrophication models the control functions are inputs of nutrients. Other forcing functions of interest could be climatic variables, which influence the biotic and abiotic components and the process rates. They are not controllable forcing functions.

2. **State variables**, as the name indicates, describe the state of the ecosystem. The selection of state variables is crucial to the model structure, but often the choice is obvious. If, for instance, we want to model the bioaccumulation of a toxic substance, the state variables should be the organisms in the most important food chains and concentrations of the toxic substance in the organisms. In eutrophication models the state variables will be the concentrations of nutrients and phytoplankton. When the model is used in a management context, the values of state variables predicted by changing the forcing functions can be considered as the results of the model, because the model will contain relationships between the forcing functions and the state variables.

3. **Mathematical equations** are used to represent the biological, chemical and physical processes. They describe the relationship between the forcing functions and state variables. The same type of process may be found in many different environmental contexts, which implies that the same equations can be used in different models. This does not imply, however, that the same process is always formulated using the same equation. First, the considered process may be better described by another equation because of the influence of other factors. Second, the number of details needed or desired to be included in the model may be different from case to case due to a difference in complexity of the system or/and the problem. Some modellers refer to the description and mathematical formulation of processes as submodels. A comprehensive overview of submodels can be found in Chapter 3.

4. **Parameters** are coefficients in the mathematical representation of processes. They may be considered constant for a specific ecosystem or part of an ecosystem. In causal models the parameter will have a scientific definition, for instance, the excretion rate of cadmium from a fish. Many parameters are not indicated in the literature as constants but as ranges, but even that is of great value in the parameter estimation, as will be discussed further. In Jørgensen et al. (2000) a comprehensive collection of parameters in environmental sciences and ecology can be found. Our limited knowledge of parameters is one of the

weakest points in modelling, a point that will be touched on often throughout the book. Furthermore, the application of parameters as constants in our models is unrealistic due to the many feedbacks in real ecosystems. The flexibility and adaptability of ecosystems is inconsistent with the application of constant parameters in the models. A new generation of models that attempts to use parameters varying according to some ecological principles seems a possible solution to the problem, but a further development in this direction is absolutely necessary before we can achieve an improved modelling procedure reflecting the processes in real ecosystems. This topic will be further discussed in Chapter 9.

5. **Universal constants**, such as the gas constant and atomic weights, are also used in most models.

Models can be defined as formal expressions of the essential elements of a problem in mathematical terms. The first recognition of the problem is often verbal. This may be recognized as an essential preliminary step in the modelling procedure and will be treated in more detail in the next section. However, the verbal model is difficult to visualize and it is, therefore, more conveniently translated into a **conceptual diagram**, which contains the state variables, the forcing functions and how these components are interrelated by mathematical formulations of processes.

Figure 2.1 illustrates a conceptual diagram of the nitrogen cycle in a lake. The state variables are nitrate, ammonium (which is toxic to fish in the unionized form of ammonia), nitrogen in phytoplankton, nitrogen in zooplankton, nitrogen in fish, nitrogen in sediment and nitrogen in detritus.

The forcing functions are: out- and inflows, concentrations of nitrogen components in the in- and outflows, solar radiation, and the temperature, which is not shown on the diagram, but which influences all the process rates. The arrows in the diagram represent the processes which are formulated using mathematical expressions in the mathematical part of the model.

Three significant steps in the modelling procedure need to be defined in this section. They are verification, calibration and validation:

- **Verification** is a test of the *internal logic* of the model. Typical questions in the verification phase are: Does the model react as expected? Is the model stable in the long term? Does the model follow the law of mass conservation? Is the use of units consistent? Verification is to some extent a subjective assessment of the behaviour of the model. To a large extent, the verification will go on during the use of the model before the calibration phase, which has been mentioned above.

- **Calibration** is an attempt to find the best accordance between computed and observed data by variation of some selected parameters. It may be carried out by trial and error or by use of software developed to find the parameters giving the best fit between observed and computed values. In some static models and in some simple models, which contain only a few well-defined, or directly measured, parameters, calibration may not be required.

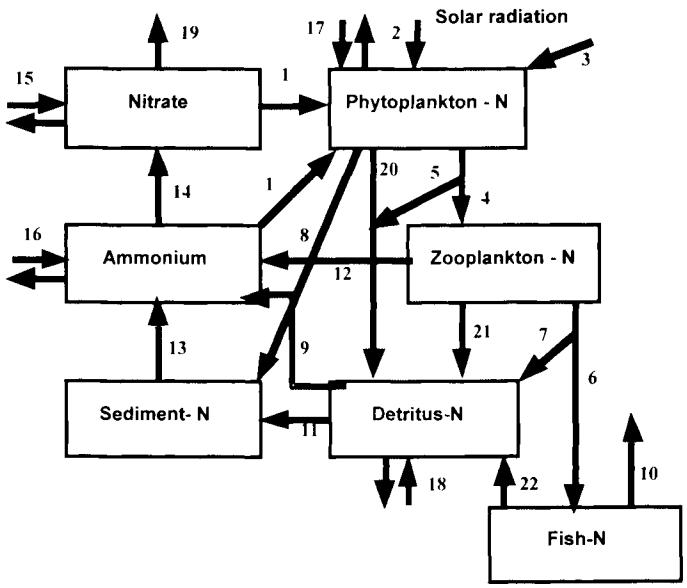

Fig. 2.1. The conceptual diagram of a nitrogen cycle in an aquatic ecosystem. The processes are: (1) uptake of nitrate and ammonium by algae; (2) photosynthesis; (3) nitrogen fixation; (4) grazing with loss of undigested matter; (5), (6) and (7) predation and loss of undigested matter; (8) settling of algae; (9) mineralization; (10) fishery; (11) settling of detritus; (12) excretion of ammonium from zooplankton; (13) release of nitrogen from the sediment; (14) nitrification; (15), (16), (17) and (18) inputs/outputs; (19) denitrification; (20), (21) and 22) mortality of phytoplankton, zooplankton and fish.

- **Validation** must be distinguished from verification. Validation consists of an objective test of how well the model outputs fit the data. We distinguish between a structural (qualitative) validity and a predictive (quantitative) validity. A model is said to be structurally valid, if the model structure represents reasonably accurately the cause–effect relationship of the real system. The model exhibits predictive validity if its predictions of the system behaviour are reasonably in accordance with observations of the real system. The selection of possible objective tests will be dependent on the aims of the model, but the standard deviations between model predictions and observations and a comparison of observed and predicted minimum or maximum values of a particularly important state variable are frequently used. If several state variables are included in the validation, they may be given different weights.

Further details on these important steps in modelling will be given in the next section where the entire modelling procedure will be presented, with additional information in Sections 2.7–2.10.

2.3 The Modelling Procedure

A tentative modelling procedure is presented in this section. The authors have used this procedure successfully several times and strongly recommend that all the steps of the procedure are used very carefully. Other scientists in the field have published other slightly different procedures, but detailed examination will reveal that the differences are only minor. The most important steps of modelling are included in all the recommended modelling procedures.

The initial focus of research is always the definition of the problem. This is the only way in which the limited research resources can be correctly allocated instead of being dispersed into irrelevant activities.

The first modelling step is therefore a **definition of the problem** and the definition will need to be bound by the constituents of **space**, **time** and **subsystems**. The bounding of the problem in space and time is usually easy, and consequently more explicit, than the identification of the subsystems to be incorporated in the model.

System thinking is important in this phase: you must try to grasp the big picture. The focal system behaviour must be interpreted as a product of dynamic processes, preferably describable by causal relationships.

Figure 2.2 shows the procedure proposed by the authors, but it is important to emphasize that this procedure is unlikely to be correct at the first attempt, so there is no need to aim at perfection in one step. The procedure should be considered as an iterative process and the main requirement is to get started (Jeffers, 1978).

It is difficult, at least in the first instance, to determine the optimum number of subsystems to be included in the model for an acceptable level of accuracy defined by the scope of the model. Due to lack of data, it will often become necessary at a later stage to accept a lower number than intended at the start or to provide additional data for improvement of the model. It has often been argued that a more complex model should account more accurately for the reactions of a real system, but this is not necessarily true. Additional factors are involved. A more complex model contains more parameters and increases the level of uncertainty, because parameters have to be estimated either by more observations in the field, by laboratory experiments, or by calibrations, which again are based on field measurements. Parameter estimations are never completely without errors, and the errors are carried through into the model, thereby contributing to its uncertainty. The problem of selecting **the right model complexity**—a problem of particular interest for modelling in ecology—will be further discussed in Section 2.6.

A first approach to the data requirement can be made at this stage, but it is most likely to be changed at a later stage, once experience with the verification, calibration, sensitivity analysis and validation has been gained.

In principle, data for all the selected state variables should be available; in only a few cases would it be acceptable to omit measurements of selected state variables, as the success of the calibration and validation is closely linked to **the quality and quantity of the data.**

It is helpful at this stage to list the state variables and attempt to gain an overview of the most relevant processes by setting up an **adjacency matrix.** The state variables are listed vertically and horizontally; 1 is used to indicate that a direct link between the two state variables is most probable, while 0 indicates that there is no link between the two components. The conceptual diagram (Fig. 2.1) can be used to illustrate the application of an adjacency matrix in modelling:

Adjacency matrix for the model in Fig. 2.1.

From To	Nitrate	Ammonium	Phyt-N	Zoopl-N	Fish N	Detritus-N	Sediment-N
Nitrate	–	1	0	0	0	0	0
Ammonium	0	–	0	1	0	1	1
Phyt-N	1	1	–	0	0	0	0
Zoopl-N	0	0	1	–	0	0	0
Fish N	0	0	0	1	–	0	0
Detritus-N	0	0	1	1	1	–	0
Sediment-N	0	0	1	0	0	1	–

The adjacency matrix is made in this case from the conceptual diagram to illustrate the application of an adjacency matrix. In practice, it is recommended that the adjacency matrix is set up before the conceptual diagram. The modeller should ask for each of the possible links: is this link possible? If yes, is it sufficiently significant to be included in the model? If "yes" write 1, if "no" write 0. The adjacency matrix shown above may not be correct for all lakes. If resuspension is important there should be a link between sediment-N and detritus-N. If the lake is shallow, resuspension may be significant, while the process is without any effect in deep lakes. This example clearly illustrates the idea behind the application of an adjacency matrix to get the very first overview of the state variables and their interactions.

Once the **model complexity**, at least at the first attempt, has been selected, it is possible **to conceptualize the model**, for instance in the form of a diagram as shown in Fig. 2.1. It will give information on which state variables, forcing functions and processes are required in the model.

Ideally, one should determine which data are needed to develop a model according to a conceptual diagram, i.e., to let the conceptual model or even some first more primitive mathematical models determine the data at least within some given economic limitation, but in real life most models have been developed *after* the data collection as a compromise between model scope and available data. There are developed methods to determine the ideal data set needed for a given model to minimize the uncertainty of the model, but unfortunately the applications of these methods are limited.

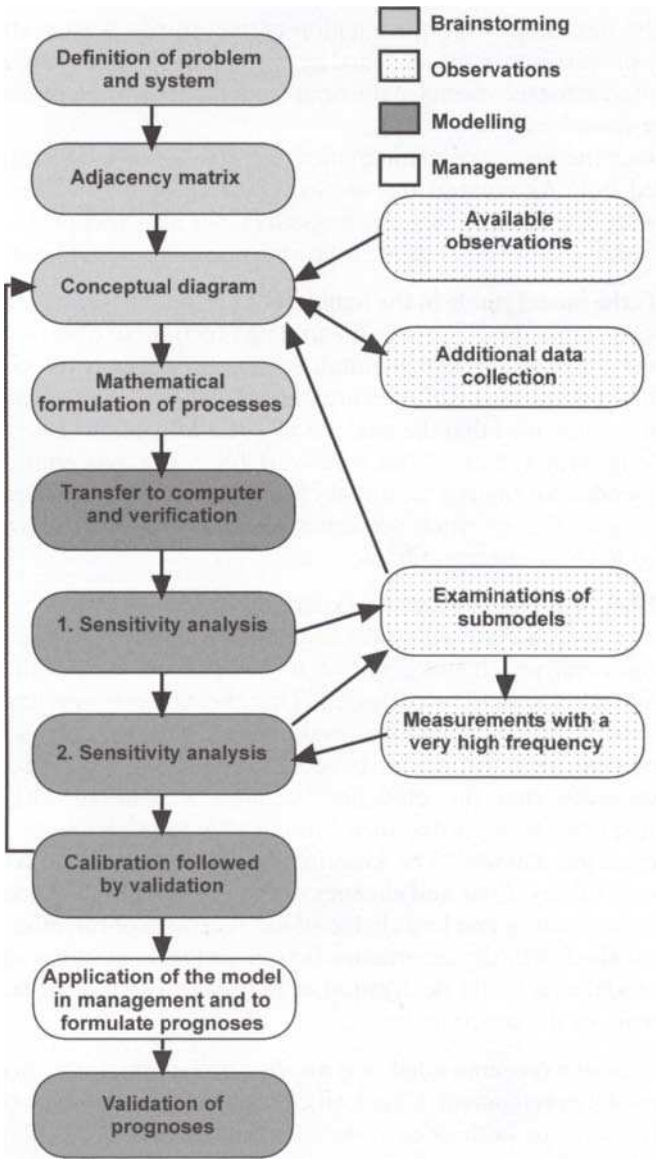

Fig. 2.2. A tentative modelling procedure is shown. As mentioned in the text, one should ideally determine the data collection based on the model, not the other way round. Both possibilities are shown because in practice models have often been developed from available data, supplemented by additional observations. The diagram shows that examinations of submodels and intensive measurements should follow the first sensitivity analysis. Unfortunately many modellers have not had the resources to do so, but have had to bypass these two steps and even the second sensitivity analysis. It is strongly recommended to follow the sequence of first sensitivity analysis, examinations of submodels and intensive measurements and second sensitivity analysis. Notice that there are feedback arrows from calibration, and validation to the conceptual diagram. This shows that modelling should be considered an iterative process.

The next step is the formulation of the processes as **mathematical equations.** Many processes may be described by more than one equation, and it may be of great importance for the results of the final model that the right one is selected for the case under consideration.

Once the system of mathematical equations is available, the **verification** can be carried out. As pointed out in Section 2.2, this is an important step, which is unfortunately omitted by some modellers (see also Section 2.6). It is recommended at this step that answers to the following questions are at least attempted:

1. **Is the model stable in the long term?** The model is run for a long period with the same annual variations in the forcing functions to observe whether the values of the state variables are maintained at approximately the same levels. During the first period state variables are dependent on the initial values for these and it is recommended that the model is also run with initial values corresponding to the long-term values of the state variables. The procedure can also be recommended for finding the initial values if they are not measured or known by other means. This question presumes that real ecosystems have long-term stability, which is not necessarily the case.

2. **Does the model react as expected?** If the input of, e.g., toxic substances is increased, we should expect a higher concentration of the toxic substance in the top carnivore. If this is not so, it shows that some formulations may be wrong and these should be corrected. This question assumes that we actually know at least some reactions of ecosystems, which is not always the case. In general, playing with the model is recommended at this phase. It is through such exercises that the modeller becomes acquainted with the model and its reactions to perturbations. Models should generally be considered to be an experimental tool. The experiments are carried out to compare model results with observations and changes of the model are made according to the modeller's intuition and knowledge of the reactions of the models. If the modeller is satisfied with the accordance between model and observations, he accepts the model as a useful description of the real ecosystem, at least within the framework of the observations.

3. **It is also recommended that all the applied units are checked at this phase of model development.** Check all equations for consistency of units. Are the units the same on both sides of the equation sign?

Sensitivity analysis follows verification. Through this analysis the modeller gets a good overview of the most *sensitive components of the model.* Thus, sensitivity analysis attempts to provide a measure of the sensitivity of either parameters, or forcing functions, or submodels to the state variables of greatest interest in the model. If a modeller wants to simulate a toxic substance concentration in, for instance, carnivorous insects as a result of the use of insecticides, he will obviously choose this state variable as the most important one, maybe besides the concentration of the toxic substance concentration in plants and herbivorous insects.

In practical modelling the sensitivity analysis is carried out by changing the parameters, the forcing functions or the submodels. The corresponding response on the selected state variables is observed. Thus, the sensitivity, S, of a parameter, P, is defined as follows:

$$S = [\partial x/x] / [\partial P/P] \tag{2.1}$$

where x is the state variable under consideration.

The relative change in the parameter value is chosen based on our knowledge of the certainty of the parameters. If, for instance, the modeller estimates the uncertainty to be about 50%, he will probably choose a change in the parameters at $\pm 10\%$ and $\pm 50\%$ and record the corresponding change in the state variable(s). It is often necessary to find the sensitivity at two or more levels of parameter changes as the relationship between a parameter and a state variable is rarely linear.

A sensitivity analysis makes it possible to distinguish between high-leverage variables, whose values have a significant impact on the system behaviour, and low-leverage variables, whose values have minimal impact on the system. Obviously, the modeller must concentrate his effort on improving the parameters and the submodels associated with the high-leverage variables.

A sensitivity analysis on submodels (process equations) can also be carried out. Then the change in a state variable is recorded when the equation of a submodel is deleted from the model or changed to an alternative expression, for instance, with more details built into the submodel. Such results may be used to make structural changes in the model. If, for instance, the sensitivity shows that it is crucial for the model results to use a more detailed given submodel, this result should be used to change the model correspondingly. The selection of the complexity and the structure of the model should therefore work hand in hand with the sensitivity analysis. This is shown as a feedback from the sensitivity analysis via the data requirements to the conceptual diagram in Fig. 2.2. A sensitivity analysis of forcing functions gives an impression of the importance of the various forcing functions and tells us which accuracy is required of the forcing function data.

The scope of the **calibration** is to improve the parameter estimation. Some parameters in causal ecological models can be found in the literature, not necessarily as constants but as approximate values or intervals. However, to cover all possible parameters for all possible ecological models, including ecotoxicological models, we need to know more than one billion parameters. It is therefore obvious that in modelling there is a particular need for **parameter estimation methods**. This will be discussed later in this chapter and further in Chapter 8, where methods to estimate ecotoxicological parameters based upon the chemical structure of the toxic compound are presented. In all circumstances it is a great advantage to give even approximate values of the parameters before the calibration gets started, as already mentioned above. It is, of course, much easier to search for a value between 1 and 10 than to search between 0 and $+\infty$.

Even where all parameters are known within intervals, either from the literature or from estimation methods, it is usually necessary to calibrate the model. Several sets of parameters are tested by the calibration and the various model outputs of state variables are compared with measured values of the same state variables. The parameter set that gives the best agreement between model output and measured values is chosen.

The need for the calibration can be explained using the following characteristics of ecological models and their parameters:

1. Most parameters in environmental science and ecology are not known as exact values. Therefore all literature values for parameters (Jørgensen et al., 1991; 2000) have a certain uncertainty. Parameter estimation methods must be used, when no literature value can be found, particularly ecotoxicological models, see, for instance, Jørgensen (1988; 1990; 1998) and Chapter 8. In addition we must accept that parameters are not constant, as mentioned above. This point will be discussed further in Chapter 9.

2. All models in ecology and environmental sciences are simplifications of nature. The most important components and processes may be included, but the model structure does not account for every detail. To a certain extent, the influence of some unimportant components and processes can be taken into account by the calibration. This will give values for the parameters that are slightly different from the real, but unknown, values in nature, but the difference may partly account for the influence of the omitted details.

3. Most models in environmental sciences and ecology are 'lumped models', which implies that one parameter represents the average values of several species. As each species has its own characteristic parameter value, the variation in the species composition with time will inevitably give a corresponding variation in the average parameter used in the model. Adaptation and shifts in species composition will require other approaches as touched on. This will be discussed in more detail in Chapter 9.

A calibration cannot be carried out randomly if more than a couple of parameters have been selected for calibration. If, for instance, ten parameters have to be calibrated and the uncertainties justify the testing of ten values for each parameter, the model has to be run 10^{10} times, which is, of course, an impossible task. Therefore, the modeller must learn the behaviour of the model by varying one or two parameters at a time and observing the response of the most crucial state variables. In some (few) cases it is possible to separate the model into several submodels, which can be calibrated approximately independently. Although the calibration described is based to some extent on a systematic approach, it is still a trial-and-error procedure.

However, procedures for automatic calibration are available. This does not mean that the trial-and-error calibration described above is redundant. If the automatic calibration should give satisfactory results within a certain time frame, it is necessary to calibrate only 6–9 parameters simultaneously. In any circumstances it will become

easier to find the optimum parameter set, the more narrow the ranges of the parameters are, before the calibration gets started.

In the trial-and-error calibration the modeller has to set up, somewhat intuitively, some calibration criteria. For instance, you may want to simulate accurately the minimum oxygen concentration for a stream model and/or the time at which the minimum occurs. When you are satisfied with these model results, you may then want to simulate the shape of the oxygen concentration versus time curve properly, and so on. You calibrate the model step by step in order to achieve these objectives step by step.

If an automatic calibration procedure is applied, it is necessary to formulate objective criteria for the calibration. A possible function could be based on an equation similar to the calculation of the standard deviation:

$$Y = [(\Sigma((x_c - x_m)^2/x_{m.a})/n]^{1/2} \tag{2.2}$$

where x_c is the computed value of a state variable, x_m is the corresponding measured value, $x_{m.a}$ is the average measured value of a state variable, and n is the number of measured or computed values. Y is followed and computed during the automatic calibration and the goal of the calibration is to obtain as low a Y-value as possible.

Often, however, the modeller is more interested in a good agreement between model output and observations for one or two state variables, while he is less interested in a good agreement with other state variables. Then he may choose weights for the various state variables to account for the emphasis he puts on each in the model. For a model of the fate and effect of an insecticide he may put emphasis on the toxic substance concentration of the carnivorous insects and he may consider the toxic substance concentrations in plants, herbivorous insects and soil to be of less importance. He may, therefore, choose a weight of ten for the first state variable and only one for the subsequent three.

If it is impossible to calibrate a model properly, this is not necessarily due to an incorrect model, but may be due to poor quality of the data. The quality of the data is crucial for calibration. It is, furthermore, of great importance that **the observations reflect the dynamics of the system.** If the objective of the model is to give a good description of one or a few state variables, it is essential that the data can show the dynamics of just these internal variables. The frequency of the data collection should therefore reflect the dynamics of the state variables in focus. Unfortunately, this rule has often been violated in modelling.

It is strongly recommended that the dynamics of all state variables are considered before the data collection program is determined in detail. Frequently, some state variables have particularly pronounced dynamics in specific periods—often in spring—and it may be of great advantage to have a dense data collection in this period in particular. Jørgensen et al. (1981) show how a dense data collection program in a certain period can be applied to provide additional certainty for the determination of some important parameters. This question will be further discussed in Section 2.9.

From these considerations, recommendations can now be drawn up about the feasibility of carrying out a calibration of a model in ecology:

1. Find **as many parameters as possible from the literature** (see Jørgensen et al., 1991; 2000). Even a *wide* range for the parameters should be considered to be very valuable, as approximate initial guesses for all parameters are urgently needed.

2. If some parameters cannot be found in the literature, which is often the case, the **estimation methods** mentioned in Section 2.9 and for ecotoxicological models in Chapter 8, should be used. For some crucial parameters it may be better to determine them by experiments *in situ* or in the laboratory.

3. A **sensitivity analysis** should be carried out to determine which parameters are most important to be known with high certainty.

4. The use of **an intensive data collection program** for the most important state variables should be considered to provide a better estimation for the most crucial parameters (see Section 2.9 for further details).

5. At this stage, the **calibration** should first be carried out using the data not yet applied. The most important parameters are selected and the calibration is limited to these, or, at the most, to eight to ten parameters. In the first instance, the calibration is carried out by using the trial-and-error method in order to to get acquainted with the model's reaction to changes in the parameters. An automatic calibration procedure is used afterwards to polish the parameter estimation.

6. These results are used in **a second sensitivity analysis**, which may give different results from the first.

7. **A second calibration** is now used on the parameters that are most important according to the second sensitivity analysis. In this case, too, both the above-mentioned calibration methods may be used. After this final calibration, the model can be considered calibrated and we can go to the next step: validation.

The calibration should always be followed by a **validation**. By this step the modeller tests the model against an independent set of data to observe how well the model simulations fit these data. It must, however, be emphasized that the validation only confirms the model behaviour under the range of conditions represented by the available data. So it is preferable to validate the model using data obtained from a period in which conditions other than those of the period of data collection for the calibration prevail. For instance, when a model of eutrophication is tested, it should preferably have data sets for the calibration and the validation, which differ by the level of eutrophication. If an ideal validation cannot be obtained, it is, however, still import to validate the model. The method of validation is dependent on the objectives of the model. A comparison between measured and computed data by use of the objective function (2.2) is an obvious test. This is often not sufficient, however, as it

may not focus on all the main objectives of the model, but only on the general ability of the model to describe correctly the state variables of the ecosystem. It is necessary, therefore, to translate the main objectives of the model into a few validation criteria. They cannot be formulated generally, but are individual to the model and the modeller. For instance, if we are concerned with the eutrophication in an aquatic ecosystem in carnivorous insects, it would be useful to compare the measured and computed maximum concentrations of phytoplankton. The discussion of the validation can be summarized by the following issues:

1. **Validation is always required** to get a picture of the reliability of the model.
2. Attempts should be made to get data for the validation, which are **entirely different from those used in the calibration**. It is important to have data **from a wide range of forcing functions** that are defined by the objectives of the model.
3. **The validation criteria are formulated based on the objectives of the model and the quality of the available data**. The main purpose of the model may, however, be an exploratory analysis to understand how the system responds to the dominating forcing functions. In this case a structural validation is probably sufficient.

2.4 Types of Model

It is useful to distinguish between various types of model and to briefly discuss the selection of model types. Pairs of models are shown in Table 2.1. The first division of models is based on the application: **scientific and management models**.

The next pair is: **stochastic and deterministic models**. A stochastic model contains stochastic input disturbances and random measurement errors, as shown in Fig. 2.3. If they are both assumed to be zero, the stochastic model will reduce to a deterministic model, provided that the parameters are not estimated in terms of statistical distributions. A deterministic model assumes that the future response of the system is completely determined by a knowledge of the present-state and future measured inputs. Stochastic models are rarely applied in ecology today.

The third pair in Table 2.1 is **compartment and matrix models**. Compartment models are understood by some modellers to be models based on the use of compartments in the conceptual diagram, while other modellers distinguish between the two classes of models entirely by the mathematical formulation as indicated in the table. Both types of models are applied in environmental chemistry, although the use of compartment models is far more pronounced.

The classification of **reductionistic and holistic models** is based on a difference in the scientific ideas behind the model. The reductionistic modeller will attempt to incorporate as many details of the system as possible to capture its behaviour. He believes that the properties of the system are the sum of the details. The holistic modeller, on the other hand, attempts to include in the model system properties of

Table 2.1. Classification of models (pairs of model types).

Type of model	Characterization
Research models	Used as a research tool
Management models	Used as a management tool
Deterministic models	The predicted values are computed exactly
Stochastic models	The predicted values depend on probability distribution
Compartment models	The variables defining the system are quantified by means of time-dependent differential equations
Matrix models	Use matrices in the mathematical formulation
Reductionistic models	Include as many relevant details as possible
Holistic models	Use general principles
Static models	The variables defining the system are not dependent on time
Dynamic models	The variables defining the system are a function of time (or perhaps of space)
Distributed models	The parameters are considered functions of time and space
Lumped models	The parameters are within certain prescribed spatial locations and time, considered as constants
Linear models	First-degree equations are used consecutively
Non-linear models	One or more of the equations are not first-degree
Causal models	The inputs, the states and the outputs are interrelated by using causal relationships
Black-box models	The input disturbances affect only the output responses. No causality is required
Autonomous models	The derivatives are not explicitly dependent on the independent variable (time)
Non-autonomous models	The derivatives are explicitly dependent on the independent variable (time)

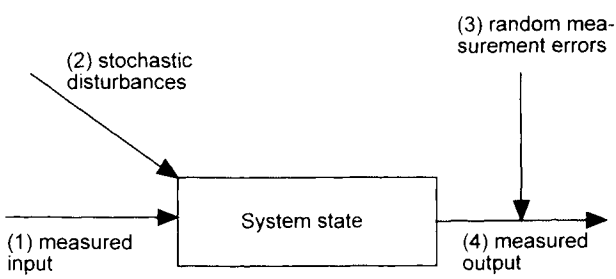

Fig. 2.3. A stochastic model considers (1) (2) and (3), while a deterministic model assumes that (2) and (3) are zero.

the ecosystem working as a system by using general principles. Here, the properties of the system are not the sum of all the details considered, but the holistic modeller presumes that the system possesses additional properties because the subsystems are working as a unit. Both types of models may be found in ecology, but the environmental chemist must, in general, adopt a holistic approach to the problems in order to gain an overview because the problems in environmental chemistry are very complex.

Most problems in environmental sciences and ecology may be described by a dynamic model, which uses differential or difference equations to describe the system response to external factors. Differential equations are used to represent continuous changes of state with time, while difference equations use discrete time steps. The steady state corresponds to the situation when all derivatives equal zero. The oscillations round the steady state are described by the use of a dynamic model, while steady state itself can be described using a static model. As all derivatives are equal to zero in steady states, the static model is reduced to algebraic equations.

Some dynamic systems have no steady state: those, for instance, that show limit cycles. This situation obviously requires a dynamic model to describe the system behaviour. In this case the system is always non-linear, although there are non-linear systems that have steady states.

Consequently, a static model assumes that all variables and parameters are independent of time. The advantage of the static model is its potential for simplifying subsequent computational effort through the elimination of one of the independent variables in the model relationship, but static models may give unrealistic results because oscillations caused, for instance, by seasonal and diurnal variations may be utilized by the state variables to obtain higher average values.

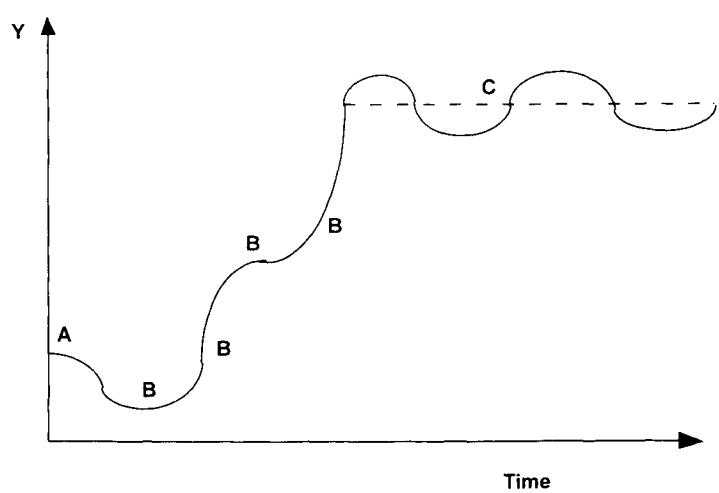

Fig. 2.4. Y is a state variable expressed as a function of time. A is the initial state and B the transient states. C oscillates round a steady state. The dotted line corresponds to the steady state that can be described by a static model.

A *distributed model* accounts for variations of variables in time and space. A typical example would be an *advection–diffusion* model for transport of a dissolved substance along a stream. It might include variations in the three orthogonal directions. However, the analyst might decide, based on prior observations, that gradients of dissolved material along one or two directions are not sufficiently large to merit inclusion in the model. The model would then be reduced by that assumption to a lumped parameter model. Whereas the lumped model is frequently based upon ordinary differential equations, the distributed model is usually defined by partial differential equations.

The causal, or internally descriptive, model characterizes the manner in which inputs are connected to states and how the states are connected to each other and to the outputs of the system, whereas the black-box model reflects only what changes in the input will affect the output response. In other words, the causal model describes the internal mechanisms of process behaviour. The black-box model deals only with what is measurable: the input and the output. The relationship may be found by a statistical analysis. If, on the other hand, the processes are described in the model using equations which cover the relationship, the model will be causal.

The modeller may prefer to use black-box descriptions in cases where his knowledge of the processes is limited. However, the disadvantage of the black box model is that it is limited in application to the ecosystem under consideration, or at least to a similar ecosystem, and cannot consider changes in the system.

If general applicability is needed, it is necessary to set up a causal model. This type is much more widely used in environmental sciences than the black-box model, due mainly to the understanding that the causal model gives the user the function of the system including the many chemical, physical and biological reactions.

Autonomous models are not explicitly dependent on time (the independent variable):

$$dy/dt = a * y^{h} + c * y^{d} + e \tag{2.3}$$

Non-autonomous models contain terms, $g(t)$, that make the derivatives dependent on time, as exemplified by the following equation:

$$dy/dt = a * y^{h} + c * y^{d} + e + g(t) \tag{2.4}$$

The pairs in Table 2.1 may be used to define the most appropriate type of model to solve a given problem. This will be discussed further in the next section in which a practical model classification will also be presented

Table 2.2 shows another classification of models. The differences among the three types of models are the choice of components used as state variables. If the model aims for a description of a number of individuals, species or classes of species, the model will be called *biodemographic.*

A model that describes the energy flows is called *bioenergetic* and the state variables will typically be expressed in kW or kW per unit of volume or area.

Table 2.2. Identification of models

Type of model	Organization	Pattern	Measurements
Biodemographic	Conservation of genetic information	Life cycles of species	Number of species or individuals
Bioenergetic	Conservation of energy	Energy flow	Energy
Biogeochemical	Conservation of mass	Element cycles	Mass or concentrations

The *biogeochemical models* consider the flow of material and the state variables are indicated as kg or kg per unit of volume or area. This model type is mainly used in ecology.

2.5 Selection of Model Type

The problem, the ecosystem characteristics and the available data base should be reflected in the choice of model type.

The two model classifications presented in Section 2.4 are useful for defining the modelling problem. Is the problem related to a description of populations, energy flows or mass flows? The answer determines whether we should develop a biodemographic, bioenergetic or biogeochemical model. Biodemographic models that include a description of age structure can be elegantly developed by a matrix model, provided that first-order processes can be assumed. This will be demonstrated in Chapter 6.

If the model is developed on the basis of a data base which has a limited quality and/or quantity, a model with relatively low complexity should be applied. A dynamic model is more demanding to calibrate and validate than a static model. Therefore, the latter type should be selected in a data-poor situation, provided of course that a description of the steady state is sufficient to solve the problem. Steady-state descriptions imply that an equation input = output for each state variable can be applied to find or estimate one (otherwise unknown) parameter. Chapter 5 will show how a steady-state model can be developed and utilized to gain a good overview of a pollution situation, even in a relatively data-poor situation. The same chapter will also show how matrix representation can be applied to give a useful mathematical description if the processes involved are first-order reactions.

Dynamic models are able to make predictions about the variations of state variables in time and/or space. Differential equations are used to express the variation. With reference to Fig. 2.5, the following differential equations are valid:

$$dPS/dt = PIN + (2) - (1) - PS \times Q/V \tag{2.5}$$

$$dPA/dt = (1) - PA * Q/V - (2) \tag{2.6}$$

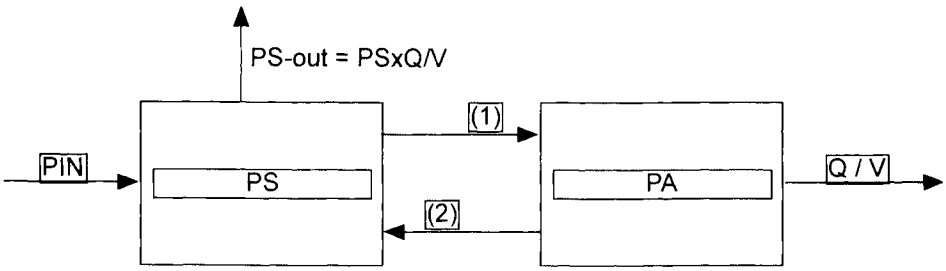

Fig. 2.5. A conceptual diagram of a simple model with two state variables, *PS* and *PA*, is shown. *PIN* and *Q/V* are forcing functions. (1) and (2) are processes.

where *PIN* represents the input (a forcing function), *Q* the flow rate out of the system, *V* the volume of the system and (1) and (2) two processes that can be formulated as mathematical equations with *PS* and *PA* as variables, for instance (1) = $kPS/(0.5 + PS)$ (a *Michaelis-Menten expression*) and (2) = $k'*PA$. *k* and *k'* are two parameters.

The corresponding steady-state model gives us two equations:

$$PIN + k'PA = PS(Q/V + k \cdot PS(0.5 + PS)) \text{ and } PA*Q/V = kPS/(0.5 + PS) - k'*PA$$

which can be used to find *k* and *k'*, presuming that we know the two state variables at steady state and the forcing functions.

Many population dynamic, *biogeochemical* and *ecotoxicological* models, however, apply differential equations, because the time variations are of importance.

Variations in both time and space require application of partial differential equations. The space variations may be considered by a *discretization*. The system can, for instance, be divided into boxes. Combinations of hydrodynamics and ecological models are typical examples of application of partial differential equations.

Fuzzy models are used when the observations used to develop the model are only indicated as ranges, classes (for instance high, medium and low), or by application of non-numeric natural language. The model results are interpreted in the same way, i.e., either as ranges or classes, but in many management and even research situations it is sufficient.

Sudden shifts are observed in ecosystems, although not very frequently. It has been demonstrated that these special cases of shifts can be described by catastrophe theory, a mathematical tool developed by Thom (1975). It is known that ecosystems are adaptable. The species can currently changed their properties to meet changing conditions (e.g., change of forcing functions). If the changes are major, there may even be a shift to other species with properties better fitted to the emerging conditions. Models that account for the change of properties of the biological components have variable parameters and are described by non-stationary, time-varying differential equations. They are often called structurally dynamic models (see, e.g., Jørgensen, 1986; 1997), because they are able to predict the changes in

properties of the biological components. They are distributed models in the sense that the *parameters* are considered functions of time and space, but while distributed models are, in most cases, based on mathematical formulations of these functions when the model is developed, we will only use the term structurally dynamic models for models that can predict the changes of the structure (shifts of the properties means shifts of the parameters). Structurally dynamic models are an important recent development in ecological modelling, because the parameters found on the basis of the observations in the ecosystem under the present prevailing conditions cannot be valid when the conditions are changed due to the adaptation. Models without dynamic structure cannot therefore give reliable prognoses, if the forcing functions are changed significantly.

The parameter variation can be determined by incorporating knowledge (*expert system*) to the relationships between forcing functions and the variation of relevant parameters. Reynolds (1995) illustrates the application of this method. Relationships between wind exposure, depth, and nutrient concentrations on the one side and the dominant phytoplankton species on the other are used to describe the change in species and thereby the *parameter shifts*. The variation can also be described by a goal function. The variation of the focal parameters is determined by *optimization* of a defined function, for instance biomass or *exergy* (for more on this thermodynamic concept, see Section 2.12). An illustrative example using exergy as goal function is presented in Chapter 9. When using this approach it is often advantageous to apply the *allometric principles* (see Section 2.9). Most of the parameters that may change are expressed by the size (length, volume). The goal function is then optimized by variation of the size as the only variable. The following procedure is applied: optimization of the goal function by varying the size → determination of the size corresponding to the optimum → determination of the parameters from the size → sometimes the parameters can be translated to species.

Structurally dynamic models should be applied whenever significant changes in the properties of the dominant organisms are expected as a result of drastic changes in the forcing functions. Up to the year 2000, the model type had only been applied 12 times. It is therefore recommended to be prudent when structurally dynamic models are applied. On the other hand, we know that ecosystems and their organisms are adaptable, which implies that when predictions resulting from radical changes of forcing functions are required, it is recommended firstly to calibrate and validate the model using the observations from a sufficiently long period of time to uncover the dynamic of the state variables. The period may contain, for instance, some seasonal changes or parameters (sizes) which may allow us to test the structurally dynamic approach in parallel by the validation. If the structurally dynamic approach yields a better or equally good validation as the fixed parameters approach, it seems feasible to apply the structurally dynamic modelling approach for the development of prognoses. If the structurally dynamic approach cannot be tested, it is still recommended to apply it for the development of prognoses, as we do know that ecosystems currently change their structure, but the prognoses should be used prudently.

Individual-oriented or individual-based models (IBM) attempt to account for the enormous variability among individuals. Usually, we apply one state variable to account for an average organism to represent a biological component. We thereby violate the individuality of individuals. Darwinian selection is only possible if individuals have different properties; these differences are crucial to the survival of species. The average species may not be able to survive under the prevailing conditions, while some individuals with a better combination of properties, such as larger size, may be survivors. In such a situation, a model based on average properties will give completely wrong results, while IBM may be better able to accord with the observations. IBM should therefore be applied as a modelling approach whenever it is of important to the modelling results that the individuals have properties different from the average. This can be examined by varying the most sensitive properties (parameters) within realistic ranges and observe if the model results are decisive, e.g., survival/no survival or abundant/scarce.

Object-oriented models (OOM) should be mentioned in this context, although they may be considered to be a particular modelling technique and not another model type. OOM uses the concept of classes. One example of a class is the definition of a population, which is the basic building block for many ecological models. Populations are characterized by variables such as mean size, age, number, reproduction, growth and mortality. Each type of population is unique although there are many similarities, such as the above-mentioned processes. We can, therefore, treat different classes of populations accordingly and need only add those particular features which need to be different in the model context. The OOP

Table 2.3. Overview of model types

Model type	Characteristics	Selection criteria
Matrix representation	linear relationships	linear equations valid, age structure required
Static models	give a good quantitative overview of steady-state (average) situation	applied in a data-poor situation where quantification is needed but changes (e.g. seasonal) are not important
Fuzzy model	give semiquantitative results or just indication of ranges	applied in a data-poor situation, semiquantitative results sufficient
Representation by differential equations	give time and/or space variations	good data base needed
Structurally dynamic models	give variations of parameters as function of time and or space by expert knowledge or goal function	prognoses under changed conditions needed. Good data base with some shifts in properties
Individual-based models	consider the different properties of individuals	where average properties (parameters) are insufficient

defines different properties in different modules that can be used in the various classes. OOP will be treated in more detail in Chapter 9, but this brief overview shows that it is a system based on model building blocks which makes a series of models more similar in structure and therefore easier to develop.

The model types presented above are practically applied model formulations, dependent on the problem, the data, the ecosystem and the objectives of the modeller. They cover most of the model types applied in practical modelling. Table 2.3 summarizes the characteristics of the various types mentioned above and give guidance on the selection of model type. It may often be more important to select the right type than to increase the complexity of the model. When, for instance, the structurally dynamic changes actually take place, an increased complexity will not solve that problem. Similarly, if the variations of the individual properties are important for the description of the ecosystem reactions, only individual based models can solve the problem satisfactorily.

Last but not least, four focal recommendations on selection of a model are presented here as a natural transition to the next section focusing on selection of model complexity and structure:

1. Remember, that the model is only as reliable as its least reliable input. This means that a balanced complexity of the *submodels* is recommended.
2. Keep the model as simple as possible and as complex as needed.
3. Remember that the most important outcome of the modelling effort may be a better understanding of the system not necessarily a reliable, quantitative prediction. This implies that the modeller should attempt to develop a model with the right structure.
4. Maintain the *system thinking*. The model is not a correct representation of reality, but an attempt to describe important system features of the system–problem complex.

2.6 Selection of Model Complexity and Structure

The literature of environmental modelling contains several methods which are applicable to the selection of *model complexity*. References are given to the following papers devoted to this question: Halfon (1983; 1984), Halfon et al. (1979), Costanza and Sklar (1985), Bosserman (1980; 1982) and Jørgensen and Mejer (1977).

It is clear from the previous discussions in this chapter that the selection of the model complexity is *a matter of balance*. On the one hand, it is necessary to include the state variables and the processes essential for the problem in focus. On the other hand—as already pointed out—it is of importance not to make the model more complex than the data set can bear. Our knowledge of processes and state variables, together with our data set, will determine the selection of model complexity. If our

knowledge is poor, the model will be unable to give many details and will have a relatively high uncertainty. If we have a profound knowledge of the problem we want to model, we can construct a more detailed model with a relatively low uncertainty. Many researchers claim that a model cannot be developed before one has a certain level of knowledge and that it is a flaw to attempt to construct a model in a data-poor situation. This is wrong, because the model can always assist the researcher by synthesis of the present knowledge and by visualization of the system. But the researcher must, of course, always present the shortcomings and the uncertainties of the model, and not try to pretend that the model is a complete picture of reality in *all* its details. A model will often be a fruitful instrument in the hand of the researcher to test hypotheses but only if the incompleteness of the model is fully acknowledged.

It should not be forgotten in this context that models have always been applied in science. The difference between the present and previous models is only that today, with modern computer technology, we are able to work with very complex models. However, it has been a temptation to construct models that are too complex: it is easy to add more equations and more state variables to the computer program, but much harder to get the data needed for calibration and validation of the model.

Even if we have very detailed knowledge about a problem, we shall never be able to develop a model that will be capable of accounting for the complete input–output behaviour of a real ecosystem and be valid for all frames (Zeigler, 1976). This model is named 'the base model' by Zeigler, and it would be very complex and require such a great number of computational resources that it would be almost impossible to simulate. The base model of a problem in ecology will never be fully known, because of the complexity of the system and the impossibility of observing all states. However, given an experimental frame of current interest, a modeller is likely to find it possible to construct a relatively simple model that is workable in that frame.

It is according to this discussion that, up to a point, a model may be made more realistic by adding ever more connections. Additions of new parameters after that point do not contribute further to improved simulation; on the contrary, more parameters imply more uncertainty, because of the possible lack of information about the flows which the parameters quantify. Given a certain amount of data, the addition of new state variables or parameters beyond a certain model complexity does not add to our ability to model the ecosystem, but only adds to unaccountable uncertainty. These ideas are visualized in Fig. 2.6. The relationship between knowledge gained through a model and its complexity is shown for two levels of data quality and quantity. The question under discussion can be formulated with relation to this figure: **How can we select the *complexity* and the structure of the model to ensure the optimum knowledge gained or the best answer to the question posed by the model?**

We shall discuss below the methods available for selecting a good model structure. If a rather complex model is developed, the use of one of the methods presented in the publications mentioned above is recommended, but for simpler models it is often sufficient to go for a model of balanced complexity, as discussed above.

Costanza and Sklar (1985) have examined 88 different models and they were able to show that the more theoretical discussion behind Fig. 2.6, is actually valid in practice. Their results are summarized in Fig. 2.7, where effectiveness is plotted versus *articulation* (= expression for model complexity). *Effectiveness* is understood as a product of how much the model is able to tell and with what certainty, while articulation is a measure of the complexity of the model with respect to number of components, time and space. The measures of articulation or complexity and of effectiveness are relative. Some other authors may have applied other measures, but it can clearly be seen by comparing Figs. 2.6 and 2.7 that they show the same type of relationship.

Selection of the correct complexity is of great importance in environmental and ecological models as already stated. By using the methods presented and discussed below, it is possible to select, by a rather objective procedure, the approximately correct level of complexity of models. However, the selection will always require the application of these methods to be combined with a good knowledge of the system being modelled. The methods must work hand in hand with an intelligent answer to the question: which components and processes are most important for the problem in focus? Such an answer is even of importance in the right use of the methods mentioned. The conclusion is therefore: know your system and your problem before you select your model, including the complexity of the model. It should not be forgotten in this context, that the model will always be an extreme simplification of nature. It implies that we cannot make a model of an ecosystem, but we *can* develop a model of some aspects of an ecosystem.

A parallel to the application of maps (see Section 1.1) can be used again: we cannot make a map (model) of a state with all its details but can only show some aspects of the geography on a certain scale. Therein lie our limitations, which are due to the immense complexity of nature. We have to accept these limitations. We cannot produce any complete model or gain any total picture of a natural system. But as some kind of map is always more useful than no map at all, some kind of model of an ecosystem is also better than no model at all. In the same way that the map gets better, the better our techniques and knowledge are, so will the model of an ecosystem become better, the more experience we gain in modelling and the more we improve our ecological knowledge. We do not need all details to get a proper overview and a holistic picture. We need some details and we need to understand how the system works at the system level.

The conclusion is, therefore, that we can never know all that is needed to make a complete model, but we can produce good workable models which can expand our knowledge of the ecosystems, particularly of their properties as systems. This is completely consistent with Ulanowicz (1979). He points out that the biological world is a sloppy place. Very precise predictive models will inevitably be wrong. It would be more fruitful to build a model which indicates the general trends and take into account the probabilistic nature of the environment.

Furthermore, it seems possible, at least in some situations, to apply models as management tool (see for instance Jørgensen and Vollenweider, 1988). Models

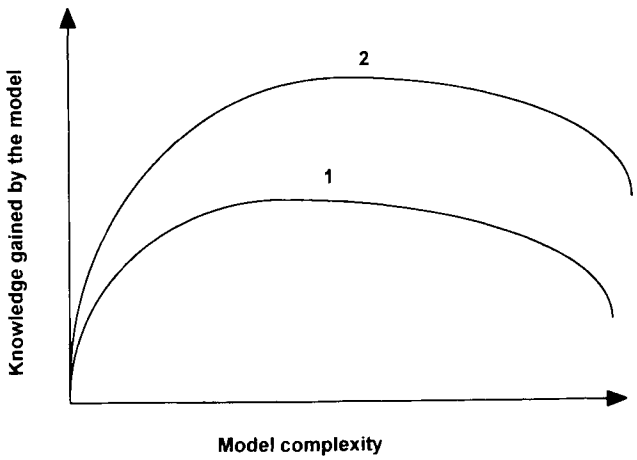

Fig. 2.6. Knowledge plotted versus model complexity measured by the number of state variables. The knowledge increases up to a certain level. Increased complexity beyond this level will not add to the knowledge gained about the modelled system. At a certain level the knowledge might even be decreased due to uncertainty caused by too high a number of unknown parameters. (2) Corresponds to an available data set, which is more comprehensive or has a better quality than (1). Therefore the knowledge gained and the optimum complexity is higher for data set (2) than for (1). Reproduced from Jørgensen (1988).

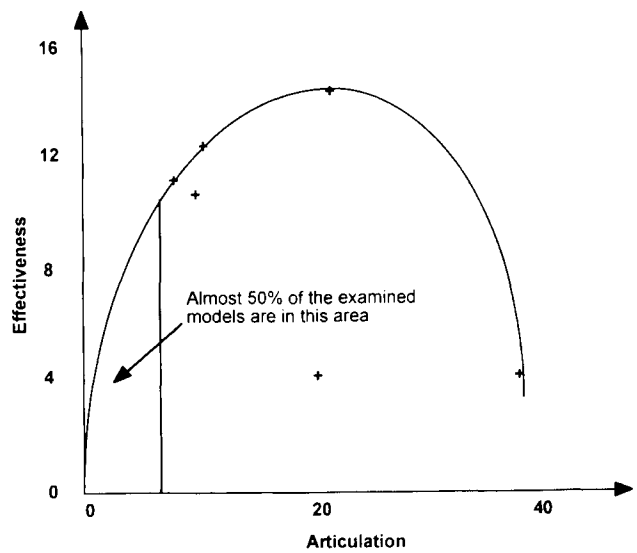

Fig. 2.7. Plot of articulation index versus *effectiveness = articulation × certainty* for the models reviewed by Costanza and Sklar (1985). As almost 50% of the models were not validated, they had an effectiveness of 0. These models are not included in the figure, but are represented by the line effectiveness = 0. Notice that almost another 50% of the models have a relatively low effectiveness due to too little articulation and that only one model has too high articulation, which implies that the uncertainty by drawing the effectiveness frontier as shown in the figure is high at articulations above 25. The figure is partly reproduced from Costanza and Sklar (1985).

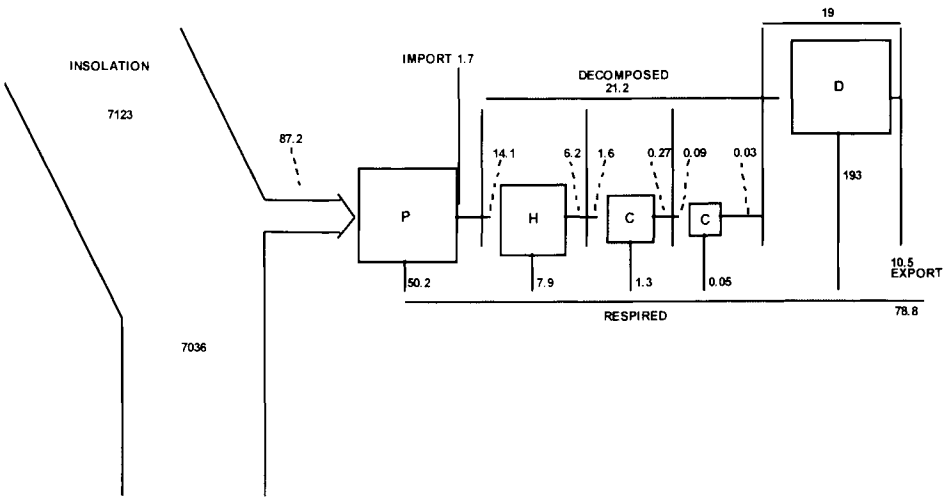

Fig. 2.8. Energy flow diagram for Silver Springs, Florida. Figures in cal/m^2/year (adapted from Odum, 1957).

should be considered as tools—tools to overview complex systems and tools to obtain a picture of the systems properties at the system level. Already a few interactive state variables make it impossible to overview how the system reacts to perturbations or other changes without a model. There are only two possibilities to get around this dilemma: either to limit the number of state variables in the model, or to describe the system using holistic methods and models, preferably using higher level scientific laws (see also the discussion about holistic and *reductionistic approaches* in Section 2.4). **The trade-off for the modeller is between knowing much about little or little about much.**

Through a good knowledge of the system, it is possible to set up mass or energy flow diagrams. These might be considered as conceptual models in their own right, but in this context the idea is to use them to recognize the most important flows for the model in question. Let us use an energy flow diagram for *Silver Springs* (see Fig. 2.8) as an example. If the goal of the model is to make predictions as to the net primary production for various conditions of temperature and input of fertilizers, it seems important to include plants, herbivores, carnivores and decomposers (as they mineralize the organic matter). A model consisting of these four state variables might be sufficient and the top carnivores, import and export can be deleted. As energy flows are different from ecosystem to ecosystem, the selected model should also be different. A general model for one type of ecosystem, e.g., a lake, does not exist; on the contrary, it is necessary to adapt the model to the characteristic feature of the ecosystem. Figures 2.9 and 2.10 show the P-flows of two *eutrophication* models for two different lakes: a shallow lake in Denmark and Lake Victoria in East Africa. From time to time the latter has a *thermocline*, which implies that the lake should be divided into at least two horizontal layers (Jørgensen et al., 1982). The food web is

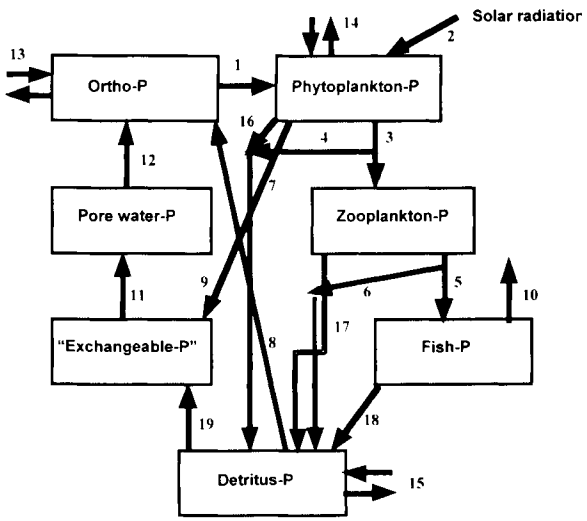

Fig 2.9. The phosphorus cycle. The processes are: (1) Uptake of phosphorus by algae; (2) photosynthesis; (3) grazing with loss of undigested matter; (4) and (5) *predation* with loss of undigested material; (6), (7) and (9) settling of phytoplankton; (8) mineralization; (10) fishery; (11) *mineralization* of phosphorous organic compounds in the sediment; (12) diffusion of pore water P; (13)–(15) inputs/outputs; (16)–(18) mortalities; (19) settling of detritus.

also different in the two lakes in that in Lake Victoria herbivorous fish graze on phytoplankton, while in the Danish lake the grazing is entirely by zooplankton. These differences were also reflected in the models set up for the two ecosystems.

In many shallow lakes the physical processes caused by the wind play an important role. In Lake Balaton the wind stirs up the sediment, which consists almost entirely of calcium compounds, having a high adsorption capacity for phosphorous compounds. Consequently, studies on Lake Balaton have shown that the mass flows of phosphorous compounds from the water column to the sediment due to this effect is significant. Therefore an adequate description of the stirring up of the sediment, the adsorption of phosphorous compounds on the suspended matter and sedimentation must be included in a *eutrophication* model for this lake.

Halfon (1983) has introduced a method which attempts to select the model structure at the conceptualization step. It is based on Bosserman's *measure of recycling* (Bosserman, 1980; 1982) and uses an index of *connectivity* as criteria for the selection of model structure. Ecosystems have a certain amount of recycling and an ecological model must mimic this recycling. If the model structure is too loose and not much recycling can be simulated, structural uncertainty is introduced into the model. Adding links or state variables improves the model connectivity and thus recycling. At a certain point additions of new links will not, however, improve the model behaviour much and therefore these additional links are useless from a model performance point of view. An example should be quoted to illustrate this method of selection model structure.

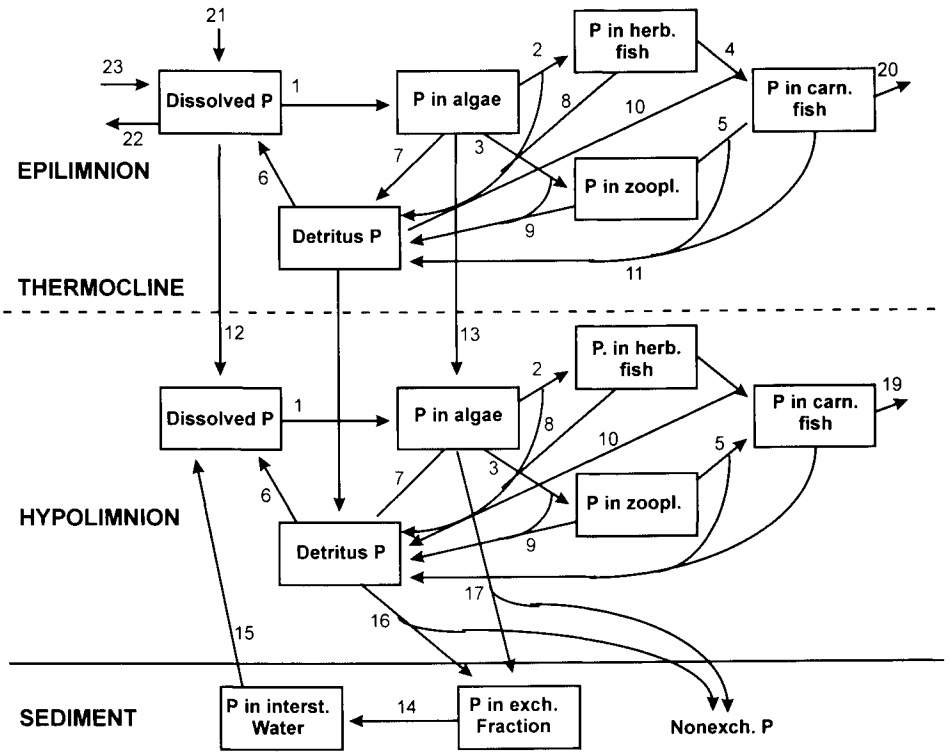

Fig. 2.10. *Eutrophication model* illustrated by use of P-cycling. Arrows indicate processes. A thermocline is considered. (1) Uptake of phosphorus by algae; (2) grazing by herbivorous fish; (3) grazing by zooplankton; (4) and (5) predation on fish and zooplankton, respectively, by carnivorous fish; (6) mineralization; (7) mortality of algae; (8)–(11) grazing and predation loss; (12) exchange of P between epilimnion and hypolimnion; (13) settling of algae (epilimnion–hypolimnion); (14) settling of detritus (epilimnion–hypolimnion); (15) diffusion of P from interstitial to lake water; (16) settling of detritus (hypolimnion–sediment) (a part goes to the non-exchangeable fraction); (17) settling of algae (hypolimnion–sediment) (a part goes to the non-exchangeable fraction); (18) mineralization of P in exchangeable fraction; (19) and (20) fishery; (21) precipitation; (22) outflows; (23) inflows (tributaries).

The pattern of interconnections among state variables can be described with an adjacency matrix A. An adjacency matrix element $A_{ij} = 1$ if a direct link i–j exists and 0 if no direct link exists (see also page 24). The direct connectivity of a model is the number of ones in the adjacency metric divided by n^2, where n is the number of rows or columns. Multi-length links of order k can be studied by looking at the elements of the matrix A^k. For example the matrix A^2 shows the position and numbers of all 2-lengths paths. The recycling measure, c, introduced by Bosserman is the number of ones in the first n matrices of the power series divided by n^3, which is equal to the number of total possible ones. c will vary between 0 and 1, when there are no paths respectively when all paths are realized.

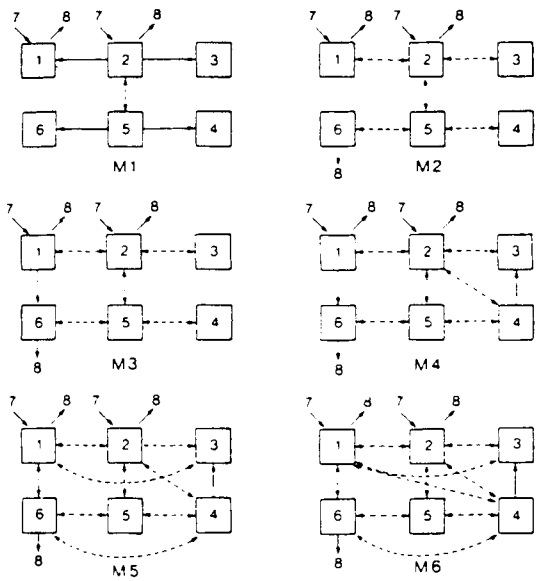

Fig. 2.11. Model structures for first set of models with six state variables. Suspended sediments (1), water (2), fish (3) benthos (4), pore water (5), bottom sediments (6), inputs (7), outputs to the environment (8). (Halfon, 1983).

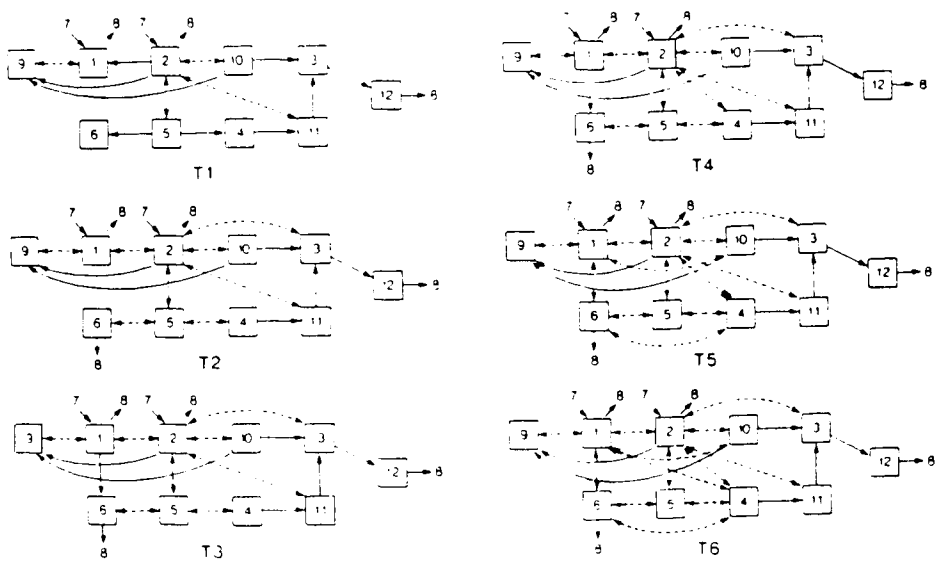

Fig. 2.12. Model structures for second set of models with ten state variables. Suspended sediments (1), water (2), fish (3), benthos (4), pore water (5), bottom sediments (6), inputs (7), outputs to the environment (8), detritus (9), plankton (10), benthic fish (11), sea gulls (12). (Halfon, 1983).

Table 2.4. Adjacency matrix of model M2. Element a_{ij}, j = 1.6 may be zero (no internal recycling) or one (internal recycling) (reproduced from Halfon, 1983).

			TO							
			1	2	3	4	5	6	7	8
	1	Susp. sed	0	1	0	0	0	0	0	1
	2	Water	1	0	1	0	1	0	0	1
F	3	Fish	0	1	0	0	0	0	0	0
R	4	Benthos	0	0	0	0	1	0	0	0
O	5	Pore water	0	1	0	1	0	1	0	0
M	6	Bottom sed.	0	0	0	0	1	0	0	1
	7	Inputs	1	1	0	0	0	0	0	0
	8	Outputs	0	0	0	0	0	0	0	0

Direct connectivity = 15/64 = 0.234.

Table 2.5. Adjacency matrix of model T2. Element a_{ij}, j = 1.12, j 7, j 8 may be equal to zero (no internal recycling) or one (internal recycling) (reproduced from Halfon, 1983).

		TO											
FROM		1	2	3	4	5	6	7	8	9	10	11	12
1	Susp. sed	0	1	0	0	0	0	0	1	1	0	0	0
2	Water	1	0	1	0	1	0	0	1	1	1	1	0
3	Fish	0	1	0	0	0	0	0	0	0	0	0	1
4	Benthos	0	0	0	0	1	0	0	0	0	0	1	0
5	Pore water	0	1	0	1	0	1	0	0	0	0	0	0
6	Bottom sed.	0	0	0	0	1	0	0	1	0	0	0	0
7	Inputs	1	1	0	0	0	0	0	0	0	0	0	0
8	Outputs	0	0	0	0	0	0	0	0	0	0	0	0
9	Detritus	1	0	0	0	0	0	0	0	0	0	0	0
10	Plankton	0	1	1	0	0	0	0	0	1	0	0	0
11	Benthic fish	0	1	1	0	0	0	0	0	0	0	0	0
12	Sea gulls	0	0	0	0	0	0	0	2	0	0	0	0

Direct connectivity = 28/144 = 0.194.

Halfon (1983) illustrates his method by two sets of models, one with six (M-models) and one with ten state variables (T-models). Each set has six model configurations of increasing complexity (connectivity). The state variables of the M-models are: suspended matter (1), water (2), fish (3), benthos (4), pore water (5), and bottom sediment (6).

Figure 2.11 shows the M-models and Fig. 2.12 illustrates the T-models. The latter has the same state variables as the M-model but with addition of detritus (9), phytoplankton (10), benthic fish (11), and sea gulls (12). The numbers 7 and 8 represent inputs and outputs respectively in both model types.

Table 2.4 shows the adjacency matrix of M2 and Table 2.5 of T2. For each set of models two analyses were done: no considerable recycling within each state variable, i.e. $a_{jj} = 0$ or some recycling $a_{ii} = 1$.

Table 2.6. Boolean powers of the M4 model adjacency matrix and their first four sums. Calculation of $\bar{c}$ (reproduced from Halfon, 1983).

A^1								A^1							
0	1	0	0	0	1	0	1	0	1	0	0	0	1	0	1
1	0	1	1	1	0	0	1	1	0	1	1	1	0	0	1
0	1	0	0	0	0	0	0	0	1	0	0	0	0	0	0
0	1	1	0	1	0	0	0	0	1	1	0	1	0	0	0
0	1	0	1	0	1	0	0	0	1	0	1	0	1	0	0
0	0	0	0	1	0	0	1	0	0	0	0	1	0	0	1
1	1	0	0	0	0	0	0	1	1	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
A^2								$A^1 + A^2$							
1	0	1	1	1	0	0	1				0				
0	1	1	1	1	1	0	1	1	1	1	1	1	1	0	1
0	1	1	1	0	0	1	1	1	1	1	1	1	0	0	1
1	1	1	1	1	1	0	1	1	1	1	1	1	1	0	1
1	1	1	1	1	0	0	1	1	1	1	1	1	1	0	1
0	1	0	1	0	1	0	0	0	1	0	1	1	1	0	1
1	1	1	1	1	1	0	1	1	1	1	1	1	1	0	1
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
A^3								$A^1 + A^2 + A^3$							
0	1	1	1	1	1	0	1	1	1	1	1	1	1	0	1
1	1	1	1	1	1	0	1	1	1	1	1	1	1	0	1
0	1	1	1	1	1	0	1	1	1	1	1	1	1	0	1
1	1	1	1	1	1	0	1	1	1	1	1	1	1	0	1
1	1	1	1	1	1	0	1	1	1	1	1	1	1	0	1
1	1	1	1	1	0	0	1	1	1	1	1	1	1	0	1
1	1	1	1	1	0	0	1	1	1	1	1	1	1	0	1
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
A^4								$A^1 + A^2 + A^3 + A^4$							
1	1	1	1	1	1	0	1	1	1	1	1	1	1	0	1
1	1	1	1	1	1	0	1	1	1	1	1	1	1	0	1
1	1	1	1	1	1	0	1	1	1	1	1	1	1	0	1
1	1	1	1	1	1	0	1	1	1	1	1	1	1	0	1
1	1	1	1	1	1	0	1	1	1	1	1	1	1	0	1
1	1	1	1	1	1	0	1	1	1	1	1	1	1	0	1
1	1	1	1	1	1	0	1	1	1	1	1	1	1	0	1
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

A^5 through A^8 are the same as A^4. All further sums are the same. $\bar{c}$ = sum of number of ones in the first eight matrices of Boolean series/n^2 = 0.682.

Table 2.7. Direct and indirect connectivity of the *adjacency matrices* for the first set of models with six state variables (reproduced from Halfon, 1983)

Model	Without internal recycling ($a_{ij} = 0$)		With internal recycling ($a_{ij} = 1$)	
	Direct connectivity	$\bar{c}$	Direct connectivity	$\bar{c}$
M1	0.15625	0.18359	0.25000	0.38281
M2	0.23438	0.44531	0.32813	0.68945
M3	0.25000	0.44922	0.34375	0.69531
M4	0.29688	0.68164	0.39063	0.71289
M5	0.37500	0.71289	0.46875	0.72852
M6	0.40625	0.72070	0.50000	0.73243

Table 2.8. Direct and indirect *connectivity* of the *adjacency matrices* for the second set of models with ten *state variables* (reproduced from Halfon, 1983)

Model	Without internal recycling ($a_{ij} = 0$)		With internal recycling ($a_{ij} = 1$)	
	Direct connectivity	$\bar{c}$	Direct connectivity	$\bar{c}$
T1	0.15972	0.33391	0.22917	0.50637
T2	0 19444	0.66898	0.26389	0.71470
T3	0.20139	0.67419	0.27083	0.71759
T4	0.21528	0.69734	0.28472	0.72454
T5	0.25000	0.71065	0.31944	0.732h4
T6	0.26389	0.71412	0.33333	0.73438

Table 2.6 shows the complete calculation for the index c of model M4. c is found as $(19 + 39 + 46 + 49 + 4 \times 49)/8^3 = 0.682$. Tables 2.7 and 2.8 summarize the results of the computations for the six M-models and six T-models both with and without internal recycling.

By looking over the results from the M-models in Table 2.7 we see a marked change between models M3 and M4, as c increases from 0.449 to 0.682. Furthermore it has been attempted to add and delete paths to the six M-models and it was found that M4 was much less sensitive to changes of the paths than model M3. Model M5 is still less sensitive to individual structural perturbations. This means that an inappropriate parametrization may have less crucial effect on the model behaviour for model M4 (or M5 and M6) than for M3. The improved structural properties of M5 and M6 are not so much better at overcoming the fact that they have more parameters and therefore more uncertain flow rates than M4. Among the M-series M4 should be preferred.

The same formal reasoning is valid for the T-series and it is concluded that T2 or T3 should be used as structural models, depending on the information one has from the system of interest. Such a structural analysis of a model cannot be done completely in a vacuum, but must be related to the system, when an application is sought.

The analysis can, however, reduce the number of arbitrary choices, as they are usually done. The method should also be used in parallel with other possible approaches and can then be considered to be a very useful tool.

The selection of *complexity* and structure of models is close to the *aggregation problem*. Aggregation is the unification of system components that are homogeneous in some properties into blocks, each being a new component with properties defined by the aggregation laws. However, to date, the theory of aggregation is still poorly developed. If the model is nonlinear, the sole method of examining whether aggregation is possible or not is to compare the model outputs of two model versions.

It can be concluded from the various methods presented that the model structure should not be selected randomly or arbitrarily, but that the modeller should use the these approaches to the problem to bring a certain objectivity into this phase of modelling. As the entire model result is greatly dependent on the model structure and complexity, it pays for the modeller to invest a little time in a proper and more objective selection of the model complexity and structure at this stage of the modelling procedure.

Jørgensen and Mejer (1977; 1979) use an examination of the inverse *sensitivity* called *the ecological buffer capacity* to select the number of state variables. The concept ecological buffer capacity is illustrated in Fig. 2.13 and it is defined as:

$$\beta = 1 / (\partial(St) / \partial F) \tag{2.7}$$

where St is a state variable and F a forcing function. It is, of course, possible to define many different buffer capacities corresponding to all possible combinations of state variables and forcing functions. However, the scope of the model will often point out

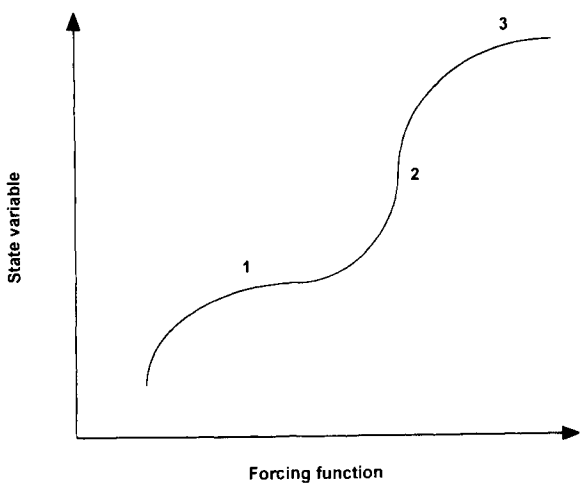

Fig. 2.13. A relationship between a state variable and a forcing function is shown. At point 1 and 3 the buffer capacity is high; at point 2 it is low.

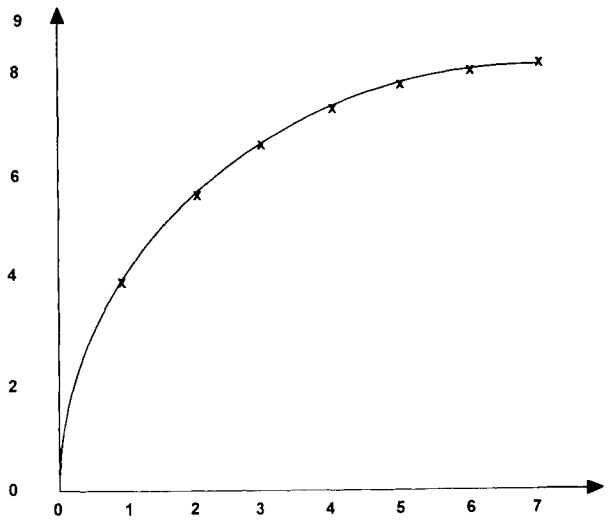

Fig. 2.14. The buffer capacity for a eutrophication model of a shallow Danish lake. In this case a model with six state variables for each of the important nutrients (C, P and N) was selected. The seventh state variable gave only minor changes to the buffer capacity. As the seventh state variable, an additional zooplankton species and an additional phytoplankton species were tested. Other possibilities could also have been tested. In this context it must be pointed out that the buffer capacity is not necessarily increasing with the number of state variables as in the case in Fig. 2.12. The *change* in buffer capacity only decreases with the number of state variables if their sequence is selected according to decreasing importance.

which buffer capacity should be in focus. For a eutrophication model, for instance, it would be the change in input of phosphorus (or nitrogen) to the concentration of phytoplankton. Now the modeller examines the relationship between the buffer capacity in focus and the number of state variables.

As long as the *buffer capacity* is changed significantly by adding an extra state variable, the model complexity should be increased. But if additional state variables only change the buffer capacity insignificantly an increased model complexity will only augment the number of parameters and thereby add to the uncertainty. Figure 2.14 illustrates the buffer capacity for a *eutrophication model* of a shallow Danish lake. In this case a model with 6 state variables for each of the important nutrients, i.e., carbon, nitrogen and phosphorus, was selected. The seventh state variable gave as seen on the Fig. 2.11 only a minor change to the buffer capacity.

Flather (1992; 1996) recommends the use of *Akaike's information criterion* (*AIC*) to select an estimated best model from the *a priori* best candidate models:

$$AIC = n \log (RSS/n)^2 + 2K$$

where n is the number of observations, RSS is the residual sum of squares (model outputs – observations) and K is the number of parameters + 1. The model with the lowest AIC is preferable. This equation is applied to select *submodels*. In principle,

the equation could also be applied to large models, but in practice a comparison of several large models would be too time consuming.

Experience shows that some model corrections can be saved until a later stage if the model has been calibrated and the validation phase indicates that improvements might be needed. However, this does not mean that corrections of the model structure at a later stage can be omitted. The methods presented for the selection of model structure are not so rigorous that the very best model is always selected in the first instance. The methods presented above will assist the modeller to exclude some unworkable models, but not necessarily to choose the very best and only right model.

2.7 Verification

The ecosystem and the problem are the basis for the *conceptual diagram*, which may be considered to be a model in its own right. Therefore Chapter 4 will be devoted to various forms of conceptual models. It will be demonstrated that it is possible to use conceptual models both as management and scientific tools. In accordance with Fig. 2.2, the conceptualization is followed by a mathematical formulation of the processes. Chapter 3 will give a survey of possible formulations of various ecological processes. Having made these two steps of the modelling procedure, the *verification* follows (again, see Fig. 2.2).

We will use the following definition of verification: "A model is said to be verified, if it behaves in the way the model builder wanted it to behave." This definition implies that there is a model to be verified, which means that not only the model equations have been set up, but also that the parameters have been given reasonable realistic values. Consequently, the sequence verification, sensitivity analysis and calibration must not be considered to be a rigid step-by-step procedure, but rather an iterative operation, which must be repeated a few times. The model is first given realistic parameters from the literature, then it is roughly calibrated and then the model can be verified, followed by a sensitivity analysis and a finer *calibration*. The model builder will have to go through this procedure several times, before the verification and the model output in the calibration phase will satisfy him.

Almost inevitably, it will be necessary at some stage during this operation to make assumptions about the statistical properties of the noise sequences idealized in the model. To conform with the properties of white noise any error sequence should broadly satisfy the following constraints: that its mean value is zero, that it is not correlated with any other error sequence and that it is not correlated with the sequences of measured input forcing functions. Evaluation of the error sequences in this fashion can therefore essentially provide a check on whether the final model invalidates some of the assumptions inherent in the model. Should the error sequences not conform to their desired properties, this suggests that the model does not adequately characterize all of the more deterministic features of the observed dynamic behaviour. Consequently, the *model structure* should be modified to accommodate additional relationships.

To summarize this part of the verification:

1. the errors (comparison model output/observations) must have mean values of approximately zero;
2. the errors are not mutually cross related;
3. the errors are not correlated with the measured input forcing functions.

Results of this kind of analysis are given very illustratively in Beck (1978). Notice that this analysis requires good estimates of standard deviations in sampling and analysis (observations).

In addition, and of equal importance, to points 1–3 above, the verification requires a test of the internal logic of the model: does the model have the foreseen causality? And are the responses to perturbations as expected?

This part of the verification is based, to a certain extent, upon more subjective criteria. Typically the model builder formulates several questions about the reaction of the model. He provokes changes in forcing functions or initial conditions and, using the model, simulates responses to those changes. If the responses are not as expected, he will have to change the structure of the model or the equations, provided that the parameter space is approved. Examples of typical questions will illustrate this operation:

- Will increased BOD_5 loading in a stream model imply decreased oxygen concentration?
- Will increased temperature in the same model imply decreased oxygen concentration?
- Will the oxygen concentration be at a minimum at sun-rise when photosynthesis is included in the model?
- Will decreased predator concentration in a prey–predator model imply, in the first instance, increased prey concentration?
- Will increased nutrient loadings in a *eutrophication model* give increased concentration of phytoplankton? etc.

Numerous other examples could be given.

Finally, the *long-term stability* of the model should be examined in the verification phase. The model is run for a long period using a certain pattern in the fluctuations of the forcing functions. It should then be expected that the state variables, too, will show a certain pattern in their fluctuations. A sufficiently long simulation period should of course be selected to allow the model to demonstrate any possible *instability*.

Verification may seem cumbersome, but it is a very necessary step for the model builder to carry out. Through verification, he learns to know his model by its reaction, and verification is furthermore an important checkpoint in the construction of a workable model. This emphasizes also the importance of good ecological

knowledge to the ecosystem, without which the right questions as to the internal logic of the model cannot be posed.

Unfortunately, many models have not been verified properly due to lack of time, but experience shows that what might at first appear to be a shortcut, will lead to an unreliable model, which at a later stage might require take time to compensate for the lack of verification. It is therefore strongly recommended that sufficient time is invested in the verification and the necessary allocation of resources is planned for in this important phase of the modelling procedure.

Illustration 2.1

Constructing a model is very time consuming if all the steps in the modelling procedure are included—something that must be done to ensure an applicable model. A rather primitive and unrealistic model has therefore been selected to illustrate some of the concepts in this chapter in a few pages.

Figure 2.5 shows the conceptual diagram of the model that we want to examine further. The phosphorus cycle in an aquatic ecosystem is modelled. We consider only two state variables: soluble phosphorus, *PS*, and phosphorus in algae, *PA*. An input of phosphorus *PIN* takes place and the output of *PS* and *PA* follows the outflow of water *Q*. The volume of the system is *V*. In addition to these forcing functions, the solar radiation available for photosynthesis can be described in this simple model as:

$$S = S_{max}(1 + \sin(0.008603 \times t)) \tag{2.8}$$

where *S* is the *solar radiation*, S_{max} is the maximum sunlight equal to 0.5 and *t* is time (the number of days). *Q*/*V* is equal to 0.01 (day^{-1}) *PIN* is 1.0 g P m^{-3}. The uptake of phosphorus by algae (process (1) in Fig. 2.5) is described as:

$$\mu = S * PS/(PS + K) \tag{2.9}$$

where μ is the growth rate and *K* is the *Michaelis–Menten constant*, here equal to 1.0 g P m^{-3}. Process 2 is described by first-order kinetics:

$$\text{Loss of algae phosphorus} = R * PA \tag{2.10}$$

where *R* is the rate constant equal to 0.1 (day^{-1}). At $t = 0$, $PA = 1.0$ g P m^{-3}.

The differential equations are:

$$\begin{aligned} dPS/dt &= (PIN - PS)\, Q/V\, (\mu - R) \times PA \\ dPA/dt &= (\mu - R - Q/V)\, PA \end{aligned} \tag{2.11}$$

The model has been written in SYSL (see Table 2.9), a P/C version of CSMP, in STELLA (see Table 2.10) and in PASCAL (see Table 2.11). STELLA is a software

Table 2.9. A simple phosphorus model. SYSL Program

```
PARAMETERS
    PARAM K = 1.0
    PARAM PIN = 1.0
    PARAM Q/V = 0.0
    PARAM R = 0.1
    PARAM SMAX = 0.5
DIFFERENTIAL EQUATIONS
    DPS = (PIN - PS) * Q/V - (μ - R) * PA                    (2.10)
    DPA = (μ - R - Q/V) * PA                                 (2.11)
INTEGRATORS FOLLOW
    PS = INTGRL (IPS, DPS)
    PA = INTGRL (IPA, DPA)
INITIAL VALUES FOR INTEGRATORS
    IN CON IPS = 0, IPA = 1.0
ADDITIONAL EQUATIONS FOLLOW
    PT = PS + PA
    μ = S * PA/(K + PS)
    S = SMAX * (1 + SIN (0.008603 * TIME))
A STATEMENT FOR PLOTTING
    SAVE 5.0, PT, PS, S, μ, PA
GRAPHIC OUTPUT STATEMENTS FOLLOW
    GRAPH (G1,DE=IBM3279) TIME (LE=10, N1=5), PA (LI=71, LE=8, N1=5, ...
    PS (LI 0 74, LE=8, N1=5)
    LABEL (G1, DE=IBM3279) A SIMPLE PHOSPHORUS MODEL
CONTROL STATEMENTS FOLLOW
    CONTROL = 365.0
END
STOP
```

The units applied in the equations are controlled. All units in Eqs. (2.10) and (2.11) are mg/l 24 h.

Table 2.10. Model equations in *STELLA*

```
PA(t) = PA(t - dt) + (P_UPTAKE - MINERALIZATION -OUTPUT_PA) * dt
INIT PA = 1.0
INFLOWS: P_UPTAKE = (SOLAR_RADIATION*PS/(1+PS))*PA
OUTFLOWS:
MINERALIZATION = 0.1*PA
OUTPUT_PA = (Q/V)*PA
PS(t) = PS(t - dt) + (MINERALIZATION + P_INPUT - P_UPTAKE - P_OUTPUT) * dt
INIT PS = 0
INFLOWS: MINERALIZATION = 0.1*PA
P_INPUT = (Q/V)*1.0
OUTFLOWS:
P_UPTAKE = (SOLAR_RADIATION*PS/(1+PS))*PA
P_OUTPUT = (Q/V)*PS
P_TOTAL = PS+PA
Q_V = 0.01
SOLAR_RADIATION = 0.5*(1.0+SIN(0.008603*TIME))
```

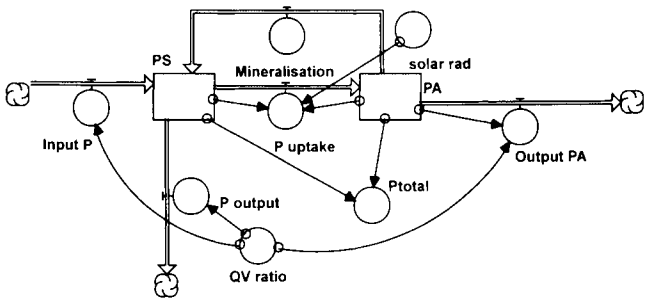

Fig. 2.15. The conceptual diagram of the model in Illustration 2.1, developed by STELLA.

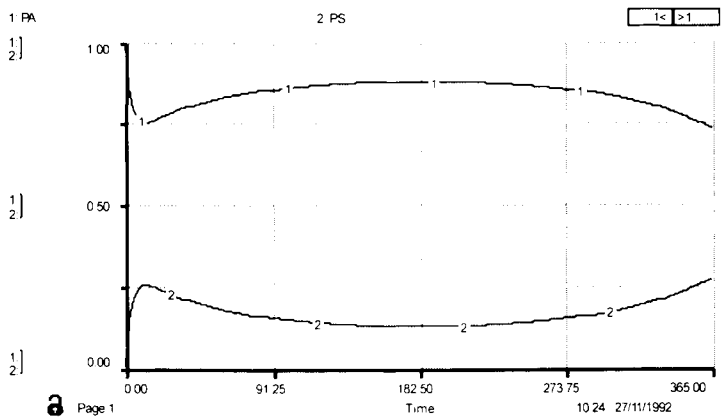

Fig. 2.16. *PS* and *PA* are plotted versus time. The model corresponds to the diagram Figs. 2.15 and 2.16 The equations are shown in Table 2.9.

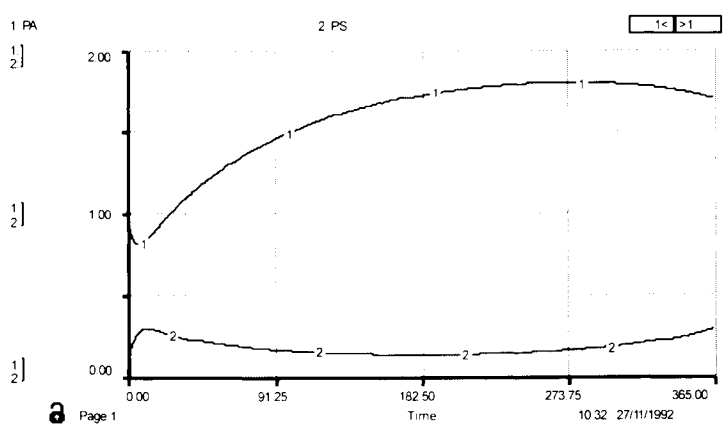

Fig. 2.17. Model response to increased phosphorus input. The concentration of phosphorus in the in-flowing water is increased from 1 mg/l to 2 mg/l.

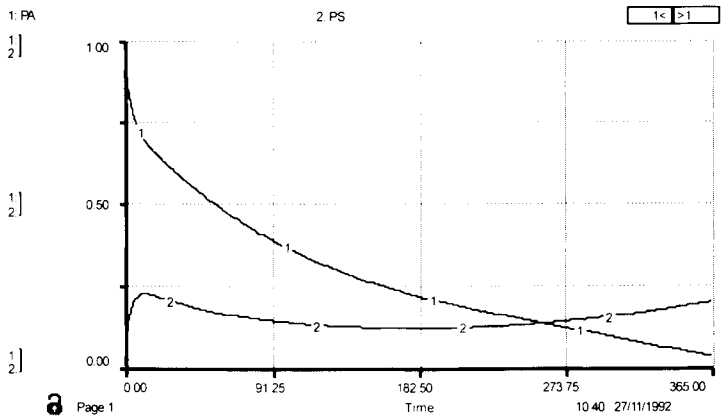

Fig. 2.18. Model response to decreased phosphorus input. The concentration of phosphorus in the in-flowing water is decreased from 1 mg/l to 0.2 mg/l.

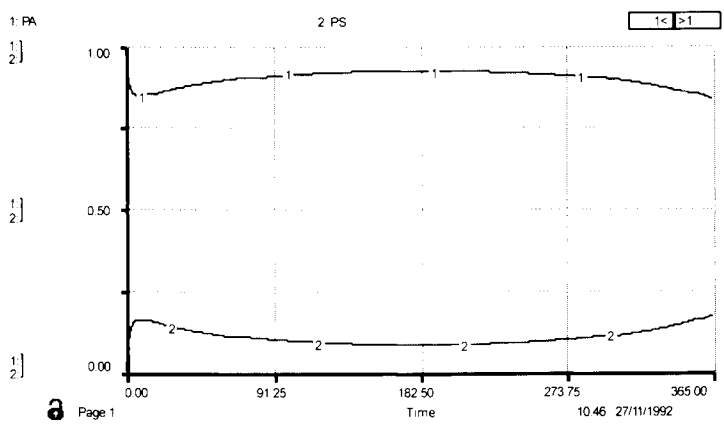

Fig. 2.19. Model response to increased solar radiation. S_{max} in the expression for solar radiation is increased from 0.5 to 0.75.

widely used in modelling. The user of STELLA needs only to draw the conceptual diagram (see Fig. 2.15) and to formulate the process equations. The differential equations are expressed by the software. Table 2.10 gives both sets of equations. Figures 2.16–2.19 give the results of a verification, where the forcing functions, i.e., PIN and S_{max} have been changed. The "internal logic" of the model is tested by recording the response of the model to increased and decreased phosphorus input and to increased solar radiation. The model's reactions to the changes performed are all according to our expectations. Increased phosphorus input and solar radiation

Table 2.11. *Pascal program* for a simple phosphorus model

```
Const
    (Initial values of state variables)
    PS: real = 0.0;
    PA: real = 0.1;
(Parameters defined as constants)
    K = 1.0;
    PIN = 1.0;
    V = 100.0;
    Q = 1.0;
    R = 0.1;
    SMAX = 0.5;
    dt = 0.5;
    MaxTime = 360;
    Time: real = 0;
    Var
    dPS: real;
    dPA: real;
    MY: real;
    PT: real;
    S: real;
    F: Text;
{Simple (Euler) integration algorithm}
Function Integrate (X,dX,dt:real) : real;
begin
    Integrate: = X + (dX*dt);
end;


Begin
    Assign(F,'outtab.txt');
    rewrite(F);
    write ln(F,'time PA PS');
    While time<=Max time do
    begin
    P:=PS + PA;
    S:=SMAX*(1.0+Sin(0.008603)*time);
    MY:=S*PS/(K+PS);
    dPS:=(PIN-PS)*Q/V-(MY-R)*PA;
    dPA:=(MY-R-Q/V)*PA;
    writeln(F,time:4:1,PA:10:4,PS:10:4);
    time:=time + dt;
    end;
    close(F);
    end.
```

give an increased phytoplankton biomass and decreased input of phosphorus implies decreased phytoplankton concentration.

The three computer languages presented above are only two of many possibilities. Odum and Odum (2000) give many examples based on *EXTEND* which is another user-friendly computer program based on preprogrammed blocks that are connected by the user to form system models. *EXTEND* has a large library of icon blocks. The computer language *C++* is also widely used to simulate ecological systems; see for instance Wilson (2000).

2.8 Sensitivity Analysis

It is important for the modeller to learn the properties of the model. The verification is an important step to obtain this knowledge: a sensitivity analysis would be the obvious next step to take. Through this analysis, the modeller gets a good overview of the most *sensitive components in the model.*

A *sensitivity analysis* attempts to provide a measure of the sensitivity of either *parameters*, forcing functions, initial values of the state variables or *submodels* to the state variables of greatest interest in the model. If the modeller wants to simulate a response of oxygen concentration in a stream to the discharge of organic matter, he will obviously choose oxygen concentration as the important state variable and will be interested in the submodels and the parameters to which the oxygen concentration is most sensitive. If, in population dynamics, the modeller wants to follow the development of a herbivorous population, the concentration or the total number of this population in a given area will be the important state variable, etc. The first step in the sensitivity analysis is therefore to answer the question: sensitive to what?

In practice, the sensitivity analysis is carried out by changing the parameters, forcing functions, initial values or submodel and observe the corresponding response on the important state variable (x). The sensitivity of a parameter, S, is defined in Eq. (2.1).

The relative change in parameters is chosen on the basis of our knowledge as to the uncertainty of the parameters. If the modeller estimates that the parameters are known within $\pm 50\%$ for instance, he would probably choose a change in the parameters at $\pm 10\%$ and $\pm 50\%$ and record the corresponding change in the state variable (x). It is often necessary to find the sensitivity at two or more levels of parameter change as the relationship between a parameter and a state variable is rarely linear; this implies that it is often crucial to know the parameters with the highest possible certainty before the sensitivity analysis is carried out. How this is possible will be discussed below and in the section on calibration. It should be added that the sensitivity most often varies with time, so it is necessary to find the sensitivity as f(time).

The interaction between the sensitivity analysis and the *calibration* could consequently work along the following lines:

1. A sensitivity analysis is carried out at two or more levels of parameter change. Relatively large changes are applied at this stage.

2. The most sensitive parameters are determined more accurately either by calibration or by other means (see next paragraph).

3. Under all circumstances great efforts are made to obtain a relatively good calibrated model.

4. A second sensitivity analysis is then carried out using narrower intervals for the parameter changes.

5. Still further improvements of the parameter certainty are attempted.

6. A second or third *calibration* is then carried out focusing mainly of the most sensitive *parameters*.

Table 2.12 shows the result of a partial sensitivity analysis on a complex eutrophication model. From the results it is evident that it is important to obtain as great a certainty as possible for the following parameters: max. growth rate of phytoplankton, max. growth rate of zooplankton, settling rate of phytoplankton, and respiration rate of phytoplankton and zooplankton. Therefore, it would be a big advantage if these parameters could be determined with great certainty by other

Table 2.12. Analysis of sensitivity (t here = time). PHYT: phytoplankton; ZOO: zooplankton; NS: soluble nitrogen and PS: soluble phosphorus. Annual average values for sensitivities (S) are shown. t illustrates change in time for occurrence of maximum values.

Definition	Parameter	S_{PHYT}	S_{ZOO}	S_{NS}	S_{PS}	t_{PHYT}	t_{ZOO}	t_{NS}	t_{PS}
Max. growth rate PHYT	CDR_{max}	0.488	0.620	−0.356	−0.392	−0.31	−0.11	−0.23	0.0
Denitrification rate	DENIT	−0.19	−0.010	−0.579	0.013	0.05	0.0	−0.70	0.0
Fish concentration	FISH	0.008	0.012	−0.011	−0.014	0.0	0.10	0.0	0.0
Initial PHYT conc.	PHYT (t=0)	−0.020	−0.044	0.032	0.033	−0.05	−0.35	−0.15	0.0
Initial ZOO conc.	ZOO (t=0)	−0.169	−0.223	0.252	0.282	0.0	−1.58	−0.43	0.0
Rate of mineralization (N)	KDN_{10} (10°C)	0.003	0.010	0.038	0.001	0.45	0.0	−0.30	0.0
Rate of mineralization (P)	KDP_{10} (10°C)	0.0	0.001	0.0	0.006	0.0	0.0	0.0	0.0
Michaelis–Menten constant (N)	KN	−0.001	−0.032	0.063	0.019	0.45	−0.05	−0.15	0.0
Michaelis–Menten constant (P)	KP	−0.003	−0.014	0.021	0.034	0.05	−0.05	−0.25	0.0
Max. growth rate ZOO	NYZ_{max}	−2.088	−4.002	2.749	4.052	−1.50	−25.95	−17.90	0.0
Mortality ZOO	MZ	2.063	1.949	−3.479	−3.350	1.30	21.50	8.40	0.0
Max. predation rate	$PRED_{max}$	0.008	0.011	−0.015	−0.016	0.0	0.10	−0.20	0.0
Max. respiration rate PHYT	RC_{max}	−0.243	−0.201	0.139	0.153	0.45	0.05	−0.35	0.0
Max. respiration rate ZOO	RZ_{max}	0.570	0.625	−0.902	−0.978	0.95	5.94	1.34	0.0
Settling rate detritus	SVD	0.0	0.0	−0.002	0.0	0.0	0.0	0.0	0.0
Settling rate PHYT	SVS	−1.042	−0.823	0.321	0.388	−0.05	0.20	0.15	0.0
Max. uptake of C	UC_{max}	0.629	0.636	−0.428	−0.481	0.05	0.10	−0.25	0.0
Max. uptake of N	UN_{max}	0.046	0.145	−0.251	−0.050	0.05	−0.05	−0.15	0.0
Max. uptake of P	UP_{max}	0.026	0.090	−0.049	−0.339	0.50	0.05	−0.15	0.0

means, e.g., by laboratory investigations aimed at a direct determination of just these parameters.

A sensitivity analysis on *submodels* (equations) can also be carried out. Here, the change in a state variable is recorded when the equation or submodel is deleted from the model or changed to alternative expressions, e.g., with more details built into the submodel. Results from such a sensitivity analysis might be used to change the structure of the model if, for example, it is found that the submodel has a great impact on the state variable in focus. The selection of the complexity and the structure of the model should therefore work hand in hand with the sensitivity analysis. There is a feedback from the *sensitivity analysis* to the *conceptual diagram*. This idea is according to the selection of model structure mentioned in Section 2.5, where all the methods presented presume that the results are used to change the conceptual diagram, i.e., the structure and complexity of the model.

If it is found that the state variable in focus is very sensitive to a certain submodel, it should be considered which alternative submodels could be used and they should be tested and/or further examined in detail either *in vitro* or in the laboratory.

It can generally be stated that those submodels that contain sensitive parameters are also submodels that are sensitive to the important state variable. But on the other hand it is not necessary to have a sensitive parameter included in a submodel to obtain a sensitive submodel. A modeller with a certain experience will find that these statements agree with his intuition, but it is also possible to show that they are correct by analytical methods.

A sensitivity analysis on forcing functions gives an impression of the importance of the various forcing functions and tells us what accuracy is required of the forcing functions' data.

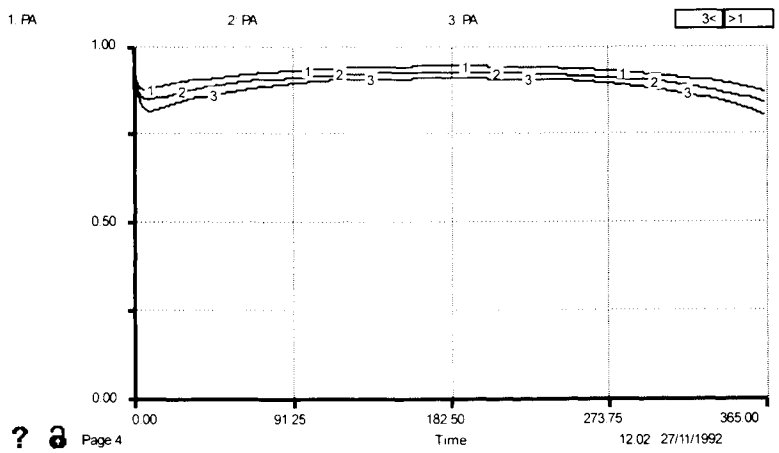

Fig. 2.20. The model response of three K-values is shown. Curve 1 corresponds to K = 0.8, curve 2 to K = 1.0 and curve 3 to K = 1.2. STELLA has facilities to perform a sensitivity analysis with the result illustrated as a graph similar to Fig. 2.2.

Illustration 2.2

The *sensitivity analysis* in Table 2.12 shows annual average values of a sensitivity analysis for a complex eutrophication model. It would generally be preferable to observe the sensitivity versus the time, as pointed out above. $PS = f(t)$ for the model presented in Illustration 2.1 is shown in Fig. 2.20. The response of three different K-values is shown. Three different values of K, *Michaelis/Menten's constant* for the uptake of phosphorus, are tested: $K = 0.8$ mg/l, $K = 1.0$ mg/l (this was the value used for all the simulations in Illustration 2.1) and $K = 1.2$ mg/l. It can be seen from Fig. 2.21 that the sensitivity is lowest in summer (the differences between the curves are smallest in summer) and highest in winter, but the differences are minor. It is therefore considered important to find the influence of K as f(time).

2.9 Parameter Estimation

Many *parameters* in causal ecological models can be found in the literature, not necessarily as constants but as approximate values or intervals. Jørgensen et al. (2000) contains about 120,000 parameters of interest to ecological modellers.

However, even if all the parameters of a model are known from the literature, it is usually necessary to calibrate the model because the biological parameters are only known as ranges. Several sets of parameters are tested by the *calibration* and the various model outputs of state variables are compared with measured or observed values of the same state variables. The parameter set that gives the best agreement between model outputs and measured state variables is chosen.

The need for calibration can be explained by the use of the following characteristics of ecological models and their parameters:

1. As mentioned above, unlike many chemical and physical parameters, it is rare that most ecological parameters are known as exact values. Therefore all literature values for ecological parameters have some degree of uncertainty.
2. All ecological models are a *simplification* of nature. The process descriptions and the system structure do not account for all the details. If the model is selected carefully it will include all important processes and components for the problem in focus, but still the details omitted (although of minor importance for the problem) might still have an influence on the result. To a certain extent, this influence can be taken into account by the calibration. The parameters might be given a value slightly different from the real, but unknown value, in nature and this difference might partly account for the influence of the omitted details.
3. Most ecological models are *lumped models*; this implies that one parameter represents the average values of several species. As each species has its own characteristic parameters, the variation in species composition inevitably gives a corresponding variation in the average parameter used in the model. Besides, the algebraic average of the parameters does not necessarily represent the right

parameter for the actual species composition. These difficulties make it almost impossible to find a correct initial value for a parameter. Here, the calibration phase will, at least to a certain extent, account for the species composition.

(4) An ecosystem is a flexible system which can meet changes in forcing functions by new properties of the state variables. This is either an adaptation of the present species or a change in species composition. It is important in many modelling contexts to include this characteristic of ecosystems into our model. This type of model is called a structurally dynamic model and will be presented in Chapter 9.

A *calibration* cannot be carried out randomly. The modeller tries to change various parameters one by one to get an acceptable accordance between observed values and model outputs for one or two state variables at a time. In a eutrophication model, for instance, it might be helpful to concentrate on the dynamic of one nutrient at a time and then, after the nutrient dynamic is acceptable, go on to the phytoplankton dynamics. Before the calibration is satisfactory, the modeller may have had to perform several hundred model runs.

Procedures for *automatic calibration* are available, but they do not make the trial and error calibration described above redundant. If the automatic calibration should give acceptable results within a certain time frame, it is necessary to calibrate only 6–9 parameters simultaneously and the smaller the uncertainties (i.e., the intervals used for allowed variations of parameters) are, the easier it will be to find the optimum parameter set. The user gives: (1) an initial guess for the parameter; (2) ranges of parameter variations; (3) a set of measured state variables; and (4) an acceptable maximum value for the standard deviation between modelled and measured values.

In the trial and error *calibration* the modeller has somewhat intuitively set up some calibration criteria. He wants to be able in the first instance to simulate fairly accurately the minimum oxygen concentration for a stream model and/or the time at which this minimum value occurs. When he is satisfied with these model results, he might want to simulate properly the shape of the oxygen concentration versus time curve, etc. He calibrates the model to achieve these objectives step by step.

If an automatic calibration procedure is used, it is necessary to formulate objective criteria for the calibration. A possible objective function such as Eq. (2.2) may be used. However, the modeller is often more interested in a *good accordance* between observations and model output for *one or a few state variables.* In that case he can choose weight for the various state variables. For a *eutrophication model*, for instance, he might choose the weight 10 for phytoplankton and the weight 5 for the nutrient concentrations, while all other state variables are given the weight 1. He might also be interested in ensuring a very high accuracy of the simulation of the maximum concentration of the phytoplankton and will therefore give an even higher weight to the phytoplankton concentration at the time when the spring bloom is expected to occur.

If it is impossible to calibrate a model, this is not necessarily due to an incorrect model; it might be due to the low quality of the observed data. The quality of the data

is crucial to the quality of the calibration. It is furthermore of great importance that **observations reflect the dynamics of the model**. If the objective of the model is to describe the dynamic behaviour of a state variable which varies from day to day, it is of course not possible to achieve a good parameter estimation based on monthly observations. This should be illustrated by an example taken from a eutrophication model.

A eutrophication model is generally calibrated based on an annual measurement series with a sampling frequency of once or twice per month. This sampling frequency is not sufficient to describe the dynamics of the lake. If it is the scope of the model to predict maximum values and related data for phytoplankton concentrations and primary production, it is necessary to have a sampling frequency that can give us an estimate of the maximum value in phytoplankton concentration and the primary production.

Figure 2.21 shows characteristic algae concentrations plotted versus time, 1 April–15 May, in a hypertrophic lake with a sampling frequency of (2) twice per month, and (1) three times per week (denoted as the "intensive" measuring program). As can be seen, the two plots are significantly different and any attempt to get a realistic calibration based on (2) will fail, provided it is the aim to model the day-to-day variation in phytoplankton concentration according to (1). This example illustrates that it is of great importance not only to have data with low uncertainty, but also data sampled with a frequency corresponding to the dynamics of the system.

This rule has often been neglected in modelling the *eutrophication* process, most probably because limnological lake data, which are not sampled for modelling purposes, are often collected with a relatively low frequency. On the other hand, the model then attempts to simulate the annual cycle, and an annual sampling program with a frequency of three per week will require too many resources. A combination of an annual *sampling program* with a frequency of one to three samples per month

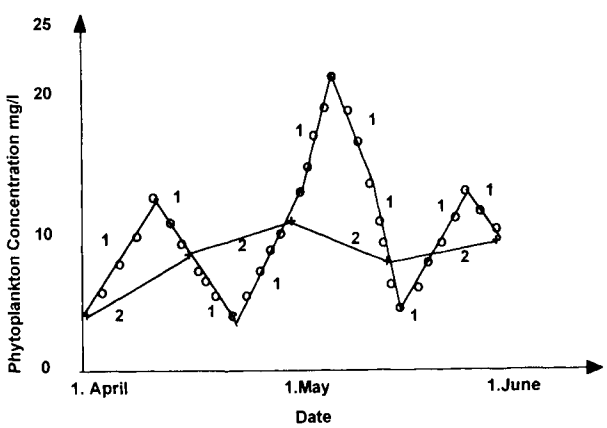

Fig. 2.21. Algae concentration plotted versus time: curve (1) = sampling frequency twice a month (+); curve (2) = sampling frequency three times a week (*). Note the difference of d(PHYT)/dt between the two curves.

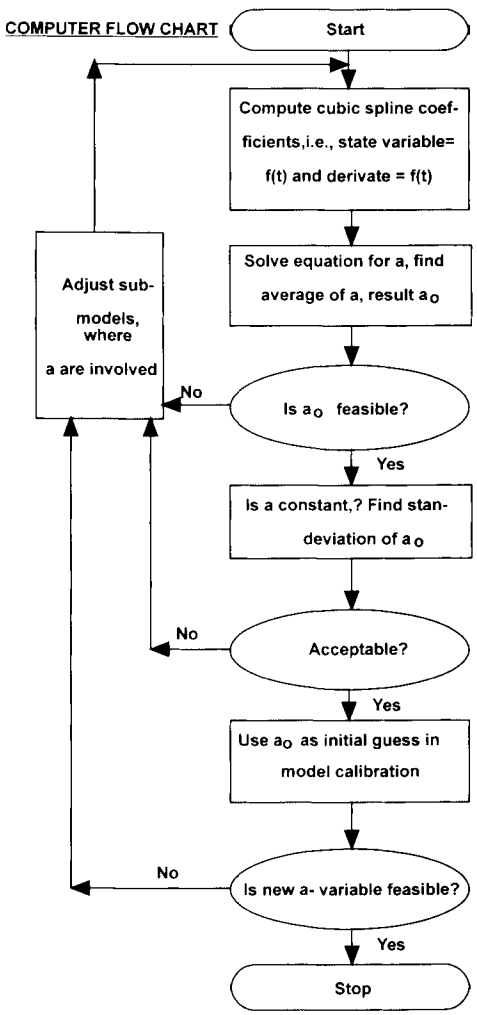

Fig. 2.22. Computer flow chart of the method applied to estimate parameters by use of "intensive measurements".

and an intensive measuring program placed in periods during which different subsystems show a maximum number of changes gives a good basis for parameter estimations.

The *intensive measuring program* can, as presented below, be used to estimate state variables' derivatives (for comparison of these estimations by low and high sampling frequency, see the slopes of curves (1) and (2) in Fig. 2.21). These estimates can be used to set up an over-determined set of algebraic equations, making the model parameters the sole unknown. An outline of the method runs as follows (see Fig. 2.22) (for further details, see Jørgensen et al., 1981).

- **Step 1**. Find cubic spline coefficients, $S_i(t_j)$, i.e., second-order time derivatives at time of observation t_j, of the spline function $s_i(t_j)$ approximating the observed variable $\psi_i(t)$, according to the *cubic spline method*. Alternatively, it is possible to find a n'th order polynomium (4–8 order is most often used) approximating the observations by an n'th order regression analysis. Several statistical software packages are available to perform such regression analyses very rapidly.
- **Step 2**. Find $\partial\psi_i(t_j)/\partial t = f(t)$ by differentiation of the function found in step 1: $\psi = f(\psi,t,a)$, where a is a parameter.
- **Step 3**. Solve the model equation of the form:

$$\partial\psi(t_j)/\mathrm{d}t = f(\psi,\partial\psi/\partial r\partial^2\psi/\partial r^2,t,a) \tag{2.14}$$

  with the average value of a, regarded as unknown.
- **Step 4**. Evaluate the feasibility of *the solution* a_0 found in Step 3. If not feasible, modify the part of the model influenced by a_0 and go to Step 1.
- **Step 5**. Choose a significance level, and perform a statistical test on constancy of a_0. If the test fails, modify appropriate *submodels* and go to Step 1.
- **Step 6.** Use a_0 as an initial guess in a computerized parameter search algorithm, such as Marquardt, Powell or steepest descent algorithms, to minimize a performance index, e.g., the one proposed in Eq. (2.2).

Although the model in hand may be highly non-linear regarding the state variables, it usually turns out that this is not the case regarding the *parameter* set a, or the subset of a that is tuned by calibration. Since the number of differential equations is greater than the number of estimable parameters, Eq. (2.14) is over-determined. It is easy to smooth the solution in some sense, but it is more important to evaluate the constancy of a_0, e.g., by variance analysis, test of normality of *white noise*, etc. Information on standard deviation of a_0 around its average value may eventually be used as point of departure for introducing *stochasticity* into the model, admitting the fact that parameters in real life may not be as constant as the modellers assume.

As a certain parameter, e.g., a_k, seldom appears at more than one or two places in the model equations, an unacceptable value of a_k found as solution to Eq. (2.14) quite accurately locates the inappropriate terms and constructs in the model. Experience with the method has shown it to be valuable as a diagnostic tool to single out unfitted model terms.

Since the method is based on *cubic spline approximation*, it is essential that observations are dense, i.e., $t_{j+1} - t_j$ should be small in the sense that local third-degree polynomials should approximate observed values well. To test whether this is fulfilled is generally difficult as the 'true' $\psi_i(t)$ function might have microscopic curls that generate oscillating derivates ($\psi_i/\mathrm{d}t$). However, if the method yields basically the same result on a random subset of observations, it may be safe to assume that

Table 2.13. Comparison of parameter values

Parameter	Parameter (Symbol)	Unit	Application of intensive measurements	Glumsø Lake*	Lyngby Lake*	Literature ranges
Settling rate	SVS = D x SA	$m\ d^{-1}$	0.30±0.05	0.2	0.05	0.1–0.6
Max. growth rate**	CDRmax (reduced)	d^{-1}	1.33±0.51	2.3	1.8	1–3
Max. growth rate**	CDRmax (model)	d^{-1}	4.71±1.8	4.11	3.21	2–6
Max. uptake rate P**	UPmax	d^{-1}	0.0072±0.0007	0.003	0.008	0.003–0.01
Min. C:biomass ratio**	FCAmin		0.4	0.15	0.15	0.3–0.7
Min. P: biomass ratio**	FPAmin		0.03	0.013	0.013	0.013–0.035
Min. N: biomass ratio	FNAmin		0.12	0.10	0.10	0.08–0.12
Max. uptake rate N**	UNmax	d^{-1}	0.023±0.005	0.015	0.012	0.01–0.035
Michaelis-Menten constant N**	KN	$mg\ l^{-1}$	0.34±0.07	0.2	0.2	0.1–0.5
Denitrification rate	DENITX	$g\ m^{-3}\ d^{-1}$	0.83±1.05			
Respiration rate**	RC	d^{-1}	0.088	0.13	0.2	0.05–0.25
Mineralization rate P	KDP10	d^{-1}	0.80±0.47	0.40	0.25	0.2–0.8
Mineralization rate N	KDN10	d^{-1}	0.21±0.11	0.05	0.15	0.05–0.3
Max. uptake rate C**	UCmax	d^{-1}	1.21±0.97	0.65	0.40	0.2–1.4

*Lyngby and Glumsø lakes have approximately the same biogeochemical characteristics and morphology.
**All parameters relate to phytoplankton.

$\{s_i(t_j)/dt\}$ represent the true rates on a day basis. After appropriate adjustment of the model equations an acceptable parameter set a_0 may eventually be obtained.

With a_0 as an initial guess, a better parameter set may be found by systematic perturbation of the set until some norm (performance index) has reached a (local) minimum. At each perturbation, the model equations are solved. Gradients $\{\delta\psi_i / \delta a_k\}$ are hardly ever known analytically. All numerical methods currently in use to solve this kind of problem fail when the number of parameters surpasses four or five, unless the initial guess is very close to a value that minimizes the performance index. This is why Steps 1 and 2 above are so important. The result of the application of what are called intensive measurements to calibrate the *eutrophication* model is summarized in Table 2.13. As can be seen, the difference in parameter estimation is pronounced. It was found to be important to use the parameters determined by intensive measurements *before* the final calibration took place.

The illustrated use of intensive measurements for a *parameter estimation* prior to the calibration was based on determinations of the actual growth of phytoplankton. By determination of the derivatives, it was possible to fit the parameters to the unknown in the model equations.

In the case referred to, measurements and observations *in vitro* were used to find the derivates. In principle, the same basic idea can be used either in the laboratory or by construction of a microcosm. In both cases the measurements are facilitated by a smaller unit, where disturbing factors or processes might be kept constant. A current record of important state variables is often possible and provides a large number of data, which decreases the standard deviation.

An example will be quoted to illustrate this method of parameter estimation. Fish growth can be described by use of the following equation:

$$dW/dt = a \times W^b \tag{2.15}$$

where W is the weight, a and b are constants. It is possible in an aquarium or in aquaculture to follow the weight of the fish versus time. If enough data are available it is easy using statistical methods to determine a and b in the above equation. In this case the feeding is known to be at the optimum level; no predator is present and the water quality, which influences growth, is maintained constant to ensure the very best growth conditions for the fish. By varying these factors it is even possible to find the influence of the water quality, and the available food on the growth parameters. It is often the results of such experiments that can be found in the literature. However, the modeller might not find the parameter for the particular species of interest to him, or cannot find the parameters in the literature under the conditions prevailing in the ecosystem he wants to model. Then he might use such experiments to determine parameters of importance to his model. Even if he can find literature values for the crucial parameters, he might still want to carry out *parameter* determinations in the laboratory or in a microcosm, if he estimates that the interval of the parameters in the literature is too wide for the most sensitive parameters.

However, parameters taken from the literature or resulting from such experiments should be applied with caution because the discrepancy between the values in the laboratory, or even the microcosm, and those in nature are much greater for biological parameters than for chemical or physical parameters. The reasons for this can be summarized as follows:

1. Biological parameters are generally **more sensitive to *environmental factors***. An illustrative example would be: a small concentration of a toxic substance could change growth rates significantly.
2. Biological parameters are **influenced by many *environmental factors***, some of which are very variable. For instance, the growth rate of phytoplankton is dependent on the nutrient concentration, but the local nutrient concentration is very dependent on the water turbulence, which again is dependent on the wind stress, etc.
3. The example in point 2 shows, furthermore, that **the *environmental factors* influencing biological parameters are interactive,** which makes it almost impossible to predict an exact value for a parameter in nature from measurements in the laboratory, where the environmental factors are all kept constant. On the other hand if the measurements are carried out *in situ* it is not possible to interpret under which circumstances the measurement is valid, because that would require the determination, simultaneously, of too many interactive environmental factors.
4. Often, determinations of biological parameters or variables **cannot be carried out** directly, but it is necessary to measure another quantity that cannot be exactly related to the biological quantity in focus. For instance, the phyto-

plankton biomass cannot be determined by any direct measurement, but it is possible to obtain an indirect measurement using the chlorophyll concentration, the ATP concentration, the dry matter 1–70 μ etc.; yet none of these indirect measurements give an exact value of the phytoplankton concentration, as the ratio of *chlorophyll* or *ATP* to the biomass is not constant, and the dry matter 1–70 μ might include other particles (e.g., clay particles). So, it is recommended in practice to apply several of these indirect determinations simultaneously to ensure that a reasonable estimate is applied. Correspondingly, the growth rate of phytoplankton might be determined by the oxygen method or the C14-method. Neither method determines the photosynthesis, but the net production of oxygen, and the net uptake of carbon, respectively, i.e., the result of the photosynthesis and the respiration. The results of the two methods are therefore corrected to account for the respiration, but obviously the correction should be different in each individual case—something that is, however, difficult to do accurately.

5. Biological parameters are finally **influenced by several *feedback mechanisms* of a biochemical nature**. The past will determine the parameters in the future. For example, the growth rate of phytoplankton is dependent on the temperature—a relationship that can easily be included in ecological models. The maximum growth rate is obtained by the optimum temperature, but the past temperature pattern determines the optimum temperature. A cold period will decrease the optimum temperature. To a certain extent, this can be taken into account by the introduction of variable parameters (see Straskraba, 1980). In other words, it is an approximation to consider parameters as constants. An ecosystem is a soft, flexible system and only with approximations can it be described as a rigid system with constant parameters (see Jørgensen, 1981; 1992a,b).

The estimation of the settling velocity as a parameter in ecological models may be crucial, as it determines the removal rate for a considered component, whether the component is suspended matter or phytoplankton. The sensitivity of this parameter to the phytoplankton concentration in a *eutrophication* model has been determined to be about –1.0 (see Table 2.12). It means that if the parameter is increased by 1%, the phytoplankton concentration will decrease by 1% (see Jørgensen et al., 1978). Let us therefore use the estimation of the settling rate as another illustration of the considerations needed in our effort to obtain a proper determination of parameters.

Settling velocity may be determined in three ways:

1. Values from previous models in the literature can be used to give a first estimation of the parameter. Tables 2.14 and 2.15 summarize values found in the literature. As can be seen, these values are indicated as ranges, and it is therefore necessary to calibrate the parameters by the use of measured values for the stated variables.
2. Values from calculations based on knowledge of the size can be used as first estimations. Because of the influence of the many factors mentioned above, a calibration is also required in this case. This method is hardly applicable for

Table 2.14. Phytoplankton settling velocities

Algal type	Settling velocity (m/day)	References
Total phytoplankton	0.05–0.5	Chen & Orlob (1975); Tetra Tech (1980); Chen (1970); Chen & Wells (1975; 1976)
	0.05–0.2	O'Connor et al. (1981); Thomann et al. (1974; 1975); Di Toro & Matystik (1980); Di Toro & Connolly (1980); Thomann & Fitzpatrick (1982)
	0.02–0.05	Canale et al. (1976)
	0.4	Lombardo (1972)
	0.03–0.05	Scavia (1980)
	0.05	Bierman et al. (1980)
	0.2–0.25	Youngberg (1977)
	0.04–0.6*	Jorgensen et al. (2000)
	0.01–4.0*	Jorgensen et al. (2000)
	0.1–2.0*	Chen & Orlob (1975)
	0.15–2.0*	Jorgensen et al. (2000)
	0.1–0.2*	Brandes (1976)
Diatoms	0.05–0.4	Bierman (1976); Bierman et al. (1980)
	0.1–0.2	Jorgensen et al. (2000)
	0.1–0.25	Tetra Tech (1980)
	0.03–0.05	Canale et al. (1976)
	0.3–0.5	Jorgensen et al. (2000)
	2.5	Lehman et al. (1975)
	0.02–14.7*	Jorgensen et al. (2000)
Green algae	0.05–0.19	Jorgensen et al. (2000)
	0.05–0.4	Bierman (1976); Bierman et al. (1980)
	0.02	Canale et al. (1976)
	0.8	Lehman et al. (1975)
	0.1–0.25	Tetra Tech (1980)
	0.08–0.18*	Jorgensen et al. (2000)
	0.27–0.89*	Jorgensen et al. (2000)
Blue-green algae	0.05–0.15	Bierman (1976); Bierman et al. (1980)
	0.08	Canale et al. (1976)
	0.2	Lehman et al. (1975)
	0.1	Jorgensen et al. (2000)
	0.08–0.2	Tetra Tech (1980)
Flagellates	0.5	Lehman et al. (1975)
	0.05	Bierman et al. (1980)
	0.09–0.2	Tetra Tech (1980)
	0.07–0.39**	Jorgensen et al. (2000)
Dinoflagellates	8.0	O'Connor et al. (1981)
	2.8–6.0**	Jorgensen et al. (2000)
Asterionella formosa	0.25–0.76**	Jorgensen et al. (2000)
Chaetoceros lauderi	0.46–1.56**	Jorgensen et al. (2000)
Chrysophytes	0.5	Lehman et al. (1975)

continued

Table 2.14 (*continuation*)

Algal type	Settling velocity (m/day)	References
Coccolithophores	0.25–13.6	Jørgensen et al. (2000)
	0.3–1.5**	Jørgensen et al. (2000)
Coscinodiscus lineatus	1.9–6.8**	Jørgensen et al. (2000)
Cyclotella meneghimiana	0.08–0.31**	Jørgensen et al. (2000)
Ditylum brightwellii	0.5–3.1**	Jørgensen et al. (2000)
Nitzschia seriata	0.26–0.50**	Jørgensen et al. (2000)
Rhizosolenia robusta	1.1–4.7**	Jørgensen et al. (2000)
Rhizosolenia setigera	0.22–1.94**	Jørgensen et al. (2000)
Scenedesmus quadracauda	0.04–0.89**	Jørgensen et al. (2000)
Skeletonema costatum	0.31–1.35**	Jørgensen et al. (2000)
Tabellaria flocculosa	0.22–1.11**	Jørgensen et al. (2000)
Thalassiosira nana	0.10–0.28**	Jørgensen et al. (2000)
T.n. pseudonana	0.15–0.85**	Jørgensen et al. (2000)
T.n. rotula	0.39–17.1	Jørgensen et al. (2000)

*Model documentation values. **Literature values. Other values: used in models.

Table 2.15. Detritus, settling rate

Item	Settling velocity (m/day)	References
Detritus	0.1–2.0	Jørgensen et al. (2000)
Nitrogen detritus	0.05–0.1	Jørgensen et al. (2000)
Faecal pellets (fish)	23–666	Jørgensen et al. (2000)

phytoplankton, because of their ability to change the specific gravity, but may be useful for other particles.

3. Measurements *in situ* by the use of sedimentation traps. It is possible to determine the distribution of the material in inorganic and organic matter, and also partly in phytoplankton and detritus, by the analysis of chlorophyll (fresh material) phosphorus, nitrogen and ash. Measurements of phytoplankton settling velocities in the laboratory will hardly give a reliable value as they do not consider the various factors *in situ*.

It has been pointed out above, that **the *calibration* is significantly facilitated if we have good initial guesses of the *parameters*.** Some might be found in the literature, but there are only a few compared with the number of parameters needed if we want to model all interesting mass flows in all relevant ecosystems. For nutrient flows the

parameters are known from the literature for the most common species only. But if we turn to flows of toxic substances in ecosystems the number of known parameters is even more limited. The earth has millions of species and the number of substances of environmental interest is about 100 000. If we want to know 10 parameters for each interaction between substances and species, the number of parameters needed is enormous. For example, if we need the interactions of, let us say, only 10 000 species with the 100 000 substances of environmental interest, the number of parameters needed is $10 \times 10.000 \times 100.000 = 10^{10}$ parameters. In Jørgensen et al. (2000) can be found 120 000 parameters and if we estimate that this handbook covers about 10% of the parameters that can be found in the entire literature, we know only about 0.012% of the required parameters. Physics and chemistry have attempted to solve this problem by setting up some general relationships between the properties of the chemical compounds and their composition and structure. This approach is widely used in *ecotoxicological modelling*, as will be shown in Chapter 8. If the necessary data cannot be found in the literature such relationships are widely used as a second best approach to the problem.

If we draw a parallel to ecology, we need some general relationships that give us some good first estimations of the parameters needed. In many ecological models used in an environmental context the accuracy required is not very high. In many toxic substance models we need only to know, e.g. whether we are far from or close to the toxic levels. More experience with the application of general relationships is needed before a more general use can be recommended. In this context it should be emphasized that in chemistry such general relationships are used very carefully.

Modern molecular theory provides a sound basis for the predictions of reliable quantitative data on the chemical, physical and thermodynamic properties of pure substances and mixtures. The biological sciences are not based on a similar comprehensive theory, although it is possible, to a certain extent, to apply the laws of basic biochemical mechanisms to ecology. Furthermore, the basic biochemical mechanisms are the same for all plants and all animals. The spectrum of biochemical compounds is wide, but considering the number of species and the number of possible chemical compounds it is very limited. The number of different protein molecules is significant, but they are all constructed from only 24 different amino acids.

This explains why the elementary composition of all species is fairly similar. For their fundamental biochemical function, all species need a certain amount of carbohydrates, proteins, fats and other compounds, and as these groups of biochemical substances are constructed from a relatively few simple organic compounds, it is not surprising that the composition of living organisms varies only a little (see tables in Jørgensen et al., 1991; 2000). It implies that if we know, for instance, the uptake rate of nitrogen for phytoplankton, we can find the approximate uptake rate of phosphorus, because the uptake rates must result in a nitrogen to phosphorus ratio of between 5:1 and 12:1, on average 1:7.

The biochemical reaction pathways are also general, as demonstrated in all textbooks on biochemistry. The utilization of *chemical energy* in the food components is basically the same for microorganisms and mammals. It is, therefore,

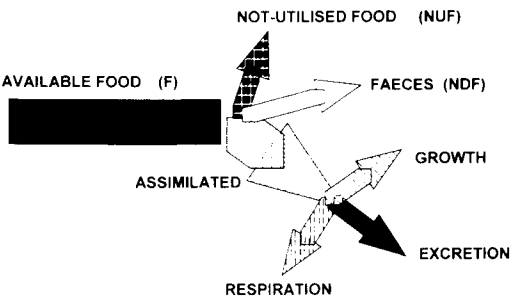

Fig. 2.23. The principle of the model of fish growth. The feed is used for respiration, excretion, growth, non-digested or not utilised. Notice that the assimilated amount of energy is $F - NUF - NDF$ and is used for respiration, excretion and growth (see Jørgensen, 1979).

possible to calculate the energy, $E1$, released by digestion of food, when the composition is known:

$$E1 = 9\frac{\text{fat}\%}{100} + 4\frac{(\text{carbohydrates} + \text{proteins})\%}{100} \tag{2.16}$$

The law of energy conservation is also valid for a biological system (see Fig. 2.23). The chemical energy of the food components is used to cover the energy needs for growth, respiration, assimilation, reproduction and losses. As it is possible to set up relationships between these needs on the one side, and some fundamental properties of the species on the other, it is possible to put a number on the items on Fig. 2.23 for different species. This is a general but valid approach to parameter estimation in ecological modelling.

The surface area of the species is a fundamental property. The surface area indicates quantitatively the size of the boundary to the environment. Loss of heat to the environment must be proportional to this area and to the temperature difference, according to the law of heat transfer. On the one hand, the rate of digestion, the lungs, hunting ground, etc. determine a number of parameters, and on the other hand, they are all dependent on the size of the animal.

It is therefore not surprising that many *parameters* for plants and animals are very much related to their size, which implies that it is possible to get very good first estimates for most parameters based only upon the size. Naturally, the parameters are also dependent on several other characteristic features of the species, but their influence is minor compared with the size, and providing good estimates is valuable in many models, at least as a starting value in the *calibration* phase.

The conclusion of these considerations must therefore be that there should be many parameters that relate to simple properties, such as size of the organism, and that such relationships are based on fundamental biochemistry and thermodynamics.

Above all, there is a strong positive correlation between *size* and *generation time*, T_g, ranging from bacteria to the biggest mammals and trees (Bonner, 1965). This

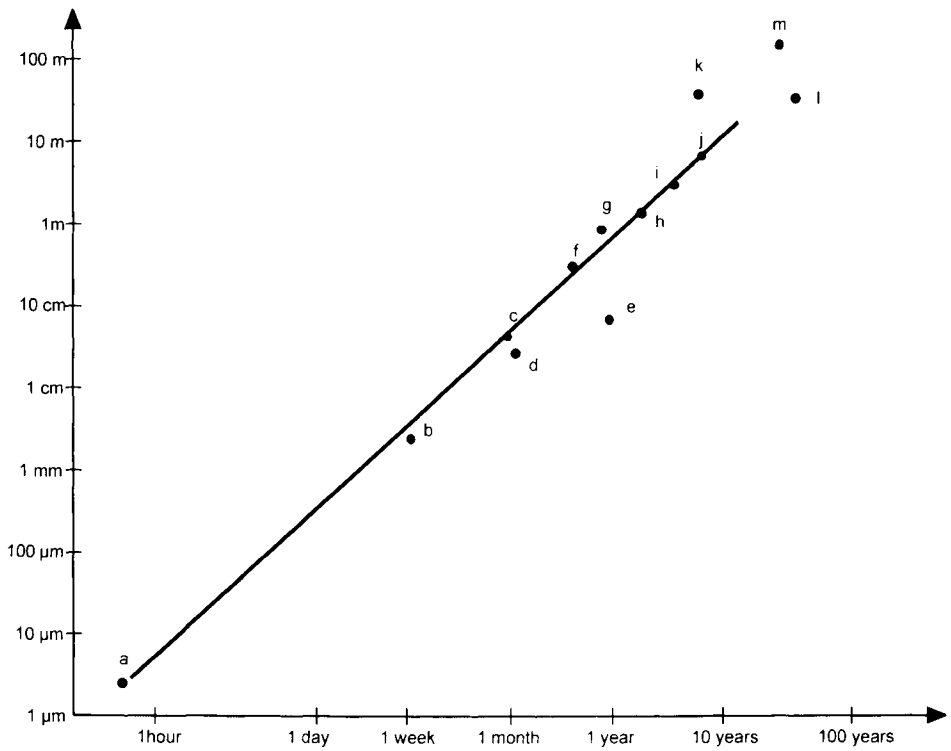

Fig. 2.24. *Length* and *generation time* plotted on a log–log scale: (a) pseudomonas, (b) daphnia, (c) bee, (d) house fly, (e) snail, (f) mouse, (g) rat, (h) fox, (i) elk, (j) rhino, (k) whale, (l) birch, (m) fir.

relationship is illustrated in Fig. 2.24 and can be explained by use of the relationship between size (surface) and total metabolic action per unit of *body weight* mentioned above. It implies that the smaller the organism, the greater the metabolic activity. The *per capitum* rate of increase, r, defined by the exponential or logistic growth equations:

$$dN/dt = rN \tag{2.17}$$

and

$$dN/dt = rN(1 - N/K) \tag{2.18}$$

respectively, is again inversely proportional to the generation time.

This implies that r is related to the size of the organism, but, as shown by Fenchel (1970), actually falls into three groups: unicellular, poikilo-therms and homeotherms (see Fig. 2.25). Thus the metabolic rate per unit of weight is related to the

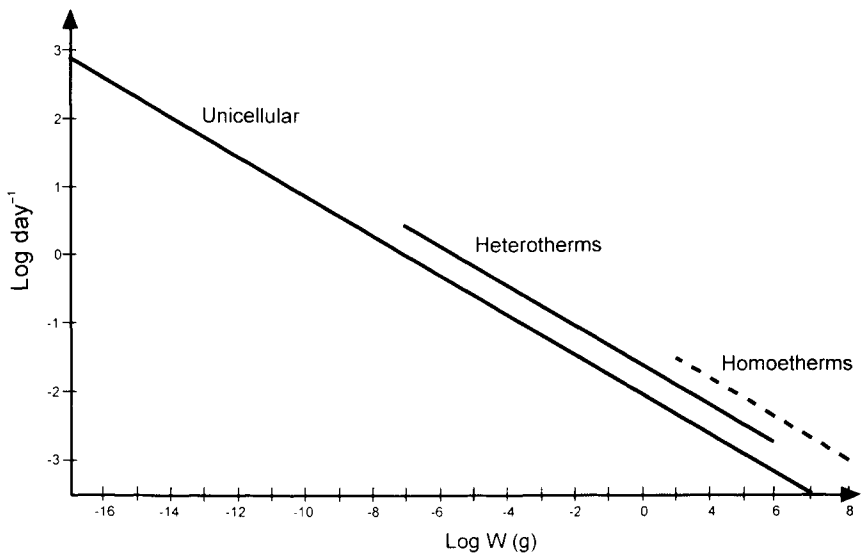

Fig. 2.25. Intrinsic rate of natural increase against weight for various animals.

size. The same basis is expressed in the following equations, giving the respiration, feed consumption and ammonia excretion for fish when the weight, W, is known:

$$\textit{Respiration} = \text{constant} * W^{0.80} \tag{2.19}$$

$$\textit{Feed Consumption} = \text{constant} * W^{0.65} \tag{2.20}$$

$$\textit{Ammonia Excretion} = \text{constant} * W^{0.72} \tag{2.21}$$

This is also expressed in Odum's equation (Odum, 1969; 1971):

$$m = k\, W^{-1/3} \tag{2.20}$$

where k is roughly a constant for all species, equal to about 5.6 kJ/g$^{2/3}$ day, and m is the metabolic rate per weight unit.

Similar relationships exist for other animals. The constants in these equations might be slightly different due to differences in shape, but the equations are otherwise the same.

All these examples illustrate the fundamental relationship in organisms between *size* (surface) and *biochemical activity*. The surface quantitatively determines the contact with the environment and thereby the possibility of taking up food and excreting waste substances.

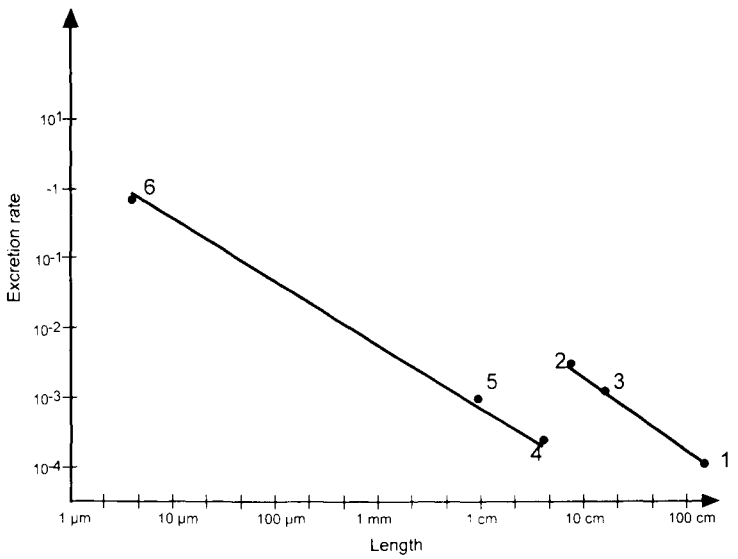

Fig. 2.26. Excretion of Cd $(24\ h)^{-1}$ plotted versus the length of various animals: (1) *Homo sapiens*, (2) mice, (3) dogs, (4) oysters, (5) clams, (6) phytoplankton.

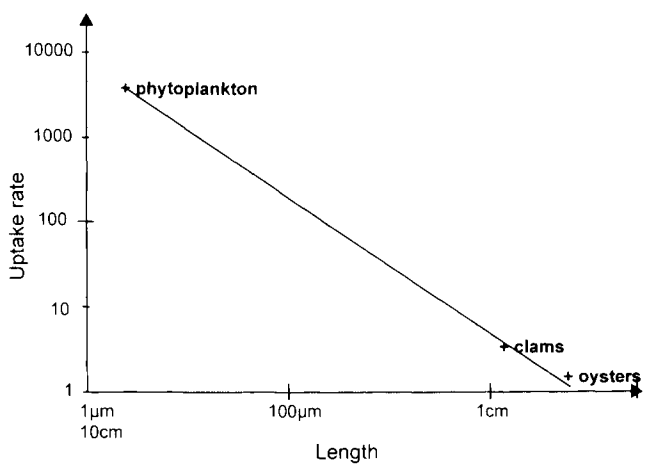

Fig. 2.27. Uptake rate (µg Cd/g 24 h) plotted against the length of various animals: phytoplankton, clams and oysters.

The same relationships are shown in Figs. 2.26–2.28, where rates of biochemical processes involving toxic substances are plotted versus size. They are reproduced from Jørgensen (1984). As can be seen, the excretion rate, uptake rate and concentration factor (for aquatic organisms) follow the same trends as the *growth rate*. This is not surprising, of course, as *excretion* is strongly dependent on metabolism

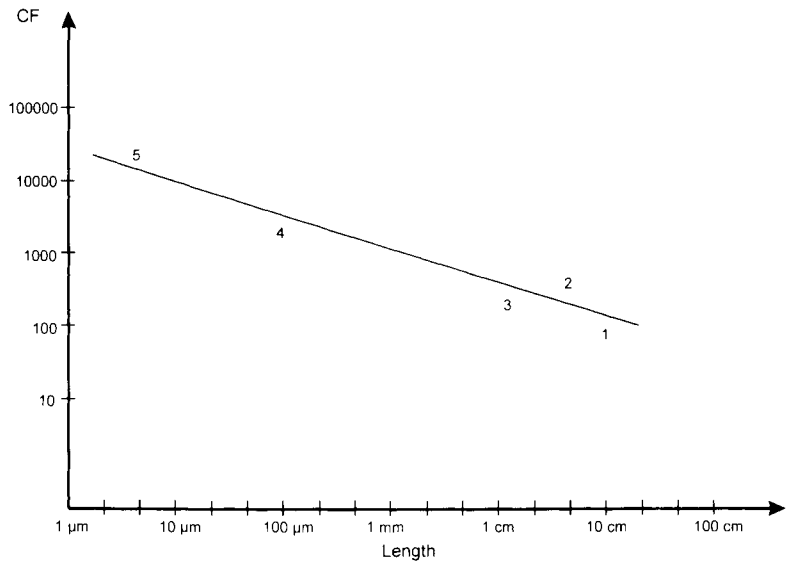

Fig. 2.28. *CF* for Cd versus size: (1) goldfish, (2) mussels, (3) shrimps, (4) zooplankton, (5) algae (brown-green).

and the direct uptake dependent on the surface. In spite of all these methods to estimate parameters, it may still in some cases be necessary to accept that a *parameter* is only known within some unacceptable large range. In such cases, it should be considered that a *Monte Carlo simulation* of the parameter be applied within, of course, the known range. The concentration factor indicating concentration in the organism vis à vis concentration in the medium also follows the same lines (see Fig. 2.28). By equilibrium the *concentration factor* can be expressed as the ratio between the uptake rate and the excretion rate, as shown in Jørgensen (1979). As most concentration factors are determined by the equilibrium, the relationship found in Fig. 2.26 seems reasonable to apply. Intervals for concentration factors are indicated here for some species according to the literature (see Jørgensen et al., 1991; 2000)

The allometric principles illustrated in Figs. 2.24–2.28 can be applied generally. In other words, it is possible to find process rates, provided these parameters are available for the element or compound under consideration for one species (because the slope is known), but preferably for several species to control the validity of the graph. When a plot similar to Figs. 2.24–2.28 is constructed, it is possible to read unknown parameters when the size of the organism is known.

It has been mentioned above that model constraints can be used to estimate unknown parameters. The chemical composition of organisms was applied to illustrate this principal method. The topic of model constraints is covered in Section 2.12. The Darwinian *survival of the fittest* is used in thermodynamic translation as a goal function to find the change in properties resulting from *adaptation* and shift in species

composition. This constraint has also been applied to estimate unknown parameters, as will be shown in Chapter 9 after the more basic theory has been presented.

This presentation of parameter estimation methods can be summarized in the following overview and recommendations.

A. Always examine the literature to find at least the range of as many parameters as possible. Jørgensen et al. (2000) which contains about 120 000 parameters can be recommended.

B. Examine processes *in situ* or in the laboratory to assess unknown parameters

C. Consider applying an intensive observation period to reveal the dynamics of the processes that are included in the model. Use the method described in Fig. 2.22 to find unknown parameters. This method often makes it possible to indicate parameters within relatively narrow ranges.

D. Always apply *allometric principles* to find parameters that are not known for the organisms included in the model, but are for other organisms. The allometric principles may also be used as a control of a parameter that is found by estimations or calibration.

E. *Ecotoxicological parameters* can be estimated by a network of methods that are based on a translation of the chemical structure to the properties of the compound. This method will be presented in detail in Chapter 8.

F. Whenever possible, use where the model constraints to estimate an unknown parameter or to control an uncertain parameter (see, for instance, how exergy can be used to determine parameters in Chapter 9).

G. Apply *calibration* of *submodels* and/or the entire model. The better the data, the more certain and reliable will be the results that the calibration offers.

The two weakest points in modelling today are: (1) to develop models that reflect the properties of the ecosystem, particularly its ability to meet changes by changing the properties of the organisms or by a shift to better fitted species, i.e., to account for current change of *parameters*; (2) to find approximately the right parameters. The first problem seems to be solved by the application of *structurally dynamic models* (see Chapter 9), while the second problem probably needs development of *additional parameter estimation methods* combined with measurements of essential parameters, although a partial solution of this problem is possible by the methods (A)–(G) mentioned above. Under all circumstances, it is recommended that sufficient time be invested in the assessment of parameters, because the model results are very dependent on the application of the right parameters. The process equations (see detail in Chapter 3) are usually quite well known, but the simulation results obtained from these process equations are very dependent on the choice of parameters.

2.10 Validation

When the modeller has terminated the calibration phase satisfactorily, the next obvious question would be: do the *parameters* found by the calibration represent the real values in the system?

Even in a data-rich situation, it may be possible by the selection of parameters to force a wrong model to give outputs that fit well with the data. **It is therefore crucial for the modeller to test the selected parameters with an independent set of data—this is called validation.** It must be emphasized that validation only confirms the model behaviour under the range of conditions represented by the available data. Consequently, it is preferable to validate the model by using data obtained from a period in which other conditions prevail than from the period of data collection used for the calibration. For instance, if a eutrophication model is applied, the ideal situation would be to have observations from the modelled ecosystem over a *wide* range of nutrient inputs, as the model is used to predict ecosystem response to changed nutrient loadings. This is often impossible, or at least very difficult, as it corresponds to a complete validation of the prognosis, which ideally takes place at a later stage of the model development. However, it may be possible and useful to obtain data from a *certain* range of nutrient loadings, for instance, from a humid and a dry summer. Alternatively, it may be possible to get data from a similar ecosystem with approximately the same morphology, geology and water chemistry as the ecosystem modelled in the first place.

Similarly, a *BOD/DO model* should be validated under a wide range of BOD-loadings, a toxic substance model under a wide range of concentrations of the toxic substances considered, and a population model by different levels of the populations etc.

If an ideal *validation* cannot be obtained, it does not imply that the model construction is useless. As mentioned in Chapter 1, models are multi-purpose tools, and if the "best" validation cannot be achieved, it is still important to validate the model. Furthermore, the model can always be used as a management tool, provided that the modeller presents all the open questions of the model to the manager. As we gain more experience in the use of the focal model and of models in general, the number of open questions will be reduced.

The method of *validation* is dependent on the objectives of the model. A comparison between measured data and model output by the use of the objective function shown in Eq. (2.2) is an obvious test. This is, however, most often insufficient as it does not focus on the main objectives of the model, but only on the general ability of the model to describe the state variables of the ecosystem correctly. It is therefore required to translate the main objectives of the model into a few validation criteria. They cannot be formulated generally, but are individual for the model and the modeller. If, for instance, a *BOD/DO model* is used to predict the water quality of a stream, it will be useful to compare the minimum concentration of oxygen predicted by the model with the corresponding measured data. For a eutrophication model

the maximum phytoplankton concentration and the maximum production could be used for validation. For a population model the modeller might be interested in the minimum or maximum level of certain species etc.

In a data-poor situation it might be impossible to meet such *validation criteria*, but it could then be useful to compare average situations, because due to the quality of data available, the model does not describe the dynamics of the system very well but can only give information of a general level or the average of important variables. The discussion on validation can be summarized as follows:

1. **Validation is always required.**
2. Attempts should be made to obtain data for the validation that are **entirely different from those used in calibration.** It is important to have data from a **wide range of the forcing functions** that are defined by the objectives of the model.
3. Validation criteria are formulated on the basis of **the objectives of model and the quality of the data.**

2.11 Ecological Modelling and Quantum Theory

How can we describe such complex systems as ecosystems in detail? The answer is that it is impossible if the description must include all details, including all interactions between all the components in the entire hierarchy and all details on feedbacks, adaptations, regulations and the entire evolution process.

Jørgensen (1997) has introduced the application of the uncertainty principles of quantum mechanics in ecology. In nuclear physics the uncertainty is caused by the observer of the incredibly small nuclear particles, while the uncertainty in ecology is caused by the enormous complexity of ecosystems.

For instance, if we take two components and want to know the relationship between them, we would need at least three observations to show whether the relationship is linear or non-linear. Correspondingly, the relationships among three components will require 3×3 observations for the shape of the plane. If we have 18 components we would correspondingly need 3^{18} or approximately 10^8 observations. At present this is probably an approximate, practical upper limit to the number of observations that can be invested in one project aimed at one ecosystem. This could be used to formulate a practical uncertainty relationship in ecology, see also Jørgensen (1990):

$$10^5 \times \Delta x / \sqrt{3^{n-1}} \leq 1 \tag{2.23}$$

where Δx is the relative accuracy of one relationship, and n is the number of components examined or included in the model.

The 100 million observations could, of course, also be used to give a very exact picture of one relationship. Costanza and Sklar (1985) talk about the choice between

the two extremes: knowing 'everything' about 'nothing' or 'nothing' about 'everything' (see also Section 2.5). The first refers to the use of all the observations on one relationship to obtain a high accuracy and certainty, while the latter refers to the use of all observations on as many relationships as possible in an ecosystem.

How we can obtain a balanced complexity in the description will be discussed further in the next section.

Equation (2.23) formulates a practical uncertainty relationship, but, of course, the possibility that the practical number of observations may be increased in the future cannot be excluded. Ever more automatic analytical equipment is emerging on the market. This means that the number of observations that can be invested in one project may be one, two, three or even several magnitudes larger in one or more decades. Yet, a theoretical uncertainty relationship can be developed. If we go to the limits given by quantum mechanics, the number of variables will still be low, compared with the number of components in an ecosystem.

One of Heisenberg's uncertainty relations is formulated as follows:

$$\Delta s \times \Delta p \geq h/2\pi \tag{2.24}$$

where Δs is the uncertainty in determination of the position, and Δp is the uncertainty of the momentum. According to this relation, Δx of Eq. (2.23) should be in the order of 10^{-17} if Δs and Δp are about the same. Another of Heisenberg's uncertainty relations may now be used to give the upper limit of the number of observations:

$$\Delta t \times \Delta E \geq h/2\pi \tag{2.25}$$

where Δt is the uncertainty in time and ΔE in energy.

If we use all the energy that the Earth has received during its lifetime of 4.5 billion years we get:

$$173\times10^{15} \times 4.5\times10^{9} \times 365.3 \times 24 \times 3600 = 2.5\times10^{34}\ \text{J} \tag{2.26}$$

where 173×10^{15} W is the energy flow of solar radiation. Δt would, therefore, be in the order of 10^{-69} s. So, an observation will take 10^{-69} s, even if we use all the energy that has been available on Earth as ΔE, which must be considered the most extreme case. The hypothetical number of observations possible during the lifetime of the Earth would therefore be:

$$4.5\times10^{9} \times 365.3 \times 3600/10^{-69} \approx \text{of } 10^{85} \tag{2.27}$$

This implies that we can replace 10^{5} in Eq. (2.21) with 10^{60} since

$$10^{-17}/\sqrt{10^{85}} \approx 10^{-60}$$

If we use $\Delta x = 1$ in Eq. (2.27) we get:

$$\sqrt{3^{n-1}} \leq 10^{60} \tag{2.28}$$

or $n \leq 253$.

From these very theoretical considerations we can clearly conclude that we shall *never* get enough observations to describe even one ecosystem in every detail. An ecosystem is what may be called a middle number system, meaning that the number of components are not as high as the number of gas molecules in a room, but may be as high as 10^{15}–10^{20}. As opposed to the gas molecules in a room, all these components are different, while there may be only 10–20 different types of gas molecules in a room.

These results are completely in harmony with Niels Bohr's *complementarity theory*, which he expressed as follows: "It is not possible to make one unambiguous picture (model) of reality, as uncertainty limits our knowledge." The uncertainty in nuclear physics is caused by the inevitable influence of the observer on the nuclear particles; in ecology it is caused by the enormous *complexity* and variability.

No map of reality is completely correct. There are many maps (models) of the same piece of nature, and the various maps or models reflect different viewpoints. Accordingly, one model (map) does not give all the information and far from all the details of an ecosystem. In other words, the theory of *complementarity* is also valid in ecology.

The use of maps in geography is a good parallel to the use of models in ecology. In the same way that we have road maps, aeroplane maps, geological maps, maps in different scales for different purposes, in ecology we have many models of the same ecosystems and we need them all if we want to get a comprehensive view of ecosystems (see also Sections 1.1 and 2.5). Furthermore, a map cannot give a complete picture. We can always make the scale larger and larger and include more detail, but we cannot get all the details—for instance, where all the cars in an area are situated at an exact moment—and even if we could, the picture would be invalid a few seconds later because we want to map too many dynamic details simultaneously (see the discussion in Sections 1.4 and 2.5). An ecosystem also has too many dynamic components to enable us to model all the components simultaneously and even if we could, the model would be invalid a few seconds later, where the dynamics of the system has changed the "picture".

In nuclear physics we need to use many different pictures of the same phenomena to be able to describe our observations. We say that we need a pluralistic view to cover our observations completely. Our observations of light, for instance, require that we consider light as waves as well as particles. The situation in ecology is similar. Because of the immense complexity we need a pluralistic view to cover a description of the ecosystems according to our observations. We need many models covering different viewpoints. This is consistent with *Gödel's Theorem* from 1931 (see Gödel, 1986), that the infinite truth can never be condensed in a finite theory. There are limits to our insight; we cannot produce a map of the world with all the possible details, because that would be the world itself.

Ecosystems must also be considered as irreducible systems in the sense that it is not possible to make observations and then reduce the observations to more or less

complex laws of nature, as is true of mechanics, for instance. Too many interacting components force us to consider ecosystems as irreducible systems. The same problem is found today in nuclear physics, where the picture of the atoms is now "a chaos" of many interacting elementary particles. Assumptions on how the particles interact are formulated as models, which are tested by observations. We draw upon exactly the same solution to the problem of complexity in ecology. It is necessary to use what is called experimental mathematics or modelling to cope with such irreducible systems. Today, this is the tool in nuclear physics, and the same tool is increasingly used in ecology.

Quantum theory may have an even wider application in ecology. Schrödinger (1944) suggests that the "jump-like changes" you observe in the properties of species are comparable to the jump-like changes in energy by nuclear particles. Schrödinger was inclined to call De Vries' mutation theory (published in 1902), the quantum theory of biology, because the mutations are due to quantum jumps in the gene molecule.

Patten (1982) defines an elementary "particle" of the environment, called an environ—previously he used the word *holon*—as a unit that can transfer an input to an output. Patten suggests that a characteristic feature of ecosystems is the *connectances*. Input signals go into the ecosystem components and they are translated into output signals. Such a "translator unit" is an environmental quantum according to Patten. The concept is borrowed from Koestler (1967), who introduced the word "holon" to designate the unit on a hierarchic tree. The term comes from the Greek "holos" = whole, with the suffix "on" as in proton, electron and neutron to suggest a particle or part.

Stonier (1990) introduces the term *infon* for the elementary particle of information. He envisages an infon as a photon, whose wavelength has been stretched to infinity. At velocities other than c, its wavelength *appears* infinite, its frequency zero. Once an infon is accelerated to the speed of light, it crosses a threshold, which allows it to be perceived as having energy. When that happens, the energy becomes a function of its frequency. Conversely, at velocities other than c, the particle exhibits neither energy nor momentum—yet it could retain at least two information properties: its speed and its direction. In other words, at velocities other than c, a quantum of energy becomes converted to a quantum of information. This concept has still not found any application in ecological modelling.

2.12 Modelling Constraints

Modellers are very much concerned about the application of the correct description of the components and processes in their models. The model equations and their parameters should reflect the properties of the model components and processes as correctly as possible. The modeller must, however, also be concerned with the right description of the system properties, and too little research has been done in this

direction. A continuous development of models as scientific tools will need to consider how to apply constraints on models according to the properties of the system. Several possible modelling constraints are mentioned below. The sequence reflects decreasing relations to physical properties and increasing relations to biological properties of the ecosystems. The ecological modelling constraints will only be mentioned briefly in this context. A more profound discussion will take place in Chapter 9, where the application of these constraints is the basis for development of what may be called next generation models.

The *conservation principles* are often used as modelling constraints. *Biogeochemical models* must follow the conservation of mass and *bioenergetical* models must equally obey the laws of energy and momentum conservation.

Energy and matter are conserved according to basic physical concepts that are also valid for ecosystems. This requires that energy and matter are neither created nor destroyed.

The expression "energy and matter" is used, as energy can be transformed into matter and matter into energy. The unification of the two concepts is possible by Einstein's law:

$$E = m\,c^2 \quad (ML^2T^{-2}) \tag{2.29}$$

where E is energy, m mass and c the velocity of electromagnetic radiation in vacuum ($= 3\times10^8$ m s^{-1}). The transformation from matter into energy and *vice versa* is only of interest for nuclear processes and does not need be applied to ecosystems on earth. We might therefore break the proposition down into two more useful propositions, when applied in ecology:

- ***ecosystems conserve matter***,
- ***ecosystems conserve energy.***

The conservation of matter may be expressed mathematically as follows:

$$dm/dt = \text{input} - \text{output} \quad (MT^{-1}) \tag{2.30}$$

where m is the total mass of a given system. The increase in mass is equal to the input minus the output. The practical application of the statement requires that a system is defined, which implies that the boundaries of the system must be indicated.

Concentration, c, is used instead of mass in most models of ecosystems:

$$V\,dc/dt = \text{input} - \text{output} \quad (MT^{-1}) \tag{2.31}$$

where V is the volume of the system under consideration and assumed constant.

If the law of mass conservation is used for chemical compounds that can be transformed to other chemical compounds, the Eq. (2.31) must be changed to:

$$V * dc/dt = \text{input} - \text{output} + \text{formation} - \text{transformation} \quad (MT^{-1}) \tag{2.32}$$

The principle of mass conservation is widely used in the class of ecological models called biogeochemical models. The equation is set up for the relevant elements, e.g., for eutrophication models for C, P, N and perhaps Si (see Jørgensen, 1976a,b; 1982a; Jørgensen et al., 1978).

For terrestrial ecosystems, mass per unit of area is often applied in the mass conservation equation:

$$A * dm_a/dt = \text{input} - \text{output} + \text{formation} - \text{transformation} \quad (MT^{-1}) \qquad (2.33)$$

where A = area, and m_a = mass per unit of area.

The *Streeter–Phelps model* (see Chapter 3) is a classical model of an aquatic ecosystem that is based upon conservation of matter and first-order kinetics (for further details, see also Chapter 3). The model uses the following central equation:

$$dD/dt + K_a \cdot D = L_0 \cdot K_1 \cdot K_T^{(T-20)} \cdot e^{-K1 \cdot t} \quad (ML^{-3}T^{-1}) \qquad (2.34)$$

where $D = C_s - C(t)$; C_s = concentration of oxygen at saturation; $C(t)$ = actual concentration of oxygen; t = time; K_a = reaeration coefficient (dependent on the temperature); L_0 = BOD_5 at time = 0; K_1 = rate constant for decomposition of biodegradable matter; and K_T = constant of temperature dependence.

The equation states that change (decrease) in oxygen concentration + input from reaeration is equal to the oxygen consumed by decomposition of biodegradable organic matter according to a first-order reaction scheme.

Equations according to (2.32) are also used in models describing the fate of toxic substances in the ecosystem. Examples can be found in Thomann (1984), Jørgensen (1991) and Jørgensen et al. (2000).

The mass flow through a food chain is mapped using the mass conservation principle. The food taken in by one level in the food chain is used in respiration, waste food, undigested food, excretion, growth and reproduction. If the growth and reproduction are considered as the net production, it can be stated that

$$\text{net production} = \text{intake of food} - \text{respiration} - \text{excretion} - \text{waste food} \qquad (2.35)$$

The ratio of the net production to the intake of food is called the net efficiency. The net efficiency is dependent on several factors, but is often as low as 10–20%. Any toxic matter in the food is unlikely to be lost through respiration and excretion, because it is much less *biodegradable* than the normal components in the food. This being so, the net efficiency of toxic matter is often higher than for normal food components, and as a result some chemicals, such as chlorinated hydrocarbons including DDT and PCB, will be magnified in the food chain.

This phenomenon is called *biological magnification* and is illustrated for *DDT* in Table 2.16. DDT and other chlorinated hydrocarbons have an especially high biological magnification, because they have a very low biodegradability and are only excreted from the body very slowly, due to dissolution in fatty tissue.

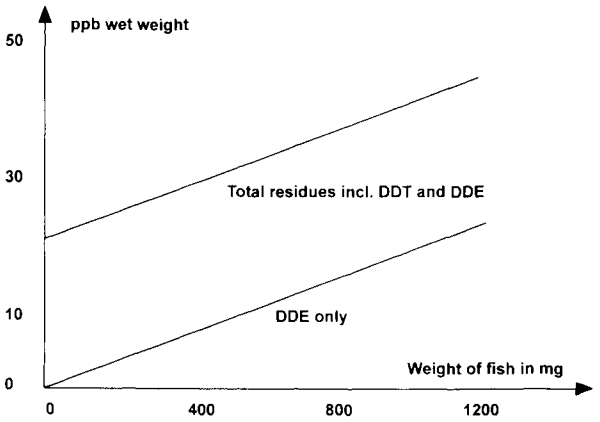

Fig. 2.29. Increase in pesticide residues in fish as the weight of the fish increases. Top line = total residues; bottom line = DDT only (after Cox, 1970).

These considerations also can explain why pesticide residues observed in fish increase with the increasing weight of the fish (see Fig. 2.29).

As man is the last link in the food chain, relatively high DDT concentrations have been observed in human body fat (see Table 2.17).

The understanding of *the principle of conservation of energy*, called the first law of thermodynamics, was initiated in 1778 by Rumford. He observed the large quantity of heat that appeared when a hole is bored in metal. Rumford assumed that the mechanical work was converted to heat by friction. He proposed that heat was a type of energy that is transformed at the expense of another form of energy, here mechanical energy. It was left to J.P. Joule in 1843 to develop a mathematical relationship between the quantity of heat developed and the mechanical energy dissipated.

Two German physicists J.R. Mayer and H.L.F. Helmholtz, working separately, showed that when a gas expands the internal energy of the gas decreases in proportion to the amount of work performed. These observations led to the first law of thermodynamics: energy can neither be created nor destroyed.

Table 2.16. *Biological magnification* (data after Woodwell et al., 1967)

Trophic level	Concentration of *DDT* (mg kg dry matter)	Magnification
Water	0.000003	1
Phytoplankton	0.0005	160
Zooplankton	0.04	~13,000
Small fish	0.5	~167,000
Large fish	2	~667,000
Fish-eating birds	25	~8,500,000

Table 2.17. Concentration of *DDT* (mg per kg dry matter)

Atmosphere	0.000004
Rain water	0.0002
Atmospheric dust	0.04
Cultivated soil	2.0
Fresh water	0.00001
Sea water	0.000001
Grass	0.05
Aquatic macrophytes	0.01
Phytoplankton	0.0003
Invertebrates on land	4.1
Invertebrates in sea	0.001
Fresh-water fish	2.0
Sea fish	0.5
Eagles, falcons	10.0
Swallows	2.0
Herbivorous mammals	0.5
Carnivorous mammals	1.0
Human food, plants	0.02
Human food, meat	0.2
Man	6.0

If the concept of internal energy, dU, is introduced:

$$dQ = dU + dW \quad (ML^2 T^{-2}) \tag{2.36}$$

where dQ = thermal energy added to the system; dU = increase in internal energy of the system; and dW = mechanical work done by the system on its environment.

Then the principle of energy conservation can be expressed in mathematical terms as follows:

U is a state variable which means that $\int_1^2 dU$ is independent on the pathway 1 to 2.

The internal energy, U, includes several forms of energy: mechanical, electrical, chemical, and magnetic energy, etc.

The transformation of solar energy to chemical energy by plants conforms with the first law of thermodynamics (see also Fig. 2.30):

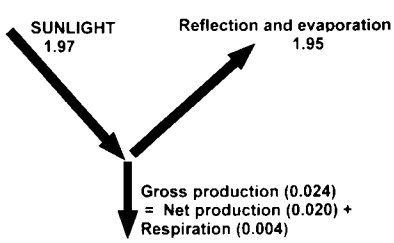

Fig. 2.30. Fate of solar energy incident upon the perennial grass-herb vegetation of an old field community in Michigan. All values in GJ $m^{-2} y^{-1}$.

Solar energy assimilated by plants = chemical energy of plant tissue growth + heat energy of respiration (2.37)

For the next level in the food chain—herbivorous animals—the energy balance can also be set up:

$$F = A + UD = G + H + UD \ (ML^2 T^{-2}) \tag{2.38}$$

where F = the food intake converted to energy (Joule); A = the energy assimilated by the animals; UD = undigested food or the chemical energy of *faeces*; G = chemical energy of animal growth; and H = the heat energy of respiration.

These considerations pursue the same lines as those mentioned in the context of Eq. (2.35), where the mass *conservation principle* was applied. The conversion of biomass to chemical energy is illustrated in Table 2.18. The energy content per g ash-free organic material is surprisingly uniform, as is illustrated in Table 2.18. Table 2.18D shows ΔH, which symbolizes the increase in enthalpy, defined as: $H = U + p \cdot V$. Biomass can be translated into energy (see Table 2.18), and this is also true of transformations through food chains. Ecological energy flows are of considerable environmental interest as calculations of biological magnifications are based on energy flows.

Table 2.18. (Source Morowitz, 1868).

(A) Combustion heat of animal material

Organism	Species	Heat of combustion (kcal/ash-free g)
Ciliate	*Tetrahymena pyriformis*	–5.938
Hydra	*Hydra littoralis*	–6.034
Green hydra	*Chlorohydra viridissima*	–5.729
Flatworm	*Dugesia tigrina*	–6.286
Terrestrial flatworm	*Bipalium kewense*	–5.684
Aquatic snail	*Succinea ovalis*	–5.415
Brachiipode	*Gottidia pyramidata*	–4.397
Brine shrimp	*Artemia* sp. (*nauplii*)	–6.737
Cladocera	*Leptodora kindtii*	–5.605
Copepode	*Calanus helgolandicus*	–5.400
Copepode	*Trigriopus californicus*	–5.515
Caddis fly	*Pycnopsyche lepido*	–5.687
Caddis fly	*Pycnopsyche guttifer*	–5.706
Spit bug	*Philenus leucopthalmus*	–6.962
Mite	*Tyroglyphus lintneri*	–5.808
Beetle	*Tenebrio molitor*	–6.314
Guppie	*Lebistes reticulatus*	–5.823

(B) Energy values in an *Andropogus virginicus* old field community in Georgia

Component	Energy value (kcal/ash-free g)
Green grass	–4.373
Standing dead vegetation	–4.290
Litter	–4.139
Roots	–4.167
Green herbs	–4.288
Average	–4.251

(C) Combustion heat of migratory and non-migratory birds

Sample	Ash-free material (kcal·g)	Fat ratio (% dry weight as fat)
Fall birds	–8.08	71.7
Spring birds	–7.04	44.1
Non-migrants	–6.26	21.2
Extracted bird fat	–9.03	100.0
Fat extracted: fall birds	–5.47	0.0
Fat extracted: spring birds	–5.41	0.0
Fat extracted: non-migrants	–5.44	0.0

(D) Combustion heat of components of biomass

Material	ΔH protein (kcal/g)	ΔH fat (kcal/g)	ΔH carbohydrate (kcal/g)
Eggs	–5.75	–9.50	–3.75
Gelatin	–5.27	–9.50	
Glycogen			–4.19
Meat, fish	–5.65	–9.50	
Milk	–5.65	–9.25	–3.95
Fruits	–5.20	–9.30	–4.00
Grain	–5.80	–9.30	–4.20
Sucrose			–3.95
Glucose			–3.75
Mushroom	–5.00	–9.30	–4.10
Yeast	–5.00	–9.30	–4.20

Many *biogeochemical models* are given **narrow bands of the chemical composition of the biomass**. Eutrophication models are either based on a constant *stoichiometric ratio* of elements in phytoplankton or on an independent cycling of the nutrients, where, for instance, the phosphorus content may vary from 0.4% to 2.5%, the nitrogen content from 4% to 12% and the carbon content from 35% to 55%.

Some modellers have used **the *second law of thermodynamics* and the concept of *entropy*** to impose thermodynamic constraints on models; see for instance Mauersberger (1985), who has used this constraint to assess process equations, too. The idea is that the second law of thermodynamics is also valid for ecosystems, and which implications can be deduced from the application of this law to ecological processes?

Ecological models contain many parameters and process descriptions and at least some interacting components, but the parameters and processes can hardly be given unambiguous values and equations, even by using the previously mentioned model constraints. This means that an ecological model in the initial phase of development has many degrees of freedom. It is therefore necessary to limit the degrees of freedom in order to come up with a workable model, which is not doubtful and non-deterministic.

Many modellers use a comprehensive data set and a calibration to limit the number of possible models. This is a cumbersome method if it is not accompanied by some realistic constraints on the model. The calibration is therefore often limited to giving the parameters realistic and literature-based intervals, within which the calibration is carried out, as mentioned in Section 2.9.

But far more would maybe be gained if it were possible to give the models more ecological properties and/or test the model from an ecological point of view to exclude those versions of the model that are not ecologically possible. **How could, for instance, the *hierarchy of regulation mechanisms* be accounted for in the models?** Straskraba (1979; 1980) classifies models according to the number of levels that the model includes from this hierarchy. He concludes that we need experience with models of the higher levels to develop structurally dynamic models. This is the topic for Chapter 9.

We know that evolution has created very complex ecosystems with many feedback mechanisms, regulations and interactions. **The coordinated co-evolution means that rules and principles have been imposed for cooperation among the biological components. These rules and principles are the governing laws of ecosystems**, and our models should follow these principles and laws as broadly as possible.

It also seems possible to limit the number of parameter *combinations* by using what could be called "ecological" tests. The maximum growth rates of phytoplankton and zooplankton may, for instance, have realistic values in a eutrophication model, but the two parameters do not fit to each other, because they will create chaos in the ecosystem, which is inconsistent with actual or general observations. Such combinations should be excluded at an early stage of the model development. This will be discussed further in Chapter 9.

Figure 2.31 summarizes the considerations of using various constraints to limit the number of possible values of parameters, possible descriptions of processes and

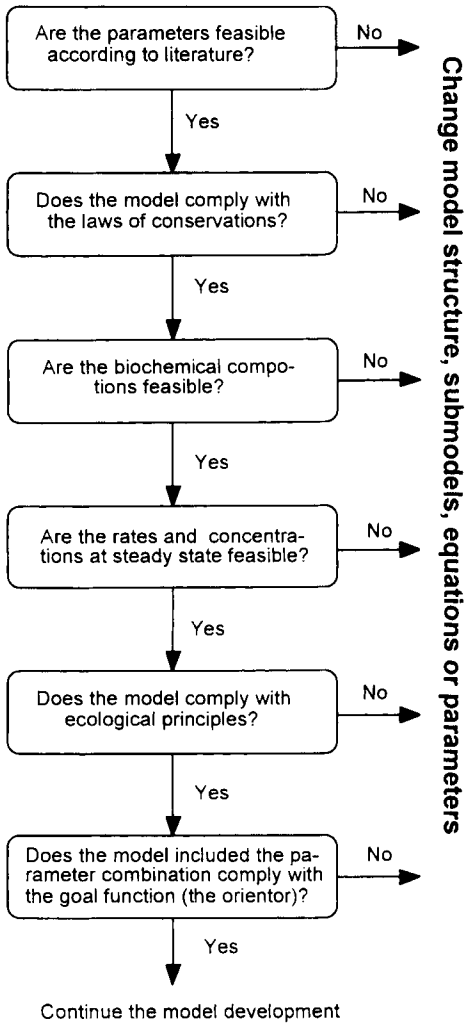

Fig. 2.31. Considerations for using various constraints by development of models. The range of parameter values particularly is limited by the procedure shown.

possible *submodels* to facilitate the development of a feasible and workable model. The two last steps of the procedure will be presented in Chapter 9, where the so-called next generation structurally dynamic models are developed.

This requires the introduction of variable parameters, governed by a goal function (an *orientor*). Several possible goal functions must be introduced before a presentation of structurally dynamic models can take place.

PROBLEMS

1. Which type of model would you select for the following problems?
   (a) Protection of a lion population in a national park.
   (b) Optimization of fishery in marine environment.
   (c) Construction of a wetland for denitrification of nitrate input from agriculture.
2. Explain the importance of verification, calibration and validation. Can models without these three steps be developed at all?
3. Find the concentration factor of cadmium for a whale estimated to have length of 20 m.
4. The ammonia excretion for a fish of 500 g is 200 mg/24 h. Estimate the ammonia excretion for a fish of 4 kg.
5. Set up an adjacency matrix for the model shown in Fig. 2.10.
6. Improve the model in Fig. 2.5 (Illustration 2.1) by adding two more state variables. Which two state variables would it be most important to add to the model when eutrophication is the focus?
7. How often would you determine the phytoplankton concentration, if a model for the diurnal variations of primary production was supposed to be determined?
8. Set up the equations for a model explaining the accumulation of DDT in fish according to Fig. 2.27. Use Eq. (2.15) to express the growth and an equation based on mass conservation, for instance, Eq. (2.32) to express the total DDT+DDE content in fish.
9. How many state variables would a model have, if all the relationships are based entirely on 100 0000 observations?

CHAPTER 3

Ecological Processes

Chapter 3 is divided in three sections to offer an overview of the major physical (3A), chemical (3B) and biological (3C) processes that can be considered in modelling an ecological system. It presents the most often used and classical models for the simulation of these processes. It does not attempt to offer a complete and detailed selection of all these models as this is beyond the scope of the chapter. For further and deeper investigation of these topics, the reader is referred to the specialized literature cited in the text or other textbooks (Marsili-Libelli, 1989; Orlob, 1977; Jorgensen and Gromiec, 1989; Chapra, 1997; EPA, 1985).

Physical processes include flow and circulation patterns, mixing and dispersion of mass and heat, water temperature, settling, adsorption, insolation and light penetration. These abiotic factors mainly concern aquatic ecosystems and their simulation is very important for setting up a good model of the whole ecosystem. The physical and chemical processes are very well known compared with the biological processes and for this reason some detailed descriptions of them are available and widely accepted by modellers. The details usually known for biological processes are much fewer than those for the physical and chemical ones. Even if a more detailed description of the physical and chemical processes could be easily provided, it is sometimes unnecessary for an ecosystem to go into detail when the biological processes have only a rough description. The result of this compromise is a trade-off between acceptable details of physical and chemical processes and a reasonable description of the bio-ecological processes. For instance, one of the most important steps of this compromise is the selection of the optimal space and time resolution of the model. While the spatial grid with 10 to 100 metres as spatial step is acceptable for physical and chemical processes in water quality models, this is very often too detailed for biological processes description, and similarly, while minutes or hours are good time steps for the physical and chemical processes description, days and months are suitable time steps for the biotic components of an ecosystem.

Part A. Physical Processes

3A.1 Space and Time Resolution

An acceptable division of the space to simulate physical processes in an ecological model must account for variation in horizontal and vertical dimensions. Aquatic ecosystems, like rivers and lakes, need some geometric representations.

The simplest one is the zero-dimensional model which simulates the system with a point and the only possibility given to the system is to change in time according to the equation

$$C = f(t)$$

where C is the simulated property, t is time and f is a function. This lumped parameter model cannot predict the spatial fluid dynamic and it is usually analytically solvable. A common example of this model is the Continuous Stirred Tank Reactor (CSTR) very often used as a first approximation of the system behaviour. It is used, for instance, to simulate water quality of shallow and small lakes where stratification does not occur and horizontal homogeneity is assumed (Fig. 3.1a).

One-dimensional models use a one-dimensional representation of the system. They assume that the system is characterized by a prevailing one-directional flow and that the properties of the water body vary along this direction. Rivers are the systems most commonly simulated by a one-dimensional model, but the vertical stratification of a deep lake, without appreciable horizontal variation of the properties can also be described by a one-dimensional representation (Fig. 3.1b).

When the system is large enough to present sensible variation of the properties, vertical and/or horizontal division is required and two or three-dimensional representation are commonly used. This is the case for temperature variation in deep and large lakes where stratification occurs (Fig. 3.1c), or water bodies with a very meandering coastline resulting in bays and gulfs where water quality is affected by a complex circulation, or in tidal estuarine water bodies (Fig. 3.1d).

Figure 3.1 shows the pattern of representation of a system in different ways, increasing in morphological complexity, which influences the spatial distribution of the properties and the model grid for an appropriate simulation of the physical processes.

As presented in Chapter 2, ecological models are distinguished on a temporal basis as being either in a steady state or in a dynamic one. The static model assumes

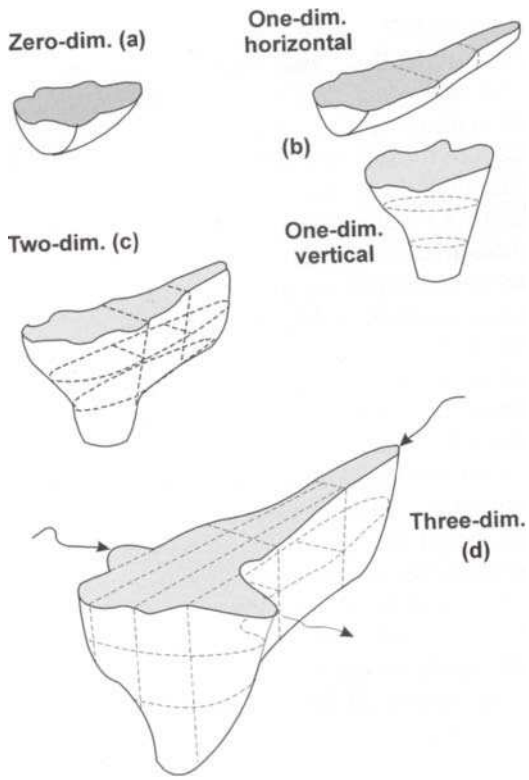

Fig. 3.1. Spatial representation of a lake with increasing morphological complexity which influences the space distribution of the properties. The grid of the distributed parameter models offers a more appropriate simulation of the physical processes.

that variables and forcing functions of the system do not change in time, at least for the simulation span. In such a case the system can show a variation in space distribution of the properties considered with the distributed parameter models, otherwise it is simulated with a zero-dimensional model. Different compartments of an ecosystem often considered in the static model and a pattern of property distribution in different compartments are also simulated in a pseudo-spatial model. As presented in Chapter 5, static models solve a wide spectrum of problems that in first approximation can be considered time invariant.

As a more detailed investigation of ecosystems is approached, time variation of the properties is immediately recognized. For instance, the meteo-climatic conditions forcing physical and biological systems are clear examples of time-varying forcing functions and the seasonal variation of primary productivity is also an evident and variable consequence of them.

These forcing functions—but also many other ecological variables—can be considered in dynamic models with different time steps ranging from minutes to

months. Such a wide range of time steps imposes the need to select one that is suitable for the model, i.e. one that does not make the physical and chemical simulation too heavy and that is not too time consuming for the biological and ecological simulation.

The procedure for selecting the appropriate time and space scale demands an *a priori* understanding of the dominant physical, chemical, biological and ecological processes occurring within the system. As is seen, the modelling procedure is a recursive process that can require several cycles to reach a good definition of the conceptual model including the appropriate time and space scale before going into the mathematical description of the processes.

Ecological models are usually set up to link together in a cascade physical, chemical, biological and ecological submodels requiring the simulation of different space and time steps and even different types of models (static, dynamic or structurally dynamic models). Instead of selecting a couple of average space and time steps for all the submodels, which is always the result of a compromise, a cascade of submodels with different space and time steps can be adopted. The results of the physical model, using a fine mesh for space representation and a short time step, are averaged over a coarser mesh and over a larger time step before being transformed into input data to the chemical model, whose results, averaged again over larger space and time steps, are transferred as input to the biological model and then to the ecological model for the final elaboration. This way of modelling an ecological system, nesting the physical, chemical, biological and ecological models, is

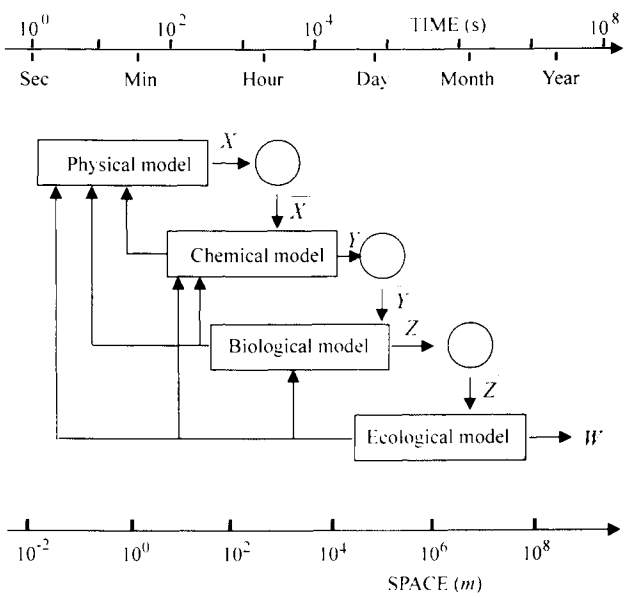

Fig. 3.2. Space and time scale ranges for some typical submodels usually chained in a complex ecological model. Circles indicate the averaging operator acting over time and space to give the input to the next submodel.

shown in Fig. 3.2. It optimizes knowledge of the physical systems gained by an appropriate space and time selection and does not lose information available for the system. Furthermore, it does not penalize too much the rest of the models characterized by a less well defined knowledge of the ecological processes. During the simulation, the characteristics of the physical and chemical environment can change according to the influence of the biotic components on them. For instance, the growth of large quantities of algae in an eutrophic water body that is accounted for in the ecological submodel, affects the light penetration and even the water circulation that are accounted for in the physical submodel. Such a cascade of submodels can include feedback that allows us to update the values of the parameters of the submodels according to the results of other submodels.

3A.2 Mass Transport

Transport of mass in fluids is one of the most relevant physical processes of ecosystems as it concerns the principal fluid media of ecosystems: air and water. For both, the process is described by the same equations, the only, but important, difference being in the values of the parameters describing the fluid and the substance moving in it.

Mass transport is an important process in environmental systems because it concerns not only the movement of pollutants but also that of nutrients and food of some ecosystem components. For this reason it is important to know how a substance moves within a medium, how it leaves a liquid phase to reach a gas phase, and which concentration it can assume in a given place at a given time.

The major processes of mass transport are *advection*, *diffusion* and *dispersion*. This section describes these processes and some combinations of them, focusing particularly on water as a major physical abiotic component of aquatic ecosystems and gas transfer between different phases.

Advection

Advection is one of the ways to move a substance in a medium: we say that a transport is advective if the substance is moving solidly with the fluid in one direction without varying its concentration. Advection refers to the transport due to the bulk movement of the medium which contains a soluble substance. The laminar motion of the water in a large river flowing very slowly in a rectilinear branch of its bed is very similar to the theoretical flow in a pipe and it is a good example of advective transport because the dominant process is the movement of the substance in the flow direction and changes in concentration are negligible. On the other and, water flowing in a mountain creek characterized by a large turbulence cannot be described by advection because mixing of substance and medium is the dominant effect of the transport.

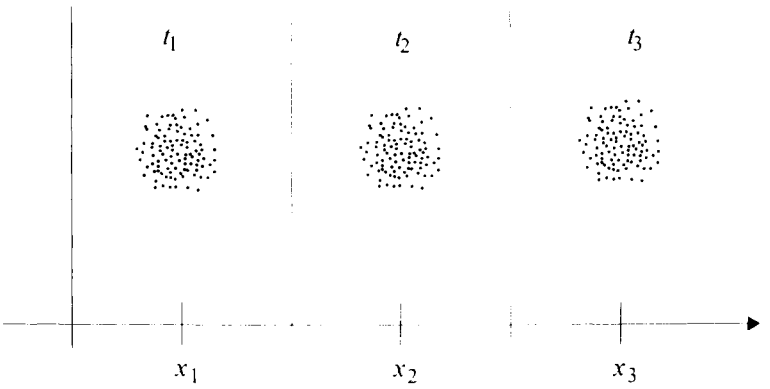

Fig. 3.3. Pictorial representation of the advective movement of a substance in a fluid, the substance concentration does not change at different times and positions.

Figure 3.3 gives a pictorial representation of the advective motion of a cloud of substance with a uniform concentration at three instants (t_1, t_2, t_3) in three positions. Concentration, shape and dimension of the cloud do not change in time moving solidly with the fluid.

The flux of a substance J [MT^{-1}] in and out of a volume of fluid, via advection can be generally described by the equation:

$$J = \pm QC \tag{3.1}$$

where: $\pm$ indicates the movement in and out of a volume, respectively; Q is the rate at which the fluid flows through the volume [L^3T^{-1}]; and C is the concentration of the substance in the volume [$M\ L^{-3}$]

The theoretical development of the equation for advective transport derives from the principle of conservation of mass. This principle applied to the fluid itself, but also to a solute or suspended substance in the fluid, can be enunciated as follows:

- the total mass of a conservative substance entering a fixed element of space in a given time must equal the increase in mass within the space, in that time.

Referring to Fig. 3.4, we assume that an incompressible fluid transporting a certain conservative substance with concentration C flows through the volume and that the fluid velocity ($\vec{v}$) has components u, v and w in the directions x, y and z.

According to Eq. (3.1), the flux of substance J_1 entering the element (positive values) through the plane 1 is equal to the concentration multiplied by the velocity and the area

$$J_1 = C\,u\,\delta y\,\delta z$$

The flux of substance J_2 leaving the element (negative values) through plane 2 can be determined by Taylor's expansion because the element is infinitesimal

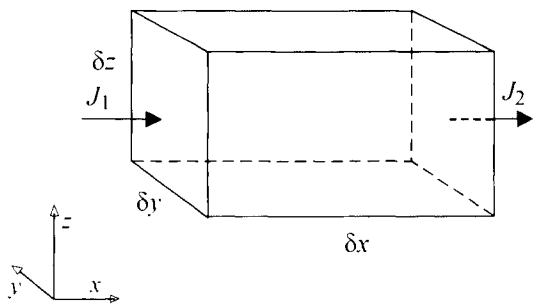

Fig. 3.4. Infinitesimal space element fixed relatively to the Earth within a fluid stream.

$$J_2 = -\left[Cu + \frac{\partial(Cu)}{\partial x}\delta x\right]\delta y\delta z$$

The net change in mass due to the flow in the x direction in time δt (and similarly for the direction y and z) is

$$J_1 + J_2 = -\frac{\partial(Cu)}{\partial x}\delta x\delta y\delta z$$

Assuming that the initial mass of substance in the element at time t is $C\delta x\delta y\delta z$, from Taylor's expansion the mass at time $t + \delta t$ is

$$\left(C + \frac{\partial C}{\partial t}\right)\delta t\delta x\delta y\delta z$$

and the rate of mass change within the element is

$$\frac{\partial C}{\partial t}\delta x\delta y\delta z$$

Equating the sum of the fluxes through all the faces of the element (decreasing in mass) with the rate of change, we obtain the following equation for conservation of mass

$$-\frac{\partial C}{\partial t} = \nabla\cdot(\vec{v}C) = \frac{\partial(Cu)}{\partial x} + \frac{\partial(Cv)}{\partial y} + \frac{\partial(Cw)}{\partial z} \tag{3.2}$$

and developing the derivatives of products

$$-\frac{\partial C}{\partial t} = C\nabla\cdot\vec{v} + \vec{v}\cdot\nabla C = C\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z}\right) + \left(u\frac{\partial C}{\partial x} + v\frac{\partial C}{\partial y} + w\frac{\partial C}{\partial z}\right)$$

the first term on the left of the equation is the rate of change of the concentration of substance in time, the second accounts for the variation in concentration C due to the expansion or compression of the fluid (and is null for an incompressible fluid), and the third is the advective term. The first and third terms can be combined by introducing a new differential operator, the substantial or total derivative dC/dt, i.e. the total rate of change of concentration in a space element moving with velocity $\vec{v} = (u, v, w)$

$$\frac{d}{dt} = \frac{\partial}{\partial t} + \vec{v} \cdot \nabla$$

Equation (3.2) is usually called the *continuity equation* and for incompressible fluids where only the advective transport occurs and for a conservative substance, $dC/dt = 0$, Eq. (3.2) becomes

$$\nabla \cdot \vec{v} = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0$$

which represents the general constraint for incompressible fluids with only advective movement.

Diffusion

Diffusion is the movement of a substance due to Brownian motion of water molecules causing the random motion of the substance molecules. Diffusion has a tendency to minimize gradients of substance concentration in a medium moving the substance from a region of high to low concentration. We say that a transport is diffusive if a substance is spreads in an immobile fluid as the effect of the molecular motion of the fluid pushing the substance molecules to change their position. As an effect of the diffusion, in an isotropic fluid, the barycentre of a cloud of substance does not change its position while the initial concentration in the space surrounding the barycentre varies. A typical diffusion transport is easily visible whenever we put a drop of dye in a glass of stagnant water: after a short time the drop enlarges and its colour intensity decreases and slowly all the water in the glass assumes a light uniform colour. Some non-isotropic diffusion of the substance in the glass, easy to see in such an experiment, is mainly due to a residual very slow advective motion of the fluid or to a difference in fluid and substance density. Figure 3.5 illustrates the diffusive transport of a cloud of substance in an immobile fluid at three instants. The peak of concentration of the substance is decreasing in time and solute substance occupies a larger space, while the centre of the cloud does not change.

Diffusion of substances with a polar structure in water is enhanced by the presence of polarities of water molecules and this is the reason why salt and sugar (polar molecules) easily diffuse in water while oil (apolar molecules) does not.

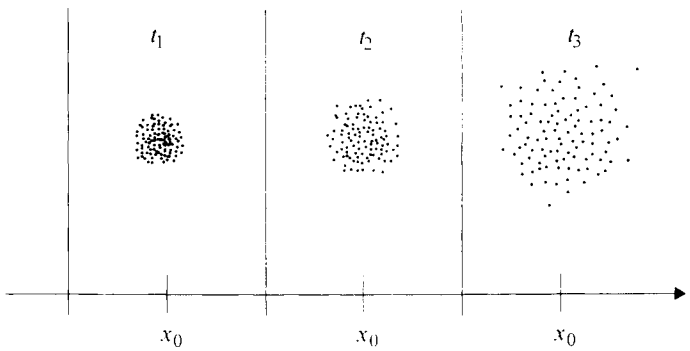

Fig. 3.5. Pictorial representation of the diffusive movement of a substance in a stagnant fluid.

Diffusion of a solid substance in a fluid occurs at a velocity lower than is the case for diffusion of liquid substance in a fluid because of the reciprocal attraction of molecules at the solid phase which is stronger than at the liquid phase. Another case of diffusion is that of a solute substance from interstitial water of sediments in the water column; in this case the lower diffusion effect is mainly due to the obstacles of porous media to the movement of the substance.

Although diffusion is generally unimportant in horizontal mass transport in ecosystems, it is theoretically important because its mathematical formulation constitutes the base for turbulent transport much more related to ecological processes than horizontal mass transport. Nevertheless, diffusion plays a major role in vertical mass transport along the water column of a water body and in this case it is ecologically important to explain phenomena such as the release of soluble substance from sediments.

The basic reason why a substance diffuses in a fluid is the difference in concentration of the substance between two points and the motion of molecules of fluid. The tendency of the system is to minimize the gradient of concentration by generating a net flux of mass from regions where the concentration is high to others where it is low. Equation (3.3) describes the diffusive transport of a mass through the boundary of a volume

$$J = D\frac{C_{out} - C_{in}}{\Delta x} \tag{3.3}$$

where D is the bulk diffusion coefficient [$L^2\ T^{-1}$], reflecting the magnitude of the mixing process through the volume boundary; and C_{out} and C_{in} are the concentrations outside and inside the volumes: if $C_{out} > C_{in}$ the movement of mass is positive (i.e. the mass is entering the volume for which the balance is taken); if $C_{out} < C_{in}$ the mass is going out.

According to the description of diffusion shown in Fig. 3.6, the mathematical formulation of the process can be given as follows. The flux J_{ab} per unit of area [$M\ L^{-2}\ T^{-1}$] of

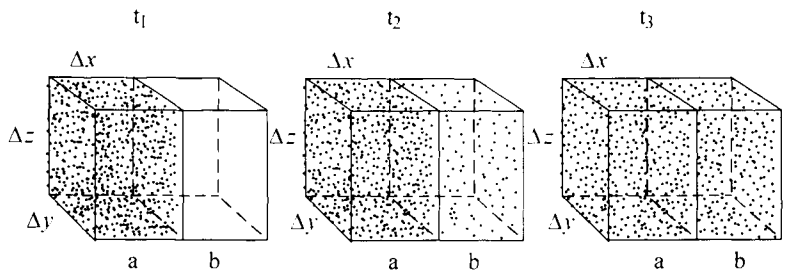

Fig. 3.6. Diffusion of mass between two completely mixed volumes a and b at three different times (t_1, t_2, t_3) until the equilibrium is reached at time t_3.

the particles of Fig. 3.6 through the interface $\Delta y\ \Delta z$ from volume a to volume b is assumed to be proportional to the number of particles near the interface (the particles are uniformly distributed in the volumes)

$$J_{ab} = n_a m_a \frac{P}{\Delta y \Delta z} = m_a \frac{P}{\Delta y \Delta z}$$

where n_a is the number of particles of mass m [M] in volume a; P is the probability of transfer across the interface [T^{-1}]: m_a is the mass of particles in a [M].

Analogously,

$$J_{ba} = m_b \frac{P}{\Delta y \Delta z}$$

and the net transfer J per unit of area is

$$J = J_{ab} - J_{ba} = P \frac{m_a - m_b}{\Delta y \Delta z} \tag{3.4}$$

Multiplying the top and bottom of the second term of Eq. (3.4) by $(\Delta x)^2$ we obtain

$$J = P(\Delta x)^2 \frac{C_a - C_b}{\Delta x}$$

taking the limit for $\Delta x \to 0$ we get

$$J = -P(\Delta x)^2 \frac{\partial C}{\partial x} \tag{3.5}$$

even if P is dependent on Δx, $P(\Delta x)^2$ is independent of the size of the volumes and constant at given conditions. It is usually indicated by D and called the *molecular diffusion coefficient* [$L^2\ T^{-1}$].

For three dimensions in Cartesian co-ordinates, assuming that D is equal in the three directions, and using the traditional notation, Eq. (3.5) is written

$$\vec{J} = -D\nabla C = -D\left(\frac{\partial C}{\partial x}, \frac{\partial C}{\partial y}, \frac{\partial C}{\partial z}\right)$$

This is the so-called *Fick's first law*. If we apply Fick's first law to an infinitesimal volume to calculate the mass balance using the principle of mass conservation, for a one-dimensional segment we can write

$$\delta m = \delta y \delta z \left[J_x - \left(J_x + \frac{\partial J_x}{\partial x} \delta x \right) \right] \delta t$$

$$\delta m = \delta y \delta z \left(-\frac{\partial J_x}{\partial x} \delta x \right) \delta t$$

dividing by the volume $\delta x \delta y \delta z$, and by δt, and then substituting Fick's first law and finally taking δt and δx as infinitesimal increments, we obtain for the x direction

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2}$$

The molecular diffusion coefficient D is equal in all the directions as is generated by isotropic brownian motion. *Fick's second law* can be written

$$\frac{\partial C}{\partial t} = D\nabla^2 C = D\nabla \cdot (\nabla C) = D\left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2} \right) \tag{3.6}$$

Equation (3.6) describes the rate of change in concentration with respect to time of a substance subject only to the molecular diffusion process. The exact solution in one coordinate of Eq. (3.6) initially concentrated at $x = 0$ is

$$C = \frac{m}{2\sqrt{\pi D t}} e^{-\frac{x^2}{4Dt}}$$

which is identical to the solution of the normal distribution: the bell-shaped curve with mean zero and variance of $2Dt$. The exact solution allows us to redraw Fig. 3.5 in a quantitative manner (Fig. 3.7) provided that the mass m is initially placed at $x = 0$, that the molecular diffusion coefficient has a typical value $D = 10^{-5}$ (cm^2/s), and that time is set at $t_1 = 50$, $t_2 = 100$, $t_3 = 150$ s.

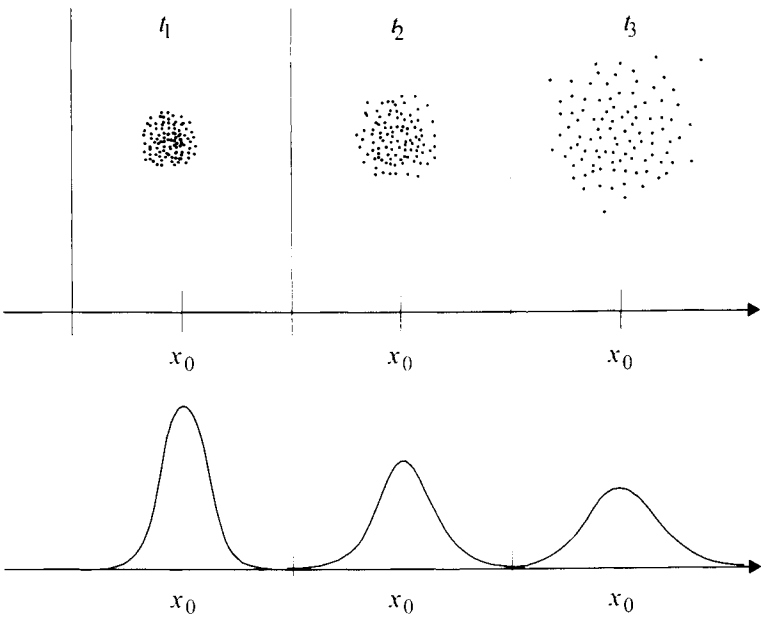

Fig. 3.7. Normal distribution, along the x axis, of particles of a substance at different times as an effect of the only molecular diffusion process as shown in Fig. 3.5.

Turbulent Diffusion

Although at the molecular scale a substance is basically diffused via random molecular movements, at larger scales it can be seen as diffusing by the effect of the large-scale eddies or turbulent movements of the fluid itself. This type of diffusion explains the horizontal diffusion of a substance in lakes using values of the diffusion coefficient larger than the molecular ones. This is the case for the outlet of a river in a bay: the river current crosses the shoreline currents of the bay creating large eddies that cause the substances dissolved in the river to diffuse in the bay. If sufficiently long observations are taken and a suitably large space scale is employed, this movement can be viewed as random and can be treated mathematically as a diffusion process.

Referring to Fig. 3.4 and Eq. (3.2) and to the conceptual description of the movement of a fluid through an infinitesimal element volume, if the fluid is not moving advectively but some variations in the velocity are admitted, the instantaneous values of the velocity $\vec{v}$ and of the concentration C can be written

$$\vec{v} = (\underline{u}+u', \underline{v}+v', \underline{w}+w'), \quad C = \underline{C}+C'$$

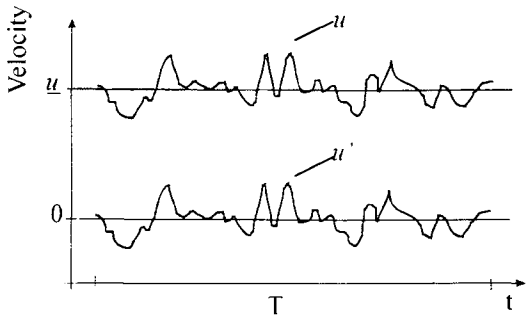

Fig. 3.8. Graphical representation of the assumption on the instantaneous velocity and its splitting in average and turbulent fluctuation terms.

where $\underline{u} = \frac{1}{T}\int_0^T u\,dt$ and so on for the others, and T is the averaging time (for instance the period of measurements); u' is the instantaneous turbulent fluctuation with average 0 as shown in Fig. 3.8 and analogously for the others.

Substituting the new expressions of $\vec{v}$ and C in Eq. (3.2) and cancelling all the terms with only one prime because of their zero average over the observation time T, and developing the derivative of products we obtain

$$-\frac{\partial \underline{C}}{\partial t} = \underline{\vec{v}} \cdot \nabla \underline{C} + \underline{C} \nabla \cdot \underline{\vec{v}} + \nabla \cdot (C' \vec{v}')$$

Given the general constraints of advective transport by incompressible fluids without sinks or sources, the term $\underline{C} \nabla \cdot \underline{\vec{v}}$ is 0 and the previous expression can be simplified to

$$\begin{aligned} -\frac{\partial \underline{C}}{\partial t} &= \underline{\vec{v}} \cdot \nabla \underline{C} + \nabla \cdot (C' \vec{v}') \\ &= \left(\underline{u} \frac{\partial \underline{C}}{\partial x}, \underline{v} \frac{\partial \underline{C}}{\partial y}, \underline{w} \frac{\partial \underline{C}}{\partial z} \right) + \left(\frac{\partial (C'u')}{\partial x}, \frac{\partial (C'v')}{\partial y}, \frac{\partial (C'w')}{\partial z} \right) \end{aligned} \tag{3.7}$$

The cross-product terms, such as $u'C'$, represent the net convection of substance due to the turbulent fluctuations and by analogy with Fick's first law, they can be expressed by an equivalent diffusive mass transport in which the mass flux is proportional to the mean concentration gradient and the flux is in the direction of the mean concentration gradient. Hence

$$u'C' = -D_x \frac{\partial \underline{C}}{\partial x}$$

and so on for the others

D_x, D_y, D_z are not necessarily the same in all directions and can vary depending upon the position in the stream and, given their origin, their magnitude is some orders larger than that of the molecular diffusion coefficient. Figure 3.9 shows the ranges of diffuse coefficient values for several processes of eddy diffusion, pure diffusion of solute substance in fluids, porous media diffusion and thermal diffusion.

If $D = (D_x, D_y, D_z)$ then Eq. (3.7) can be rewritten as

$$-\frac{\partial C}{\partial t} = \vec{v} \cdot \nabla C - \nabla \cdot (D \cdot \nabla C) \tag{3.8}$$

The last equation is the three-dimensional convective diffusion equation which, in its general form, has an analytical solution only in very special cases.

Turbulent diffusion is scale-dependent; generally, the horizontal turbulent diffusion coefficient in oceans and large lakes varies with a 4/3 power of the length scale of the phenomenon

$$D_h = A_D L^{4/3}$$

where D_h is the horizontal diffusion coefficient; A_D is the dissipation parameter of the order of 0.005 when D_h units are (cm^2/s); L is the length scale of the phenomenon often taken as the size of the horizontal grid spacing, since this approximates the minimum scale of eddies which can be reproduced by the model.

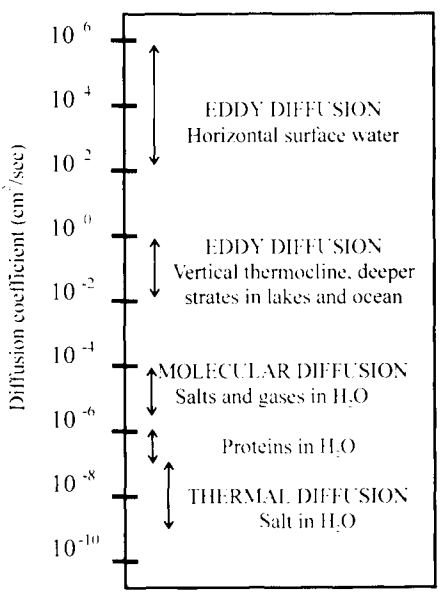

Fig. 3.9. Ranges of diffusion coefficient values for several processes.

Dispersion

The combination of the two main processes of mass transport—advection and diffusion (pure or turbulent)—is usually the real process responsible for the movement of a substance in a fluid. In one dimension the phenomenon can be represented by the equation

$$J_x = Cu - D_x \frac{\partial C}{\partial x}$$

Remembering that the mass balance applied to an infinitesimal volume, as seen for Fick's second law, gives in one co-ordinate the following relation

$$\frac{\partial C}{\partial t} = -\frac{\partial J_x}{\partial x}$$

substituting in the last the value just obtained for J_x and assuming a constant D_x, we get the *advection–diffusion equation*

$$\frac{\partial C}{\partial t} = D_x \frac{\partial^2 C}{\partial x^2} - \frac{\partial Cu}{\partial x} \tag{3.9}$$

which can easily also be written in three dimensions with possible different values of the diffusion coefficient in the three directions. The exact solution of Eq. (3.9) in the case of an instantaneous release of substance in a mono-directed flow with constant advection is

$$C(x,t) = \frac{m}{2\sqrt{\pi D t}} \cdot e^{-\frac{(x-ut)^2}{4Dt}}$$

The effect of the *advective–diffusive process* is shown in Fig. 3.10 which is obtained from Fig. 3.7 moving to the right the axis of the bell-shaped curve with a constant velocity.

Even if the combination of advection and diffusion is a good model of the movements of a substance in a fluid and adequately describes the environmental process of mass transport, the advective transport is often too simple a description because it does not account for the differences in velocity that occur in a moving fluid due to the shear stress of the bottom. These differences in velocity generate a transversal diffusion that adds to advection and diffusion and, together, are usually called *dispersion*. Provided that enough time is taken to mix the substance, this process can be modelled by a Fickian process. In the environment, dispersion is usually predominant when the strong shears developed by large mean flow and constraining banks is dominant as in rivers, estuaries and lagoons and if a short time scale is considered. For long-term simulation, mixing is more similar to a turbulent diffusion and it can be simulated with this last more handy model.

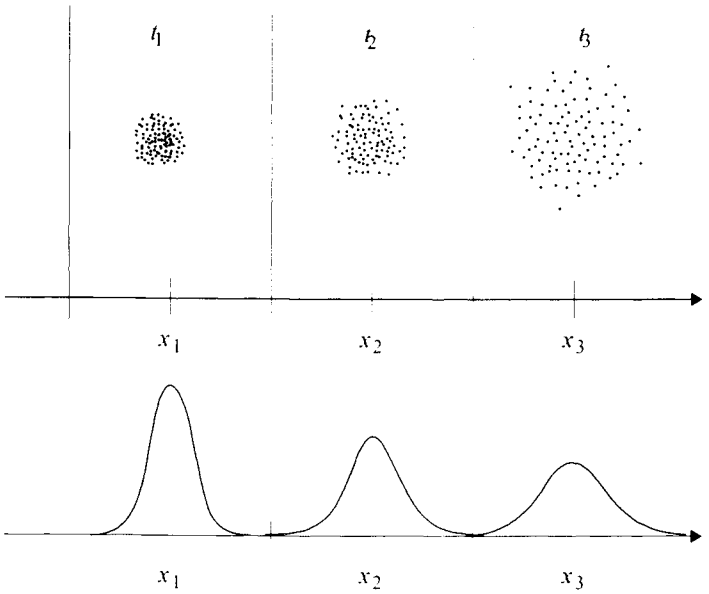

Fig. 3.10. Effect of a simultaneous advection and diffusion process on a substance released as an impulse at $t = 0$ in the position $x = 0$.

Mass Transfer at a Two-phase Interface

As we have seen in the presentation of diffusion processes, if the concentrations of a substance are different in two parts of a system, diffusion tends to adjust the equilibrium between the parts. The adjustment depends on the magnitude of the difference usually called *driving force* and on the surface of the interface through which the transfer occurs. The matter through which the substance has to transfer offers a resistance to this migration that is usually accounted for by a *mass transfer coefficient* which incorporates the effect of turbulence and of the type of substance molecules and depends on temperature.

For a system with a gas–liquid interface, at the equilibrium, as commonly occurs in environmental stagnant aquatic systems between air and water, we can imagine that the substance moves by diffusion across two films, one of gas and one of liquid with different thicknesses δ_g and δ_l, as shown in Fig. 3.11. The diffusion coefficients D_g for gas and D_l for liquid are also different. The resulting mass-transfer velocities in the laminar layer are for gas $k_g = D_g/\delta_g$ and for liquid $k_l = D_l/\delta_l$, respectively.

At the equilibrium the concentrations of the substance in the two phases are connected by *Henry's law*: at the interface the concentration C_i of any gas, not reacting with the solvent, dissolved in a liquid is directly proportional to the partial pressure p_i of gas at the interface

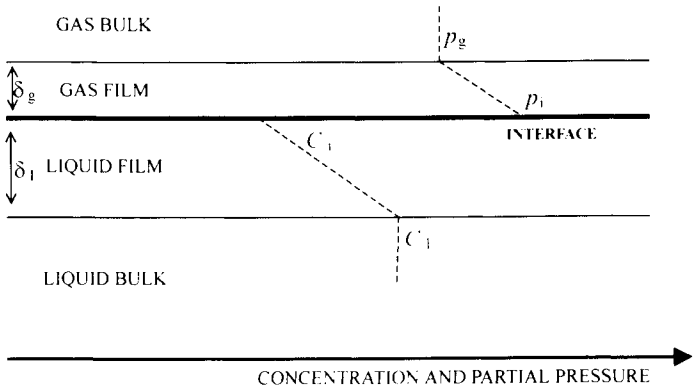

Fig. 3.11. Mass transfer at the interface between a liquid and a gas phase (layer model).

$$C_i = \frac{P_i}{He} \tag{3.10}$$

where *He* is Henry's constant, i.e. the ratio of the partial pressure of the gas to the concentration of the substance in the liquid at saturation. The rate at which the substance is transported across the liquid film is

$$J_l = k_l(C_i - C_l) \tag{3.11}$$

The rate at which the substance is transported across the gas film is

$$J_g = (k_g/RT)\,(p_g - p_i) \tag{3.12}$$

Assuming that $J_l = J_g = J$, substituting (3.10) in (3.11) and solving for p_i (3.11) and (3.12) we get:

$$J = \frac{p_g - C_l}{\dfrac{RT}{K_g He} + \dfrac{1}{k_l}}$$

where $\dfrac{RT}{K_g He} + \dfrac{1}{k_l}$ is the net transfer velocity across the gas–liquid interface (m/s) provided by the driving force due to the difference between the bulk gas pressure p_g and the bulk liquid concentration C_l. Note the analogy to the formulation for two resistors in series in an electrical circuit.

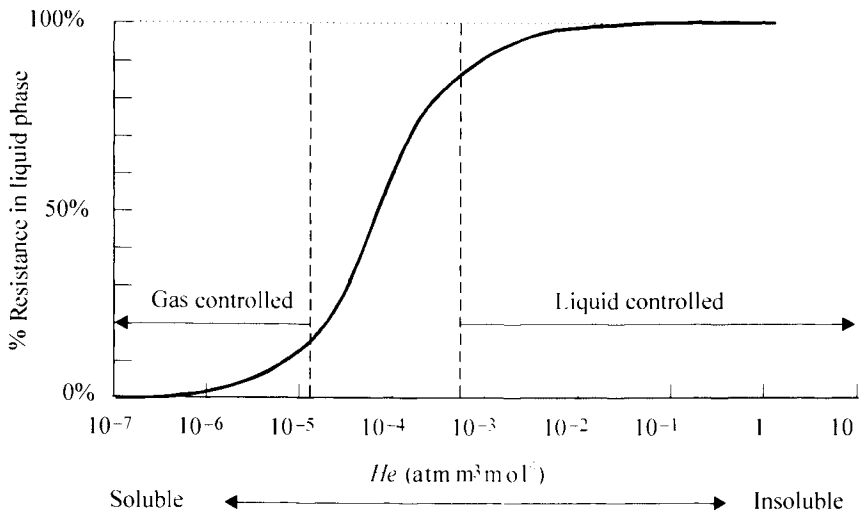

Fig. 3.12. Percent resistance to gas transfer in liquid phase for some environmentally important gases as a function of *He*, for lakes (modified after Mackay, 1977).

An application of *Whitman's two film theory* of mass-transfer of environmentally important substances and toxicants is shown in Fig. 3.12.

Values of log(*He*) for a number of substances of environmental interest are listed in Table 3.10 of Section 3B.7. The higher the *He*, the more the liquid phase resistance controls the mass transfer. This means, for instance, that the transfer of CO_2 (log*He* = –1.57) or methane (log*He* = 0.19) from water is almost totally dependent on their concentration in water, those of Dieldrin (log*He* = –4.96) and Lindane (log*He* = –6.45) depend on the concentration of these pesticides in air, while NH_3 (gaseous ammonia), that can be toxic for aquatic life, is right in the middle. This justifies the usual attention paid in the eutrophication models in modelling NH_3 concentration and to the stripping process of this gas from water, as a consequence of turbulence.

The assumption of stagnant water is very restrictive. In order to model non-stagnant water we can conceptualize the water as consisting of parcels brought to the surface for periods of time. While at the surface, exchange between the water parcel and air takes place according to the two-phase mass transfer theory. The difference between the two conceptualizations consists in the time of contact of the fluid parcel at the interface and can be modelled by a liquid surface renewal rate r_l [T^{-1}] in the following way

$$J = \sqrt{D_l r_l}(C_i - C_l)$$

as shown in Section 3C.1, the re-aeration coefficient in rivers, k_r, can be computed in many different ways and it is strictly connected to the renewal rate.

3A.3 Mass Balance

The mass balance is a very primary principle of ecological modelling. It usually considers the fate of substances entering and leaving a system in various ways. The modelling approach to the mass balance tries to simplify the system with some general assumptions that are very useful. If we refer to an aquatic system, we could assume the system to be:

- completely mixed, dominated by dispersion and zero-dimensional like a lake;
- dominated by advection like a river where it is possible to assume that substances entering a branch of the river are leaving it in the same sequence as they enter;
- affected by both advection and dispersion like estuaries.

All these assumptions lead us to a specific type of models, known, respectively, as *CSTR* (*Continuous Stirred Tank Reactor*), *PFR* (*Plug Flow Reactor*) and *MFR* (Mixed Flow Reactor).

Mass Balance for a Well Mixed System

The well mixed system (CSTR) is the simplest way to model an aquatic system; the basic assumption is that the concentration C of a given substance in the volume V of the system is always uniformly distributed in space. If a change in time of the concentration occurs instantaneously the new concentration is distributed all over the system. For CSTR a lumped parameter model of mass balance can be summarized as follows.

$$Accumulation = input - output \pm reaction$$

Accumulation of mass M over time t can be mathematically written as

$$Accumulation = \Delta M/\Delta t$$

and because $M = VC$ accumulation can also be written as $\Delta VC/\Delta t$, if V is constant, as we can usually assume over short time span.

$$Accumulation = V(\Delta C/\Delta t)$$

and if $\Delta t \rightarrow 0$, *Accumulation* can be written as $V(\partial C/\partial t)$.

Input represents the mass entering the volume from a variety of sources and different ways. This entering mass is called load and is usually indicated by L. It is a function of time and indicates the rate of mass (MT^{-1}) entering the system at time t. If the only source of a lake is the influent river with a flow Q ($L^3\,T^{-1}$) the input can be written

$$Input = L(t) = Q\,C_{in}(t)$$

where $C_{in}(t)$ is the average inflow concentration (ML^{-3}).

Output represents the mass leaving the volume from a variety of sources and different ways. It usually includes the main processes: outflow and settling.

$$Output = QC + vA_sC$$

where v is the apparent settling velocity (LT^{-1}), A_s is the sediment deposition area, C is the concentration and Q the flow in the outlet.

Reaction is a way of leaving the system for the mass by chemical transformation into other substances. The most common way to account for this process is a first-order kinetic

$$Reaction = kM = kVC$$

where k is the parameter that accounts for the reaction depending on the mass of the system.

The total balance for the system is

$$V(\delta C/\partial t) = L(t) - QC - vA_sC - kVC \tag{3.13}$$

and for a steady state ($\delta C/\partial t = 0$)

$$C = \frac{L}{Q + vA_s - kV}$$

if we put $(Q + vA_s - kV) = a$, we get $C = L/a$ and $C = C_{in}(Q/a)$ where Q/a is usually said to be the transfer function because it shows how an entering concentration is transformed into a leaving one.

For a system in steady state, as we can assume for a lake, the volume V is constant and, provided that precipitation is equal to evaporation, Q is constant and we can define the residence time of a lake $t_w = V/Q$.

If the system is not in steady state, the general mass balance is given by Eq. (3.13). Dividing by V and putting $\lambda = (Q/V - v/h - k)$ where h is the depth of the system (lake) and λ is the eigenvalue of the non-homogeneous linear, first-order differential equation.

$$(\partial C/\partial t) + \lambda C = L(t)/V \tag{3.14}$$

the general solution for the homogeneous associated equation is

$$C = C_0 e^{-\lambda t}$$

when $C(0) = C_0$, the general solution of Eq. (3.14) is

Table 3.1. List of the most relevant loading functions and solutions of the CSTR model for these forcing functions.

LOADING FUNCTION $L(t)$		SOLUTION
Pulse	$m\delta(t)$	$C = \frac{m}{V} e^{-\lambda t}$
Dirac delta	$\delta(t)$	
Step	$L(t) = 0 \; t < 0$ $L(t) = L \; t \geq 0$	$C = \frac{L}{\lambda V}(1 - e^{-\lambda t})$
Linear $L(t) = \beta t$		$C = \pm\frac{\beta}{\lambda^2 V}(\lambda t = 1 + e^{-\lambda t})$
Exponential $L(t) = L_0 e^{-\beta t}$		$C = \frac{L_0}{V(\lambda - \beta)}(e^{-\beta t} - e^{-\lambda t})$

$$C = C_0 e^{-\lambda t} + C_p$$

where C_p is a particular solution depending on the shape of the loading function $L(t)$.

For several ideal loading functions it is easy to have the exact solution of Eq. (3.14) and Table 3.1 summarizes the most relevant ones.

CSTRs are also useful to describe more complex systems for which the assumption of a single CSTR is not acceptable. Such a system can be described by a distributed parameters model using a network of CSTRs eventually with feedback as shown in Fig. 3.13.

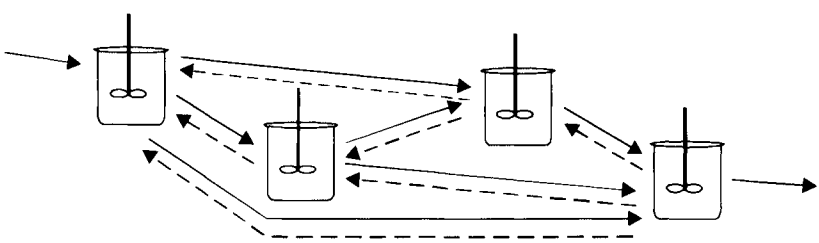

Fig. 3.13. Network of CSTRs useful to simulate complex systems.

Each CSTR is characterized by a proper volume V_i and kinetic constant k_i and outflow Q_i from the i-esim CSTR to the other and by a load L_i from the other CSTRs into the i-esim including the external environment.

Another important application of CSTR models concerns a zero-dimensional system with complex transfer processes. According to the general hydraulic theory series of CSTRs (Chow, 1964), a cascade of n CSTRs characterized by the same parameters can be used to simulate the attenuation of the entering concentration of a substance in a porous media. This model has been used, for instance, to simulate the response of an agricultural watershed to a load of fertilizers applied to crops (Zingales et al., 1984). The general solution of the model is

$$C_n = \left(\frac{Q}{Q+kV}\right)^n C_0$$

Mass Balance for a Non Well Mixed System

If a variation of concentration C occurs along a longitudinal axis x of an elongated system such as a river (as depicted in Fig. 3.14), and if the assumption of a uniform distribution of concentration on a transversal section $A_c = BH$ can be done, the mass balance is given for a differential element of length Δx by the following equation

$$\Delta V \, \partial C/\partial t = J_{in} A_c - J_{out} A_c \pm reaction \tag{3.15}$$

with the usual meaning of symbols.

A *Plug Flow Reactor (PFR)* model assumes that advection dominates the mass transfer and substances entering the reactor will leave it in the same sequence as they enter it.

$$J_{in} = uC$$

where $u = Q/A_c$ is the velocity, and

$$J_{out} = u(C + (\partial C/\partial x)\Delta x)$$

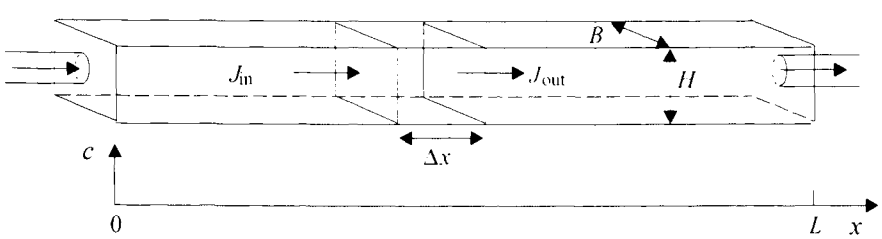

Fig. 3.14. Mass balance scheme for an elongated system like a river.

if the reaction is assumed as a first-order one

$$reaction = k\,\Delta V\,\underline{C}$$

where $\underline{C}$ is the average concentration over Δx.

Equation (3.15) can be written

$$\Delta V\,\partial C/\partial t = u\,A_c\,C - u\,A_c\,(C + (\partial C/\partial x)\Delta x) - k\,\Delta V\,\underline{C}$$

Rearranging the equation, dividing by ΔV and taking the limit of $\Delta x \rightarrow 0$ and consequently $\underline{C} \rightarrow C$, we get

$$\partial C/\partial t = -u\,\partial C/\partial x - kC$$

at steady state, if we assume $C = C_0$ at $x = 0$, we get

$$C = C_0 e^{-kx/u}$$

If both advection and dispersion are significant, such as for turbulent transport in a river, the proper model is a *Mixed Flow Reactor* (*MFR*) where the components of the mass balance assume the following form

$$J_{in} = uC - E\,\partial C/\partial x$$

where the second term is Fick's law and E is the turbulent (eddy) diffusion coefficient.

$$J_{out} = u(C + (\partial C/\partial x)\Delta x) - E\,(\partial C/\partial x + \partial/\partial x(\partial C/\partial x)\Delta x)$$

Equation (3.15) is now written

$$\Delta V\,\partial C/\partial t = u\,A_c C - E\,A_c\,\partial C/\partial x - u\,A_c(C + (\partial C/\partial x)\Delta x) - E\,A_c(\partial C/\partial x + \partial/\partial x(\partial C/\partial x)\Delta x) - k\,\Delta V\,\underline{C}$$

Rearranging, as before, the last mass balance equation we get

$$\partial C/\partial t = -u(\partial C/\partial x) - E\,A_c(\partial^2 C/\partial x^2) - k\,\underline{C}$$

at steady state with the usual initial conditions

$$0 = -u(\partial C/\partial x) - E\,A_c\,(\partial^2 C/\partial x^2) - k\,C$$

and the second-order differential equation can be solved in a variety of ways. For a general solution of this equation, refer to Chapra (1997).

3A.4 Energetic Factors

Solar Radiation

The most important factor driving the evolution of the ecosystem is the energy flow and the main source of energy for ecosystems is solar energy. For this reason, modelling solar radiation is of great importance because it is the principal forcing function for models of heat budget, photosynthesis, primary productivity and photolysis. Solar energy reaching the earth's surface depends on the day, the hour and the latitude of the place because of the earth's rotation on its axis and around the sun. Table 3.2 shows the energy entering the troposphere with different wavelengths and its fate. As we can simply understand from the table, only 46% of the energy entering the troposphere reaches the earth's surface and the major part of this energy has wavelengths in the ranges ultraviolet and visible. After utilization by ecological systems, an equal quantity of energy leaves the planet. Unfortunately, during the last century, human activities have increased the concentration of CO_2 and other gases in the atmosphere. These gases have generated the well known *greenhouse effect* and the related global warming. Because the energy balance, at the earth scale, is no longer in equilibrium, the flow of energy through the atmosphere changes, both in quantity and quality, in terms of wavelengths, and we can roughly say that each photon entering the surface with short wavelengths generates about 20 outgoing photons with long wavelengths. This fact is explained by the formula

$$E = h\nu = h(c/\lambda)$$

where the energy of a photon E is inversely proportional to the wavelength, so shorter wavelengths have higher energy than longer ones. This degradation of energy quality supports life on earth.

An important variable in the model of solar radiation is the longest duration, P, of light in a day, commonly named the *photoperiod*, expressed as part of the 24 hours. Equation (3.16) indicates a way of calculating the photoperiod for a given day, n, of the year and for a given latitude ϕ

$$P(n,\phi) = (2 \arccos(-tg\phi tg\delta)) / 360 \tag{3.16}$$

where δ, the *solar declination* (angle between the line connecting sun and earth and the equatorial plane) is expressed by the following function

$$\begin{aligned}\delta(y) = 0.38092 &- 0.76996 \cos(y) + 23.2650 \sin(y) \\ &+ 0.36958 \cos(2y) + 0.10868 \sin(2y) \\ &+ 0.01834 \cos(3y) - 0.00392 \sin(3y) \\ &- 0.00392 \cos(4y) - 0.00072 \sin(4y) \\ &- 0.00051 \cos(5y) + 0.00250 \sin(5y)\end{aligned}$$

Table 3.2. Fate of solar radiation flowing through the troposphere and reaching the earth's surface

Total Energy	% Band	Wave length (μm)	Absorbed by
about 1360 W m^{-2}	9% ultraviolet	< 0.12	by O_2 and N_2 at 100 km
		0.12–0.18	by O_2 at 50 km
		0.18–0.30	by O_3 at 25–50 km (1)
		0.30–0.34	partially by O_3
		0.34–0.40	4% absorbed and reflected
	41% visible	0.40–0.71	46% almost entirely reaching the earth's surface and reflected after utilization by ecosystem and wavelength degradation
	50% infrared	0.71–3	50% absorbed and reflected by CO_2, N_2O at 10 km (2)

(1) Reduction of O_3 in the troposphere due to the increased CFC concentration is reducing the quantity of the energy with this wavelength that is reflected, increasing the global warming and the damages due to ultraviolet rays.
(2) The increase of CO_2 generates the greenhouse effect, reduces the reflected infrared energy and increases the global warming.

where y, the *yearly angle* in degrees, is given by the following relation (3.17) (France and Thornley, 1984) with the convention that the first day of the year is the 1st March to avoid the problem of leap-years.

$$y(n) = 360\ ((n - 21) / 365) \tag{3.17}$$

The absolute value of the argument of the arcos, ($tg\phi tg\delta$), must be less than 1. In fact the maximum solar declination (δ) is 23.5° and $tg(23.5) = 0.434$, the maximum absolute value for latitude (ϕ) is 66.5°, because $tg(66.5) = 2.2998 < (1/0.434) = 2.3041$. This justifies the fact that for latitudes larger than the latitude of polar circles (66.5°) the day (or night) can be 24 hours long and consequently the photoperiod 1 (or 0).

The *daily solar radiation* at a given latitude is modelled by a sinusoidal formula for the clear sky condition and is calculated by multiplying the clear sky solar radiation (W m^{-2}) times the photoperiod. Attention must be paid to the photoperiod when the unit is expressed per hour or second and to the unit of solar radiation.

Usually, solar radiation is measured in W m^{-2} but sometimes other units are used, such as, for instance, the English system unit BTU (British Thermal Unit) ft^{-2} day^{-1} (= 0.131 W m^{-2}) or the Langley day^{-1} (Ly = 1 cal cm^{-2} which means 1 Ly = 0.483 W m^{-2}) and Kcal m^{-2} h^{-1} (= 1.16 W m^{-2}) or cal m^{-2} s^{-1} (= 4.18 W m^{-2}) or in MJ m^{-2} day^{-1} (= 86.4 W m^{-2}).

Figure 3.15 shows a simple plot to estimate the daily clear sky solar radiation Q_{sc} due to the short waves, as a function of latitude and day of the year (30 to 300 Kcal m^{-2} h^{-1}).

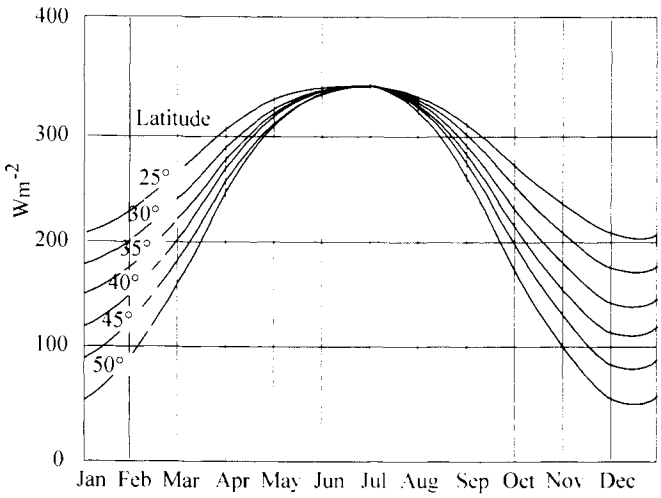

Fig. 3.15. Clear sky radiation due to short wavelengths, according to Hamon et al. (1954).

The net short-wave radiation $Q_{sn} = Q_{sc} - Q_{sr}$ (Q_{sr} = reflected short-wave radiation) is lower than the clear sky radiation (Q_{sc}) because of clouds and can be estimated by the following relation due to Ryan and Harleman (1973)

$$Q_{sn} = 0.94\ (1 - 0.65\ C^2)$$

where C is the fraction of sky covered by clouds and the constant 0.94 roughly accounts for reflected short-wave radiation Q_{sr}, usually ranging from 4 to 20 W m^{-2}.

Even if this model is easy to be set up, it is very dependent on the average cloud coverage of the site and for this reason it can be unreliable.

The example in Fig. 3.16 shows how it can work for one site yet fail for another when the clouds are not uniformly distributed over the year. Fortunately, average solar radiation does not change too much from point to point in a site and measured data of such a forcing function are usually available from the weather forecasting offices. This is the reason why, in environmental models, the solar radiation is simulated by regression on measured data by the formula

$$I\ (n) = a + b \sin y \tag{3.18}$$

where a and b are parameters that have to be estimated on real data and y is given by relation (3.17).

Figure 3.16a shows a set of daily radiation data gathered at Venice (Italy) during 1985 and the simulation obtained by relation (3.18). Figure 3.16b shows similar data for Manila (Philippines): it is easy to compare and appreciate the different agreement of the model with solar radiation data for a temperate and tropical place and to conclude that for the latter, the model would be changed and adapted.

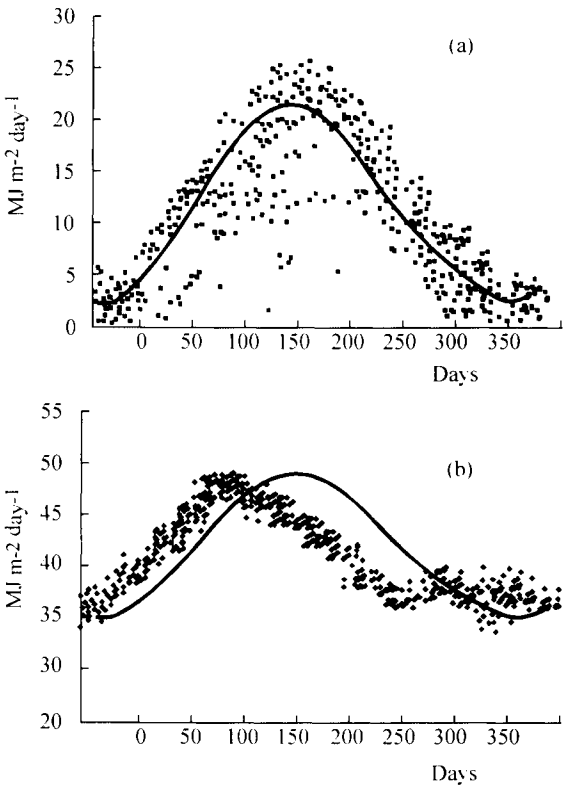

Fig. 3.16. Daily radiation data gathered (a) at Venice (Italy) and (b) at Manila (Philippines) and the relative simulation curve, obtained by Eq. (3.18).

The total radiation budget

$$Q_{in} = Q_{sc} - Q_{sr} + Q_{lc} - Q_{lr} - Q_{br}$$

is the sum of two positive terms, the *gross short-wave radiation*, Q_{sc}, and the gross *long-wave*, Q_{lc} (260 to 420 W m^{-2}), both with a wide range of values, and of three negative terms the two reflected Q_{sr}, Q_{lr} (6 to 17 Wm^{-2}) and a *back radiation* Q_{br} (255 to 400 W m^{-2}), numerical values are valid for a latitude close to that of the Mediterranean sea. This budget shows how a quantity of energy equal to that entering as long wavelengths is almost totally reflected as long wavelength radiation and the rest is leaving the earth after degradation as heat reflection and other radiation.

The long-wave *incident radiation*, Q_{lc}, is due to atmospheric radiation, the major emitting substances are water vapour, carbon dioxide and ozone. The approach generally adopted to compute this flux is the empirical estimation of an overall atmospheric emissivity of Swinbank (1963) (in BTU ft^{-2} day^{-1})

$$Q_{lc} = 1.16\ 10^{-13}\ (1 + 0.17C^2)\ (T_a + 460)^6$$

where T_a is the dry bulb air temperature in Fahrenheit.

The long-wave back radiation Q_{br} is the largest back flux of energy and a water body is evaluated according to the water surface emissivity (in cal m^{-2} s^{-1})

$$Q_{br} = 0.97\ \sigma\ T_w^4 \tag{3.19}$$

where σ is the *Stefan–Boltzman constant* (= 5.667 10^{-8} W m^{-2} K^{-4}) and T_w is the surface water temperature in Kelvin. A good linearization of relation (3.19) in the range from 0 to 30°C is given by the U.S. Army Corps of Engineers (1974) where Q_{br} is expressed in cal m^{-2} s^{-1} and T_w is the water temperature in °C

$$Q_{br} = 73.6 + 1.17\ T_w$$

Solar radiation varies during the day as a sinusoidal curve, and relation (3.20) describes the variation of the intensity I as a function of t (hours of the day)

$$I(t) = \frac{I(n)}{P(n,\phi)}\left(1 + \cos\left[(t - 0.5)\frac{360}{P(n,\phi)}\right]\right) \tag{3.20}$$

t can range over the photoperiod that is a fraction of the day and if we normalize the day length to 1, t can range between $0.5 - (P(n,\phi)/2)$ and $0.5 + (P(n,\phi)/2)$, out of this interval the light is zero because of night, due to the fact that the intensity is always positive the cos is shifted up by 1, relation (3.20) is finally normalized to the total daily solar radiation $I(n)$ given by relation (3.18).

Light Extinction

The solar radiation just modelled refers to the energy reaching the earth surface. In aquatic ecosystems, the solar radiation of interest for primary productivity is that penetrating the water surface. Light is one of the main factors affecting plant growth. Because many of the materials frequently dissolved or suspended in aquatic systems absorb or scatter light, light entering at the surface is attenuated as it penetrates the water. Light intensity is therefore a function of depth and of water content and it is essentially defined by the *Lambert–Beer law*

$$I(z) = I_0 e^{-\gamma z} \tag{3.21}$$

where I is the light intensity at depth z below the surface, I_0 is the light intensity at the surface and γ is the light extinction coefficient (L^{-1}). The surface light intensity photosynthetically active, used in the algal growth formulations, corresponds only to

the visible range, which is typically about 50% of the total solar radiation provided by relation (3.20). Almost all non-visible radiation is absorbed within the first metre below the surface (Orlob, 1977).

The *light extinction coefficient* is usually defined as a linear sum of several extinction coefficients representing each component of light absorption (water, colour, particulate turbidity due to non-living and living matter such as phytoplankton). If in the model we can assume that the major cause of the extinction is the self-shading effect of the algal bloom, a linear or quadratic relation to the phytoplankton concentration of the living matter extinction coefficient can be assumed

$$\gamma = \gamma_0 + a_1 A \qquad \text{or} \qquad \gamma = \gamma_0 + a_1 A + a_2 A^b$$

where γ_0 is the extinction coefficient due to all the other factors, A is the algae concentration and a_1, a_2, b are coefficients related to the self-shading effect.

Temperature

The temperature of air and water, as well as solar radiation, is another important abiotic factor driving the primary productivity of ecosystems. It is strictly linked to solar radiation which constitutes the only source of energy for ecosystems, but it also depends on other factors such as cloud presence, wind, humidity and pressure. Temperature variations of an ecosystem are strongly influenced by the thermal capacity of a large mass of ecosystem (air, water and land) contributing towards smoothing and delaying the variation of temperature driven by solar radiation.

On a long time scale of seasons, temperature follows a deterministic behaviour driven by solar radiation; on a short time scale of days temperature shows a stochastic behaviour driven by the meteo-climatic variations. Usually the daily temperature $T(n)$ of day n is modelled by relation (3.22)

$$T(n) = D(n) + R(n) \tag{3.22}$$

where $D(n)$ is the deterministic term describing the seasonal variation and $R(n)$ is a random term describing the difference between the value predicted by $D(n)$ and the real one.

As for solar radiation, $D(n)$ can be described by the following equation

$$D(n) = a + b \sin(y - \phi)$$

where a and b are parameters that have to be fitted with experimental data, y is given by Eq. (3.17) and ϕ is the angle that represents a delay of d days in respect to the solar radiation usually given by $\phi = (360/365)d$.

The random term $R(n)$ can be estimated by auto-regressive models using a noise signal. Where the auto-covariance is largely explained by the temperature a few days before (typically 5 days) because larger time span variations (e.g. 30 days) are accounted for by the deterministic value.

Relation (3.22) can be used to describe the temperature of an ecosystem but, for aquatic environments, temperature variations could be better simulated using a deterministic model accounting for meteo-climatic factors. The model simulates the temperature of a water body accounting for the heat flows at the interface between water and air and remembering that the thermal capacity of water is 1 and that it does not vary so much for small variations of temperature, pressure and humidity of the ecosystem. The temperature at time $t + \Delta t$ is calculated by the following equation

$$T_w(t + \Delta t) = T_w(t) + \Delta t[T(t) + Ex(t) - Ev(t) - Re(t)]$$

on the basis of T_w at time t and the fluxes of solar radiation $I(t)$ as expressed in Eq. (3.18) and that of heat exchange at the air–water surface

$$Ex(t) = k_{Ex}(T_a - T_w)$$

where k_{Ex} is the thermal conductivity accounting also for wind effects, and T_a and T_w are the temperature of air and water at the interface at time t, respectively. The flux of heat due to evaporation is given by the relation

$$Ev(t) = k_{Ev} H(P_w - P_a)$$

where k_{Ev} is an evaporation conductivity, H is the latent heat of evaporation, and P_w is the saturation pressure of water vapour estimated by the relation

$$P_w = 4.75 + 0.375\, T_w + 0.0065\, T^2_w + 0.0004\, T^3_w$$

and P_a is the partial pressure of water vapour in air estimated by

$$P_a = 4.75\, h_r + 0.375\, T_a + 0.0065\, T^2_a + 0.0004\, T^3_a$$

where h_r is the relative humidity of air. And finally $Re(t)$ is the reflected radiation on water surface expressed by

$$Re(t) = k_{Re}(T_w - T_a)$$

where k_{Re} is the reflection conductivity.

3A.5 Settling and Resuspension

Settling and *resuspension* are physical processes of importance in ecological modelling because they move matter and substances commonly used in ecological systems from the aquatic environment to the benthic one and *vice versa*. Similar processes also occur in air, usually called deposition and wind erosion; although important for terrestrial ecosystems they are not considered in the following part of this chapter.

Settling and resuspension are both described by physical relations that can be used in modelling an aquatic ecosystem. They are complicated by strong interactions with the biotic processes. For instance, the physiological state of phytoplankton cells affects the sedimentation rate; on the other hand, bioturbation of sediments affects their pellet size and the gluing effect changes to some order of magnitude the critical shear stress that regulates resuspension. A simple description of these mechanisms of transport is given here; for further details of the biotic influence on processes we recommend specialized literature such as Hakanson (1983).

The physics of the settling phenomenon for particles that are non-flocculating in a dilute suspension is described by classical mechanics. We assume that such a particle is not aggregated to others to form larger aggregates (the formation of flocculates is mainly due to changes in pH or the concentration of some ions of metal that facilitate this process) and due to the assumed dilute solution, the particle is not affected by the presence of the other particles. Settling is therefore a function solely of the properties of the fluid and of the characteristics of the particles.

According to Newton's second law of motion, we can write

$$m\frac{\partial v}{\partial t} = F_g - F_b - F_f \tag{3.23}$$

where v is the linear settling velocity of particle of mass m and t is time.

F_g is the gravitational force given by

$$F_g = \rho_p \cdot V \cdot g$$

where ρ_p is the particle density, V is its volume and g is the gravitational acceleration; F_b is the buoyant force expressed by

$$F_b = \rho_f \cdot V \cdot g$$

where ρ_f is the fluid density.

F_f is the frictional force, function of different particles' parameters such as roughness, size, shape, velocity of the particle, density and viscosity of fluid; it can be expresses as

$$F_f = (C_d A \rho_f v^2)/2$$

where C_d is Newton's dimensionless drag coefficient, and A is the projected particle area in the direction of flow.

After an initial transition period the settling velocity becomes constant and the right term of Eq. (3.23) is zero and we get

$$v = \sqrt{\frac{2g(\rho_p - \rho_f)V}{C_d \rho_f A}} \tag{3.24}$$

If the particle is assumed spherical of diameter d the term V/A is equal to $2d/3$.

C_d is a function of the *Reynolds number*

$$\mathrm{Re} = \frac{d\rho_f v}{\mu}$$

where μ is the fluid viscosity, C_d depends also on the shape of the particle as shown in Fig. 3.17 where, if the Reynolds number is lower than 10^0 (laminar flow), C_d can be approximated by a straight line, if $10^0 < \mathrm{Re} < 10^3$, C_d can be approximated by $C_d = 24/\mathrm{Re}$ from these considerations and from Eq. (3.24) we get *Stoke's law*

$$v = \frac{g}{18\mu}(\rho_p - \rho_f)d^2$$

if $\mathrm{Re} > 10^3$ (turbulent flow), C_d for cylinder is approximately 1 and

$$v \approx 1.82\sqrt{\frac{(\rho_p - \rho_f)dg}{\rho_f}}$$

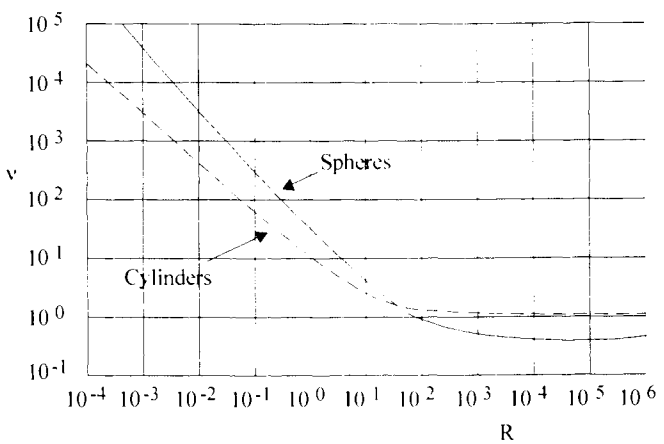

Fig. 3.17. Variation of the drag coefficient v with Reynolds (Re) number (after Fair et al., 1968).

When, as for some cases of ecological interest, the shape of the particle is not spherical or cylindrical, as with some phytoplankton cells, Stoke's law can be modified using an equivalent radius R, based on a sphere of equivalent volume, and a shape factor F that for small diatoms has been found to be 1.3, for large ones 2.0 and 1 for the other algae groups (Scavia, 1980) and we get

$$v = \frac{2}{9}\frac{gR^2}{\mu F}(\rho_p - \rho_f) \tag{3.25}$$

Many other factors, such as for instance the physiological state of the algae (TetraTech, 1980), can affect settling of algae cells and Eq. (3.25) can be further complicated.

In spite of such a detailed physical description of settling, many models describe the process by a first-order reaction equation

$$\frac{\partial m}{\partial t} = -s\, m$$

where s is the removal rate by settling usually expressed like the ratio between v and the depth d.

Alternatively the following equation is also used

$$sm = v\frac{\partial Ph}{\partial t}$$

where Ph is the phytoplankton concentration.

The settling rate is temperature dependent, and various expressions have been suggested to account for this dependence, the most used is

$$v_T = v_{Tr}\sqrt{\frac{T}{T_{ref}}}$$

where T is the absolute temperature and T_{ref} is a reference one.

Straskraba and Gnauk (1985) suggest considering for the sedimentation rate s the relations

$$s = \frac{1}{3}\frac{\rho_p - \rho_w}{\mu}$$

and the dependence on temperature of viscosity (μ) and on the density of water (ρ_w) are accounted for by

$$\mu = 0.178/(1 + 0.0337\,T + 0.00022T^2)$$
$$\rho_w = 0.999879 + 6.02602\,10^{-5}\,T - 7.99470\,T^2 + 4.36926\,T^3$$

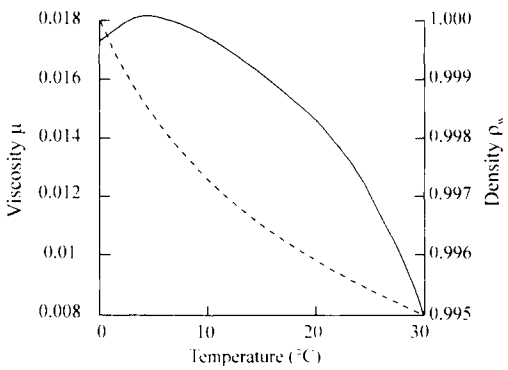

Fig. 3.18. Viscosity (dashed line) and density (solid line) of water plotted versus temperature of water.

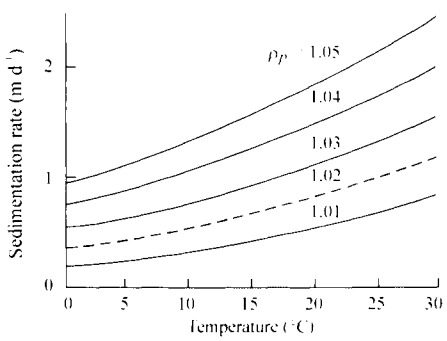

Fig. 3.19. Sedimentation rate of phytoplankton cells versus temperature of water for different densities of the phytoplankton cell ρ_p.

The plots of these functions are shown in Fig. 3.18 and, as a consequence, they get for the sedimentation rate s the relation shown in Fig. 3.19 for different values of the density of algae ρ_p.

Resuspension is the process that removes a particle from the sediment and moves it in the water body. The mechanism of resuspension in a lake is schematically represented in Fig. 3.20. It depends on several factors:

- energy delivered by the wind to the water surface depending on wind velocity U and on fetch F (the length of exposed water surface in the direction of the wind);
- waves, whose significant wave height H_s, and significant wave period T_s, depend on wind velocity and fetch;
- energy in the water, due to the circular eddies, dissipate with the depth H and exert a shear stress τ at the bottom;
- type of sediment described by grain size and consolidation state, which determine the critical shear stress τ_c.

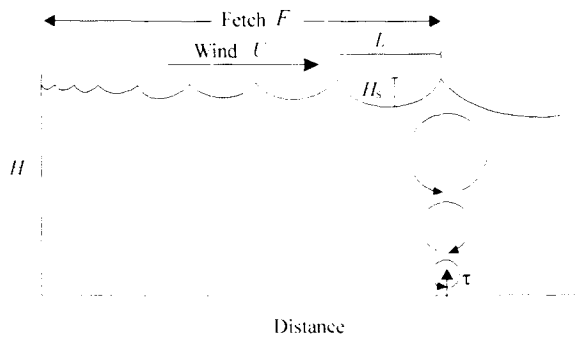

Fig. 3.20. Mechanism of resuspension generated by wind velocity and depending on fetch and water depth.

The amount of sediments ε scoured from the bottom can be calculated with

$$\varepsilon = 0 \quad \tau < \tau_c$$
$$\varepsilon = (\alpha_{ti}/t_d)\,(\tau - \tau_c)^3 \quad \tau > \tau_c$$

where the usual values for the constants are $\alpha_{ti} = 0.008$ and $t_d = 7$.

For shallow waters, where resuspension can easily mobilize sediments and pollutants, the shear stress can be approximated by

$$\tau = 0.003\, u^2$$

where u is the velocity created by waves at the bottom; usually the velocity at 15 cm over the bottom is considered. It can be generated by wind and also by currents. If we consider the wind effect, we can use the following formula to calculate it

$$u = \frac{\pi H_s}{T_s} \frac{100}{\sinh(2\pi H/L)}$$

H_s, T_s, and L can be estimated or calculated by more complex formulas that can be found in specialized texts (Chapra, 1997).

Due to the difference between the shear stress and the critical one, resuspension can occur at a given velocity. Figure 3.21 tries to depict how different processes of erosion, transport and accumulation occur at different values of previous factors u and type of sediments described as grain size and consolidation state.

For sandy material where the problem of cohesion and consolidation is negligible, a relation can be stated between some crucial factors, and the critical shear stress can be calculated by

$$\tau_c = k\rho_p(\beta - d)\frac{du}{dz}$$

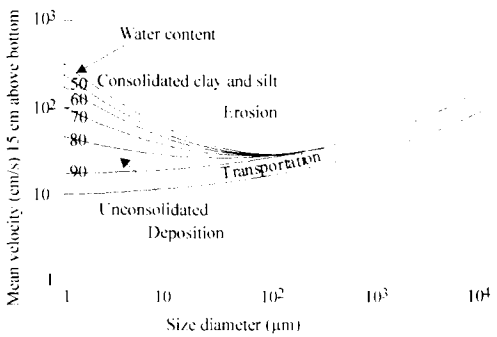

Fig. 3.21. Erosion, transportation and deposition (= accumulation) velocities for different grain sizes. Possible values for various stages of consolidation are indicated, as given by the water content (Postma, 1967).

where τ_c is the critical shear stress (drag force or force per surface) $[ML^{-1} T^{-2}]$, k is a constant usually equal to 0.013, ρ_p is the density of the particles $[ML^{-3}]$, β is a measure of spacing between particles usually constant, d is the particle diameter [L], u is the velocity of water at a distance z from the bottom.

Unfortunately the reality is far from being as simple as described in the last formula. As an example, Fig. 3.22 shows the spread of real data around the model line and shows how much the relationship between the water content of the sediment and the critical shear stress depends on the type of cohesive sediment. The previous relation for resuspension provides the order of magnitude of the critical shear stress but a description of the shear stress of cohesive sediments must include a parameter expressing, directly or indirectly, the glue properties of the deposit (McCall and Fisher, 1979; Fukuda and Lick, 1980). The problem of measuring the glue properties has not yet been fully explored and the difference between net and total deposition in lakes is largely unsolved (Smith, 1975; Fukuda and Lick, 1980).

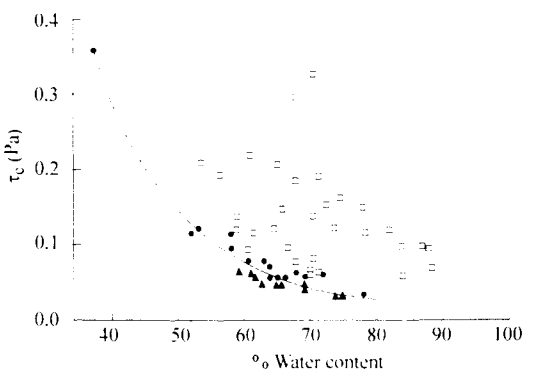

Fig. 3.22. Critical entrainment stress, τ_c, of oxidized box cores as a function of sediment water content. Filled circles: box cores of shale-based sediments. Filled triangles: runs made in flume experiment with the entire flume covered with shale-based sediments. Open squares: box cores collected from locations in Lake Erie (McCall and Fisher, 1980).

Part B. Chemical Processes

3B.1 Chemical Reactions

Reaction Types

Before going in detail about the modelling of a chemical reaction, we must recall some general definitions.

Reactions can be heterogeneous because they involve more than one phase and the reaction usually occurs at the phase interface. Writing a chemical reaction using the usual symbols, if necessary, the phase is specified with by a g (gas), l (liquid), or s (solid) in brackets after the chemical symbol of the element or of the substance, thus H_2O(l) means water at liquid phase. If the reaction occurs in a single phase it is said to be *homogeneous*. This type of reaction is the most usual and relevant in ecological modelling, particularly in water quality modelling.

Let A, B, C, D be four chemical substances, "[A]" usually denotes the concentration of "A" and "a" its stoichiometric coefficient, the number of moles of A involved in the reaction. A chemical reaction is usually written

$$a\mathrm{A} + b\mathrm{B} \rightarrow c\mathrm{C} + d\mathrm{D};$$

the symbol $\rightarrow$ indicates an *irreversible reaction* proceeding from left to right transforming the reactants A and B into the products C and D. If the inverse reaction

$$c\mathrm{C} + d\mathrm{D} \rightarrow a\mathrm{A} + b\mathrm{B}$$

can contemporarily occur, the global reaction

$$a\mathrm{A} + b\mathrm{B} \leftrightarrow c\mathrm{C} + d\mathrm{D}$$

is said to be a *reversible reaction*.

A common example of an irreversible reaction of interest for ecological systems is the decomposition of organic matter in aerobic environments

$$\mathrm{C_6H_{12}O_6} + 6\mathrm{O_2} \rightarrow 6\mathrm{CO_2} + 6\mathrm{H_2O}$$

which transforms glucose (representing organic matter) to dioxic carbon and water. It takes place, for instance, any time that sewage is discharged into a river.

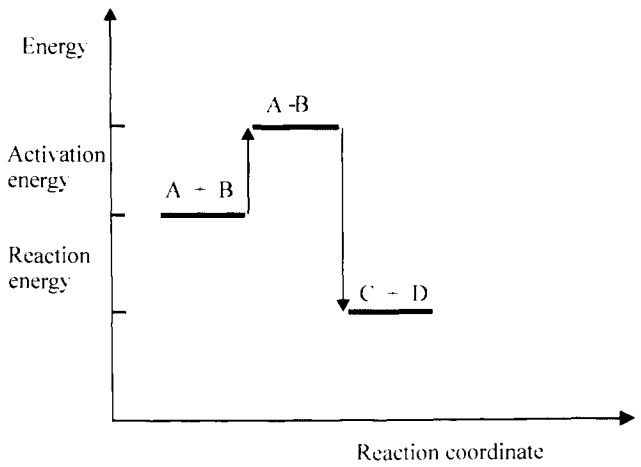

Fig. 3.23. Energetic diagram of an irreversible reaction.

An irreversible reaction occurs provided that:

- molecules of A and B have contact;
- the contact has a sufficient energy;
- the contact happens in a reactive position of the molecule.

When the contact satisfies the two last conditions it is said to be effective.

The mechanism of the reaction is

$$\underset{\text{Reactants}}{A + B} \rightarrow \underset{\text{effective contact}}{} \underset{\text{activated complex}}{A \cdot B} \rightarrow \underset{\text{products}}{C + D}$$

and the energetic diagram of this reaction is reported in Fig. 3.23.

The *activation energy* of a reaction can be reduced by the use of a catalyst.

A *catalyst* is a substance that enters a reaction but does not appear, neither as a reactant, nor as a product. The catalyst is not consumed during the reaction and it does not affect its equilibrium; it varies the velocity of the reaction because a lower activation energy allows a larger number of molecules to react.

Reaction Kinetics

The kinetics, or rate of a reaction, can be expressed quantitatively by the law of mass action

$$d[A]/dt = -k f([A], [B], [C], [D]) \tag{3.26}$$

where k is the constant of the reaction usually depending on temperature, and f is a function of the concentration of substances involved in the reaction. The functional

Table 3.3. Solutions of the law of mass for the most common orders of reaction

Reaction order	Differential form	Explicit form	Linear form
Zero	$\frac{dc}{dt} = -k$	$c = c_0 - kt$	$c = c_0 - kt$
First	$\frac{dc}{dt} = -kc$	$c = c_0 \cdot e^{-kt}$	$\ln c = \ln c_0 - kt$
Second	$\frac{dc}{dt} = -kc^2$	$c = c_0 \cdot \frac{1}{1 + c_0 kt}$	$\frac{1}{c} = \frac{1}{c_0} + kt$
n-Order	$\frac{dc}{dt} = -kc^n$	$c = c_0 \cdot \frac{1}{[1 + (n-1)kc_0^{n-1}t]^{\frac{1}{n-1}}}$	$\frac{1}{c^{n-1}} = \frac{1}{c_0^{n-1}} + (n-1)kt$

relationship f is commonly determined experimentally and assumes the general form of

$$f = [A]^{\alpha}[B]^{\beta}[C]^{\gamma}[D]^{\delta}$$

the index $n = \alpha + \beta + \gamma + \delta$ is called the order of the reaction and can also assume non-integer values.

The most common reactions depend on a single substance concentration, indicated in the following by C, and the *law of mass* (3.26) assumes the form

$$dC/dt = -kC^n$$

Table 3.3 summarizes the solutions of this differential equation for the most common order of reaction.

A practical method to decide the order of a reaction and the consequent model that has to be adopted, is to put in a graph the values of concentration [C], or their logarithm log[C], or their inverse values 1/[C], at different times, and fit them by a linear function. The best fitting line will indicate the order of the reaction. Data reported in Fig. 3.24 refer to the same set of data and clearly show that the reaction, to which they refer, is a first-order one according to the equation of Table 3.3 because plot b is clearly the best fit.

Temperature Effects

The constant reaction k depends on temperature and the *Arrhenius equation* governs this dependence

$$k(T) = A\, e^{-(E/RT)}$$

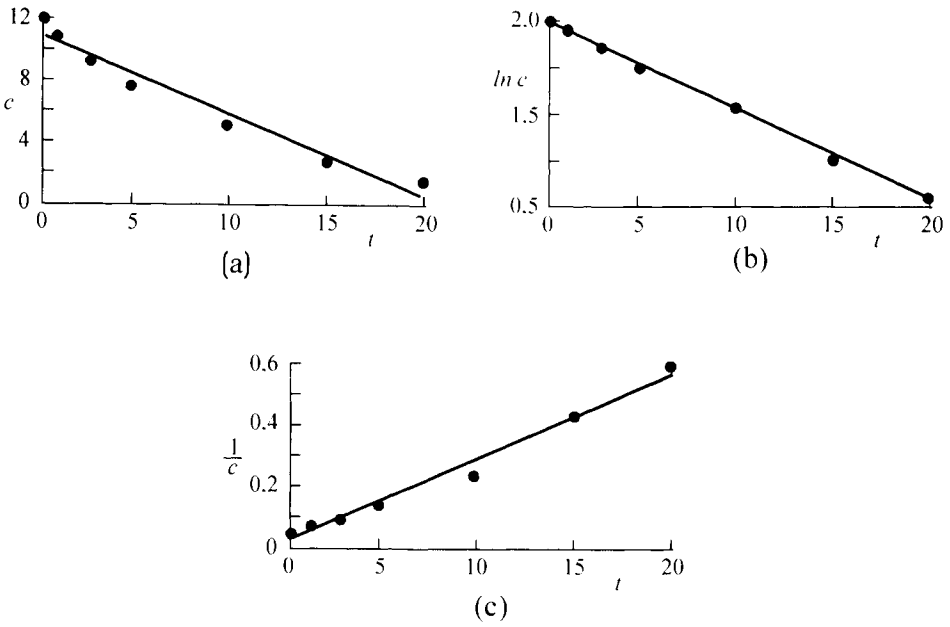

Fig. 3.24. Procedure to select the order of a reaction by the graphical method (Chapra, 1997).

where, T is the absolute temperature in Kelvin, R is the universal gas constant, E is the activation energy of the reaction, and A is a frequency factor accounting for the percentage of affective contacts.

The difference of distinct values of k at different temperatures T_1 and T_2 can be evaluated as their ratio

$$k(T_1)/k(T_2) = e^{(E(T1-T2))/RT1T2}$$

Because the reactions of ecological interest usually occur in a very narrow range of temperature (273–313°K), the product T_1T_2 is relatively constant, the quantity $\theta = e^{(E/(RT1T2))}$ is also relatively constant and the value of $k(T)$ can be evaluated by

$$k(T) = k_{20}\,\theta^{(T-T20)}$$

provided that the values of k at temperature of 20°C, k_{20}, and that of θ are known for a given reaction. Figure 3.25 shows the effect of temperature variation on the reaction constant k for various values of θ referring to different reactions of ecological interest.

The temperature dependence of a reaction is also often expressed by the quantity

$$Q_{10} = \frac{k_{20}}{k_{10}} = \theta^{10}$$

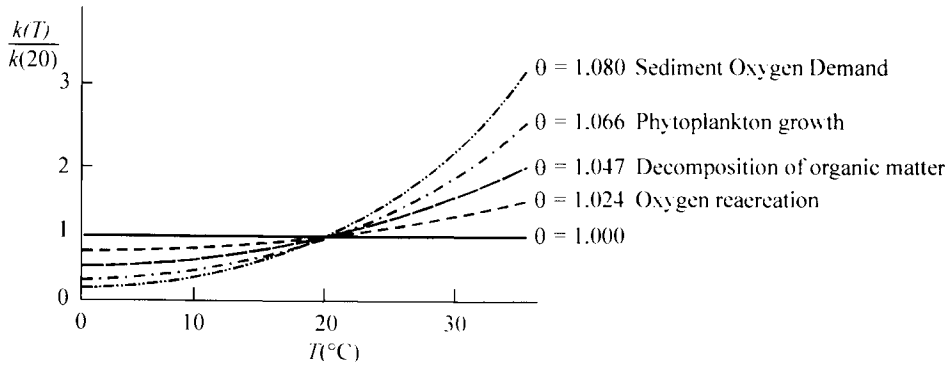

Fig. 3.25. Values of k at different temperatures for some reactions of ecological interest.

Enzymatic Reactions

Many chemical reactions of biological interest are catalysed by an enzyme. An enzyme often consists of complex proteic molecules formed by peptidic chains.

The fold of these chains forms an activation site where the reactants, usually called substrate in these reactions, can react with lower activation energy and transform into products.

The mechanism of an *enzymatic reaction* is represented by

$$S+E \underset{k_2}{\overset{k_1}{\longleftrightarrow}} ES^* \xrightarrow{k_3} P+E_0$$

where S indicates the substrate, P the products, E and E_0 the enzyme, ES^* the activated complex and k_i the reaction constants.

In the enzymatic reaction:

- the enzyme is not consumed and the enzyme released with the formation of the product can be reused by the substrate;
- the first reaction producing the activated complex ES^* is a reversible reaction, which implies that the velocity of the direct reaction is equal to the inverse one ($k_1 = k_2$);
- the activated complex ES^*, is an unstable substance, which implies that the second reaction is irreversible.

The kinetic equations of the enzymatic reactions are:

$$\frac{dS}{dt} = -k_1 \cdot E \cdot S + k_2 \cdot ES^*$$

$$\frac{dES^*}{dt} = k_1 \cdot E \cdot S - (k_2 + k_3) \cdot ES^*$$

$$\frac{dP}{dt} = k_3 \cdot ES^*$$

The first step of the reaction is at the steady state and we can assume that the concentration of ES^* is almost constant,

$$\frac{dES^*}{dt} \cong 0,$$

from this assumption and from the second kinetic equation we can write

$$k_1 \cdot E \cdot S - (k_2 + k_3) \cdot ES^* = 0$$

$$E \cdot S = \frac{(k_2 + k_3)}{k_1} \cdot ES^* = k_m \cdot ES^*$$

The fact that the enzyme is not consumed means that

$$E_0 = E + ES^* \text{ and } E = E_0 - ES^*$$

Substituting this result in the previous equation we have

$$(E_0 - ES^*) \cdot S = k_m \cdot ES^*$$

$$ES^* = E_0 \cdot \frac{S}{S + k_m}$$

and substituting this result in the third kinetic equation we obtain

$$\frac{dP}{dt} = k_3 \cdot E_0 \cdot \frac{S}{S + k_m}$$

because

$$\frac{dP}{dt} = -\frac{dS}{dt}$$

the kinetic of the enzymatic reaction is usually written

$$-\frac{dS}{dt} = \mu(S) = \mu_{max} \frac{S}{S + k_m}$$

and called the *Michaelis–Menten kinetic equation*.

$\mu(S)$ is a function of the substrate S, where μ_{max} represents the maximum velocity of the reaction and k_m is related to the enzyme.

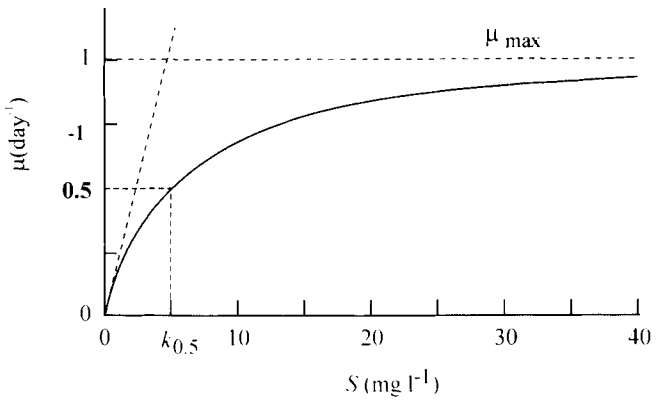

Fig. 3.26. Plot of the Michaelis–Menten kinetic.

The plot of the Michaelis–Menten kinetic equation is shown in Fig. 3.26 at different values of the substrate.

When the substrate is abundant ($S \to +\infty$) the function is asymptotically tending to μ_{max} and the kinetic is a zero-order one whose velocity is maximum and does not depend on the quantity of S.

When the substrate is not abundant ($S \to 0$), the kinetic is almost a first-order one and

$$-\frac{dS}{dt} = \frac{\mu_{max}}{k_s}$$

when $S = k_s$, the velocity of the kinetic is half of the maximum velocity reached at the saturation; for this reason k_s is also said to be the "semi-saturation constant".

If we write the Michaelis–Menten equation in this form:

$$\frac{1}{\mu(S)} = \frac{1}{\mu_{max}} + \frac{k_s}{\mu_{max}} \cdot \frac{1}{S}$$

we obtain a linear form of it that is easier to plot.

Sometimes, reactions of biological interest may contemporaneously depend on more than one substrate; this is the typical case of the photosynthesis reaction depending on the nutrients, nitrogen and phosphorus. Such a multiple dependence can be written:

$$\mu(S_1, S_2, \ldots, S_n) = \mu_{max} \cdot \left(\frac{S_1}{S_1 + k_1} \cdot \frac{S_2}{S_2 + k_2} \cdot \ldots \cdot \frac{S_n}{S_n + k_n} \right)$$

The global velocity of the reaction depends on the scarcest substrate; this fact is usually called *Liebig's law* of limiting factor.

3B.2 Chemical Equilibrium

Many processes in ecological systems can be modelled by a kinetic equation, but the time to complete the chemical reaction ranges from 3 to 10 times a semi-reaction time, $t_{1/2}$, and such a time is much lower than the usual time step used to model the ecosystem process. Many of the ecological models deal with the final steady-state equilibrium of the system and the equilibrium of the reactions becomes more important than the kinetic itself. If we assume that chemical reactions of ecological interest occur in diluted solution, the concentration of the substances provides an adequate approximation of their activities and the reaction at the equilibrium can be written

$$a[\mathrm{A}] + b[\mathrm{B}] \leftrightarrow c[\mathrm{C}] + d[\mathrm{D}]$$

The rates r_d and r_i of the direct and inverse reactions are

$$r_d = k_d[\mathrm{A}]^a[\mathrm{B}]^b = k_i[\mathrm{C}]^c[\mathrm{D}]^d = r_i$$

The equilibrium constant K can be defined as

$$K = k_d/k_i = [\mathrm{C}]^c[\mathrm{D}]^d/[\mathrm{A}]^a[\mathrm{B}]^b$$

The equilibrium constant of a reaction depends on the pressure and temperature.

Reactions of environmental interest usually occur at an atmospheric pressure that is not so variable as to induce strong variations in the values of the equilibrium constant. On the contrary, the temperature of the environment can vary in a broad range and models have to account for the effects of such a variation on the equilibrium of the reaction.

From thermodynamics we know that:

$$\ln K(T) = \frac{-\Delta G^0(T)}{R \cdot T}$$

and

$$\Delta G^0(T) = \Delta H^0(T) - T\Delta S^0(T)$$

where K is the equilibrium constant; T is the absolute temperature; G^0 is the standard free energy of the reaction; R is the gas constant; H^0 is the standard enthalpy; S^0 is the standard entropy.

In many cases ΔS^0 does not change significantly over the temperature range of interest and, as the pressure is constant, we can use the *Gibbs–Helmoltz equation*:

$$\frac{\partial}{\partial T}\left(\frac{\Delta G^0(T)}{T}\right)_P = \frac{\partial}{\partial T}\left(\frac{-\Delta H^0(T) + T\Delta S^0(T)}{T}\right) = -\frac{\Delta H^0(T)}{T^2}$$

from this equation we get

$$\frac{\partial(\ln K(T))_p}{\partial T} = \frac{\partial}{\partial T}\left(-\frac{\Delta G^{\circ}(T)}{T}\cdot\frac{1}{R}\right)_p = \frac{1}{R}\cdot\frac{\Delta H^{\circ}(T)}{T^2}$$

Integration of this equation between T_1 and T_2 gives a function describing the dependence of k on temperature

$$\ln K(T_2) - \ln K(T_1) = \frac{1}{R}\cdot\int_{T_1}^{T_2}\frac{\Delta H^{\circ}}{T^2}\,\mathrm{d}T$$

Provided that the change in molecular heat capacity ($\Delta c_p(T)$), between reactants and products are evident:

$$\Delta H^{\circ}(T) = \int_{T_1}^{T_2} n\Delta c_p(T)\mathrm{d}T$$

and the dependence on temperature of the equilibrium constant can be calculated by c_p tables available in chemical and physical handbooks.

An important application of this equilibrium constant is connected with the ionic equilibrium for water dissociation

$$H_2O \leftrightarrow H^+ + OH^-$$

The equilibrium constant is

$$K = [H^+]\,[OH^-]/[H_2O]$$

The concentration of water $[H_2O]$ in a diluted aqueous solution is much greater than the ion ones. It may be assumed at constant level because it is decreased by a very small quantity by the ionization, consequently the ionic product of water K_w can be defined

$$K_w = [H^+]\,[OH^-]$$

and its value at 25°C is equal to 10^{-14}. This means that the concentration of the ion H^+ is 10^{-7}. In chemistry the concentration of H^+ is very important and a special function of it is defined as

$$pH = -\log_{10}[H^+]$$

pH is short for the French words "puissance d'Hydrogene" (power of intensity of hydrogen). pH is used to distinguish acid solutions, pH < 7, from basic ones, pH > 7. The pH of pure water and neutral solutions is 7.

The chemical equilibrium constant is also of importance for environmental reasons because it explains the availability of metal ions in aquatic environments, which could be harmful for biota.

Metals are usually bound to some ligand Y, in solid form in the sediment; if a ligand L in liquid form, exists in the interstitial water (pore water), the following chemical equilibria occur:

$$MeY_{(s)} + L_{(l)} \leftrightarrow MeL_{(l)} + Y_{(s)} \tag{3.27}$$

$$MeL^{(n-m)+}{}_{(l)} \leftrightarrow Me^{n+} + L^{m-} \tag{3.28}$$

Given the values of equilibrium for the two reaction constants, if the concentrations of reactants are known, it is possible to calculate the concentration of free metal ion, Me^{n+}, which is of great interest for environmental purposes.

The former two reactions show that ligand availability (in liquid form) increases the solubility of the metal in complex form $MeL_{(l)}$ and regulates the free ion metal availability.

Provided that electrons donors are present in water ($L^{m-} = me^-$), a change in the oxidation number of metal can occur with the consequent change in the free ion metal toxicity.

The most common coordination number for metals of environmental interest are shown in Table 3.4. It is important to note that only even coordination numbers are more frequently present.

The ligand concentrations in pore-seawater have an almost constant value, as shown in Table 3.5. Unfortunately, the concentration of ligands in freshwater is much more variable than that in seawater and depends on pollution; organic ligands are usually more concentrated in freshwater than in seawater.

As a consequence of this, free ion metal concentration in freshwater is usually higher than in seawater.

Humic acid and fulvic acid play an important role in the availability of metals, especially in freshwater because of their high bonding capacity (200–600 meq/100 g humic acid). It has been estimated that approximately two thirds of their bonding capacity are available for complexation (Rashid and King, 1971).

In the environment, the availability of metal ion compared with the total quantity of metal is important because the ionized form affects the concentration of metals in the biota.

Table 3.4. Coordination numbers of some ions of environmental interest

Cu^+	2	Fe^{3+}	4, 6
Ag^+	2	Cu^{2+}	4, 6
Hg_2^{2+}	2, 4	Ni^{2+}	4, 6
Li^+	4	Hg^{2+}	2, 4
Be^{2+}	4, 6	Fe^{2+}	6
Al^{3+}	4, 6	Mn^{2+}	4, 6

Table 3.5. Molar concentration (M) of some ligands in interstitial sea-water (reducing conditions)

Ligand	Concentration	Ligand	Concentration
Total soluble carbonate	$8 \cdot 10^{-3}$	Glutamic acid	$1.09 \cdot 10^{-6}$
Total soluble borate	$6 \cdot 10^{-4}$	Glycerine	$4 \cdot 10^{-6}$
Total soluble silicate	$5 \cdot 10^{-4}$	Glycolic acid	$7.9 \cdot 10^{-6}$
Ammonia	$4 \cdot 10^{-4}$	Histidine	$2.58 \cdot 10^{-7}$
Nitrite	$7 \cdot 10^{-7}$	p–Hydroxybenzoic acid	$4.35 \cdot 10^{-7}$
Nitrate	$1.4 \cdot 10^{-6}$	Hydroxyproline	$3.05 \cdot 10^{-7}$
Orthophosphate	$2.5 \cdot 10^{-5}$	Lactic acid	$1.11 \cdot 10^{-7}$
Sulphide	$5 \cdot 10^{-4}$	Leucine	$7.63 \cdot 10^{-7}$
Sulphate	$2.8 \cdot 10^{-2}$	Lysine	$6.85 \cdot 10^{-7}$
Fluoride	$8 \cdot 10^{-4}$	Malic acid	$1.49 \cdot 10^{-5}$
Chloride	0.5	Methionine	$1.34 \cdot 10^{-7}$
Bromide	$8 \cdot 10^{-4}$	Ornithine	$8.47 \cdot 10^{-7}$
Iodide	$5 \cdot 10^{-7}$	Proline	$1.74 \cdot 10^{-7}$
Acetic acid	$2 \cdot 10^{-4}$	Serine	$1.9 \cdot 10^{-6}$
Alanine	$1.12 \cdot 10^{-6}$	Threonine	$8.4 \cdot 10^{-7}$
Arginine	$1.15 \cdot 10^{-7}$	Tryptophan	$9.8 \cdot 10^{-8}$
Aspartic acid	$1.2 \cdot 10^{-6}$	Tyrosine	$5.24 \cdot 10^{-7}$
Citric acid	$1.04 \cdot 10^{-6}$	Valine	$5.13 \cdot 10^{-7}$

$MeY_{(s)}$ in reaction (3.27) is in equilibrium with the ionic form of Me^{n+} of reaction (3.28) and Y^{p-} and

$$p\ Me^{n+} + n\ Y^{p-} = Me_pY_n$$

Given the solubility product of the compound Me_pY_n

$$S = [Y^{p-}]^n \cdot [Me^{n+}]^p$$

and the concentration $[Y^{p-}]$, the rate $\beta_{Me} = [Me^{n+}]/[Me_{tot}]$, can be calculated by

$$\beta_{Me} = \frac{\sqrt[p]{\frac{S}{[Y^{p-}]^n}}}{[Me_{tot}]}$$

In the same way, once the metal is in ionized form, it can be complexed by a ligand according to equilibrium (3.28). The availability of L^{m-} is a consequence of other equilibria

$$L^{m-} + H^+ \rightarrow HL^{(m-1)-};\ HL^{(m-1)-} + H^+ \rightarrow H_2L^{(m-2)-}...$$

between the compounds that the ligand can form with H^+, $H_xL^{(m-x)-}$, and the ionized form of the ligand and H^+.

The rate $\beta_L = [L^{m-}]/[L_{tot}]$, is of environmental interest and can be calculated, provided that the equilibrium constant of the previous ionization step of $H_xL^{(m-x)-}$ are known and also the total concentration of the ligand.

3B.3 Hydrolysis

The term *hydrolysis* covers processes which proceed with water, hydrogen ions and hydroxide ions, and result in the introduction of a hydroxyl group OH^- in the structure of the compound. Hydrolysis may give rise to the solubility of metal ions as for the case of Al^{3+} in the reaction to form hydrate of Al:

$$Al(OH)_3 + 3H^+ + nH_2O \rightarrow Al(H_2O)_{n+3}^{3+}$$

or to the formation of insoluble compounds, often hydroxides, as for Fe in the reaction forming $Fe(OH)_3$, which is very insoluble and precipitate to the sediments

$$Fe^{3+} + 3H_2O \rightarrow Fe(OH)_{3(s)} + 3H^+$$

The increased solubility of heavy metals with decreasing pH due to formation of metal-aqua-ions has great environmental interest. As pH decreases as a result of acidic precipitation in areas with low pH buffer capacities, the toxic effect of metal ions is increased significantly.

As an example of these relations, Fig. 3.27 illustrates the aluminium concentration in clear-water lakes in Sweden and Norway as a function of pH, in consequence of acid precipitation that supports the reaction.

Metal ions are able to form a number of species as a result of hydrolysis such as aqua-, hydroxo-, hydroxo-oxo- and oxo-complexes. This implies that multivalent metal ions are able to participate in a series of consecutive proton transfers:

$$Fe(H_2O)_6^{3+} = Fe(H_2O)_5OH^{2+} + H^+ = Fe(H_2O)_4(OH)_2^+ + 2H^+$$
$$Fe(OH)_3(H_2O)_{3(s)} + 3H^+ = Fe(OH)_4(H_2O)_{2(s)}^- + 4H^+$$

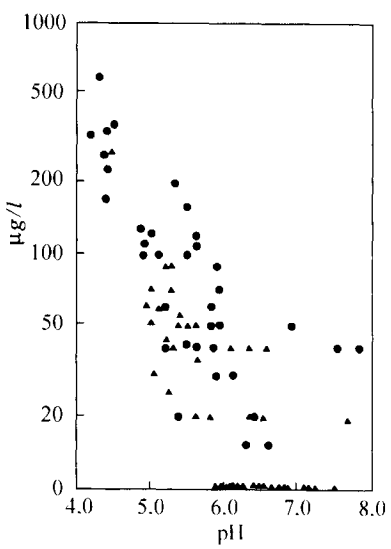

Fig. 3.27. Aluminium concentration in clear-water lakes in Sweden and Norway as function of pH (Jorgensen and Johnson, 1989).

Hydrolysis of inorganic compounds is of major environmental interest; however, hydrolysis of organic compounds in the aquatic environment is of equal interest. Organic pollutants can undergo reactions with water, resulting in the introduction of a hydroxyl group, OH^-, into the chemical structure:

$$RX + H_2O = ROH + HX$$
$$RCOX + H_2O = RCOOH + HX$$

Hydrolysis reactions are catalysed by oxonium and/or hydroxyl ions, which implies that the rate of hydrolysis, $d[A]/dt$ of a certain chemical compound A, is given by the equation:

$$\frac{d[A]}{dt} = k_H \cdot [A] = k_A \cdot [H^+] \cdot [A] + k_B \cdot [OH^-] \cdot [A] + k_N \cdot [H_2O] \cdot [A] \qquad (3.29)$$

where k_H is a pseudo first-order rate constant at a given pH, while k_A and k_B are second-order rate constants, because the reaction depends on the concentration of two reactants, $[H^+]$ and [A], or $[OH^-]$ and [A]. k_N is the second-order rate constant for neutral reaction of a chemical compound with water, which may be expressed as a pseudo first-order rate constant. Equation (3.29) indicates that the rate of hydrolysis is strongly dependent on pH, unless k_A and k_B are equal to zero.

The mechanisms of hydrolysis, including predictive test methods to estimate kinetic rates of hydrolysis of various compounds, have been studied by Mabey et al. (1978), Wolfe et al. (1978) and Tinsley (1979). Table 3.6 gives some examples of hydrolysis rates of some halogenated compounds.

Given the long half-time of some of these reactions, compared with environmental processes and usual ecological model time steps, hydrolysis of organic compounds can require a dynamic model, instead of the steady-state approach typical of the chemical equilibria.

3B.4 Redox

Many inorganic ions are dominant participants in environmental *redox processes* and Table 3.7 shows the equilibrium constant and the standard electrode potential of pertinent redox processes in aquatic conditions for some of these ions.

It is obviously of importance to describe in which chemical species various inorganic components can be found in aquatic environments under different conditions of availability of protons and electrons that can shift the equilibrium of the reaction.

This can be done in a simple, graphical representation using pe–pH diagrams like that for Fe in Fig. 3.28; pe is a parallel to the pH definition (dealing with protons), and it is defined as the negative logarithm of the relative electron activity:

$$pe = -\log(e).$$

Table 3.6. Hydrolysis rates and $t_{1/2}$ at 25°C and pH = 7 of some halogenated compounds

Compound	Rate constants (1/s)			$t_{1/2}$
	k_N	k_A	k_B	
CH_3F*	$7.44 \cdot 10^{-10}$	$5.82 \cdot 10^{-14}$	$7.44 \cdot 10^{-10}$	30 yr
CH_3Cl*	$2.37 \cdot 10^{-8}$	$6.18 \cdot 10^{-13}$	$2.37 \cdot 10^{-8}$	339 days
CH_3Br*	$4.09 \cdot 10^{-7}$	$1.41 \cdot 10^{-11}$	$4.09 \cdot 10^{-7}$	20 days
CH_3I*	$7.28 \cdot 10^{-8}$	$6.47 \cdot 10^{-12}$	$7.28 \cdot 10^{-8}$	110 days
$CH_3CHClCH_3$*	$2.12 \cdot 10^{-7}$		$2.12 \cdot 10^{-7}$	38 days
$CH_3CH_2CH_2Br$*	$3.86 \cdot 10^{-6}$		$3.86 \cdot 10^{-6}$	26 days
$((CH_3)_2Cl)CCH_3$*	$3.02 \cdot 10^{-2}$		$3.02 \cdot 10^{-2}$	23 sec
CH_2Cl_2*	$3.2 \cdot 10^{-11}$	$2.3 \cdot 10^{-15}$	$3.2 \cdot 10^{-11}$	704 yr
$CHCl_3$		$6.9 \cdot 10^{-11}$		3500 yr
$CHBr_3$#		$3.2 \cdot 10^{-11}$		686 yr
CCl_4		$4.8 \cdot 10^{-7}$		7000yr (1 ppm)
$C_6H_5CH_2Cl$	$1.28 \cdot 10^{-5}$		$1.28 \cdot 10^{-5}$	15 h

*$k_A = k_N$; $k_B << k_N$
#$k_A = k_B$; $k_N << k_B$

Table 3.7. Equilibrium constants and standard electrode potential for selected redox reactions of environmental interest.

Reaction	log$K$ (25°C)	E_0 (25°C)
$Na^+ + e = Na(s)$	–46.0	–2.71
$Zn^{2+} + 2e = Zn(s)$	–26.0	–0.76
$Fe^{2+} + 2e = Fe(s)$	–15.0	–0.44
$Co^{2+} + 2e = Co(s)$	–9.5	–0.28
$V^{3+} + e = V^{2+}$	–8.8	–0.26
$2H^+ + 2e = H_2(g)$	0	0
$S(s) + 2H^+ + 2e = H_2S$	+0.47	+0.14
$Cu^{2+} + e = Cu^+$	+2.7	+0.16
$AgCl(s) + e = Ag(s) + Cl^-$	+3.7	+0.22
$Cu^{2+} + 2e = Cu(s)$	+12.0	+0.34
$Cu^+ + e = Cu(s)$	+18.0	+0.52
$Fe^{3+} + e = Fe^{2+}$	+13.1	+0.77
$Ag^+ + e = Ag(s)$	+13.5	+0.80
$Fe(OH)_3(s) + 3H^+ + e = Fe^{2+} + 3H_2O$	+18.8	+1.06
$IO_3^- + 6H^+ + 5e = {}^1/_2 I_2(s) + 3H_2O$	+104	+1.23
$MnO_2(s) + 4H^+ + 2e = Mn^{2+} + 2H_2O$	+42	+1.23
$Cl_2(g) + 2e = 2Cl^-$	+46	+1.36
$Co^{3+} + e = Co^{2+}$	+31	+1.82

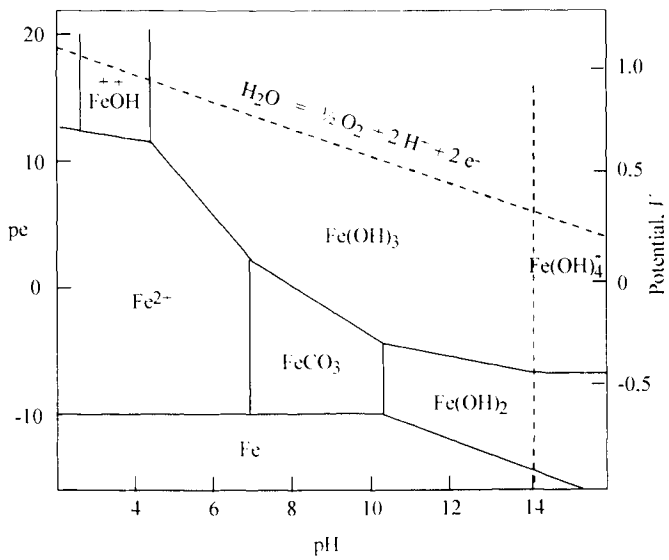

Fig. 3.28. pe–pH diagram for Fe.

There is a number of ways to calculate pe, provided that we know some relations. pe is related to E, the electrode potential, by:

$$\text{pe} = \frac{F \cdot E}{2.3 \cdot R \cdot T} \text{ and } \text{pe}^0 = \frac{F \cdot E^0}{2.3 \cdot R \cdot T}$$

where F is the symbol for the unit Faraday equal to 1 mole of electrons and 2.3 is the conversion factor between natural and decimal logarithms.

The Nernst equation states that:

$$E = E^0 + \frac{2.3 \cdot R \cdot T}{nF} \cdot \log\left(\frac{[\text{ox}]}{[\text{red}]}\right)$$

where [ox] and [red] are respectively the concentration of the oxidized and reduced forms in the reaction and n is the number of moles of electrons involved in the equilibrium, and we get

$$\text{pe} = \text{pe}^0 + \frac{1}{n} \cdot \log\left(\frac{[\text{ox}]}{[\text{red}]}\right)$$

Because $nF \cdot E = \Delta G$, pe is also a measure of the free energy, ΔG:

$$\text{pe} = -\frac{\Delta G}{n \cdot 2.3 \cdot RT} \text{ and } \text{pe}^0 = -\frac{\Delta G^0}{n \cdot 2.3 \cdot RT}$$

If ΔG and ΔG^0 refer to the half reaction written in the form of reduction, cf. Table 3.7, and because

$$\log K = -\left(\frac{\Delta G^0}{2.3 \cdot RT}\right)$$

pe is related to the equilibrium constant as follows

$$\text{pe} = \frac{\log K}{n}$$

The use of these equations can be illustrated by the following example:

$$Fe^{3+} + e = Fe^{2+}$$

For this process from Table 3.7, we have: $E^0 = 0.77$ and, at 25°C,

$$\log K = 13.2;$$

$$\text{pe}^0 = \frac{F \cdot 0.77}{2.3 \cdot R \cdot 298},$$

and because $\frac{F}{2.3 \cdot R \cdot T} = \frac{1}{0.059}$

$$\text{pe}^0 = 1 \cdot \frac{0.77}{0.0059} = 13.1$$

An example of an application of these calculations is the pe of an acid solution with the molar concentration of $[Fe^{3+}] = 10^{-3}$ and $[Fe^{2+}] = 10^{-2}$

$$\text{pe} = \text{pe}^0 + \frac{1}{n} \cdot \log\left(\frac{[Fe^{3+}]}{[Fe^{2+}]}\right) = 13.1 + \frac{1}{1} \cdot \log(10^{-1}) = 12.1$$

The importance of redox processes in the environmental context can be illustrated by examples.

If FeS_2 (pyrite) is exposed to air, e.g. by reduced water level in mines, the following processes occur:

$$2FeS_2 + 2H_2O + 7O_2 = 2FeSO_4 + 2H_2SO_4$$
$$2FeSO_4 + \tfrac{1}{2}O_2 + H_2SO_4 = Fe_2(SO_4)_3 + H_2O$$
$$Fe_2(SO_4)_3 + 6H_2O = Fe(OH)_3(s) + 3H_2SO_4$$
$$2FeS_2 + 7H_2O + 7.5O_2 = Fe(OH)_3 + 8H^+ + 4SO_4^{2-}$$

As will be seen, the formation of considerable amounts of sulphuric acid occurs, resulting in extremely low pH values, which in many cases have caused great damage to the environment.

Another example is related to the release of phosphorus from sediments in aquatic ecosystems as a consequence of eutrophication. Phosphorus in sediments is usually bound as iron(III)phosphates, but if the conditions are changed from aerobic to anaerobic, because of anoxia caused by eutrophication, the following process will occur:

$$FePO_4(s) + HS^- + e = FeS + HPO_4^{2-}$$

with further increase of phosphate available for algal growth.

Edginton and Callender (1970) mention a third example. Lake Michigan has ferromanganese nodules, which contain unexpectedly large concentrations of arsenic (up to 345 ppm, but averaging 108 ppm). Under aerobic conditions, the nodules are stable, but under anaerobic conditions arsenic will be released. As arsenic is highly toxic to mammals and also carcinogenic, it is obviously of great importance to formulate the redox processes in the Lake Michigan sediment to provide predictions for the release of arsenic.

All organic matter will suffer oxidation if present in an aerobic environment for a sufficiently long time. If reduced material is sufficiently abundant, the oxygen dissolved in interstitial water or at the sediment–water interface of aquatic ecosystems will be exhausted. Oxidation of organic matter, however, will continue by denitrification and sulphate reduction. All these processes can, in principle, occur by pure chemical oxidation, but in general the microbiological oxidation plays a far more important role.

3B.5 Acid–Base

Acid–base reactions are of a great environmental interest, because almost all processes in the environment are dependent on pH. A few illustrative examples are included in the following list:

1. Ammonia is toxic to fish and the ratio of ammonium to ammonia is known to be dependent on pH.
2. Carbon dioxide is toxic to fish and the ratio of hydrogen carbonate to carbon dioxide is dependent on pH.
3. The fertility of fish and zooplankton eggs is highly dependent on pH.
4. All biological processes have a pH-optimum, which is usually in the range 6–8. This implies that algal growth, microbiological decomposition, nitrification and denitrification are all influenced by pH.

5. The release of heavy metals ions from soil and sediment increases very rapidly with decreasing pH. Heavy metal ions are precipitated at pH 7.5 or above.

It is therefore understandable that assessments, computations or predictions of pH and the buffer capacities are important elements in many models in environmental chemistry.

The buffer capacity β is defined as the variation of the concentration C of a species, given a variation of pH:

$$\beta = \frac{dC}{dpH}$$

pH and β are often found by using an additional submodel. The application of the double logarithmic representation of proteolytic species is recommended here, because this method is easy to use even for rather complex acid–base systems. The concentrations of proteolytic species are characterized by the total alkalinity, Alk., and pH. The total alkalinity is experimentally determined by adding an excess of a standard acid (e.g. 0.1 M), boiling off the carbon dioxide formed and titrating back to a pH of 6. During this process, all the carbonate and hydrogen carbonate are converted to carbon dioxide and volatized and all the borate is converted to boric acid. The amount of standard acid used (i.e. the acid added minus the base used for back titration) corresponds to the alkalinity, and the following equation is valid:

$$k\mathrm{Al} = [H_2BO_3^-] + 2[CO_3^-] + [BO_3^-] + ([OH^-] \cdot [H^+]),$$

where [] are the molar concentrations.

In other words, the alkalinity is the concentration of hydrogen ions that can be taken up by proteolytic species present in the sample examined.

Obviously, the higher the alkalinity, the better the solution is able to maintain a given pH value if acid is added. The buffering capacity and the alkalinity are proportional (see, e.g., Stumm and Morgan, 1970).

Each of the proteolytic species in an aquatic system has an equilibrium constant. If we consider the acid HA and the dissociation process:

$$HA \rightarrow H^+ + A^-$$

we have

$$K_a = \frac{[H^+] \cdot [A^-]}{[HA]}$$

where K_a is the equilibrium constant.

When the composition of the aquatic system is known, it is possible to calculate both the alkalinity and the buffering capacity, using the expression for the

equilibrium constants. However, these expressions are more conveniently used in logarithmic form. If we consider the expression for K_a for a weak acid, the general expression (3.30) may be used in a logarithmic form:

$$\mathrm{pH} = pK_a + \log\left(\frac{[\mathrm{A}^-]}{[\mathrm{HA}]}\right) = pK_a + \log([\mathrm{A}^-]) - \log([\mathrm{HA}]) \qquad (3.30)$$

It is often convenient to plot the concentrations of HA and A^- versus pH in a logarithmic diagram as in Fig. 3.29. If C denotes the total concentrations $C = [\mathrm{HA}] + [\mathrm{A}^-]$, we have at low pH:

$$[\mathrm{HA}] \approx C$$
$$\log[\mathrm{A}^-] = \mathrm{pH} - pK_a + \log C$$

This means that $\log[\mathrm{A}^-]$ increases linearly with increasing pH, the slope being +1. The line goes through $(\log C, pK_a)$ as $\mathrm{pH} = pK_a$ gives $\log[\mathrm{A}^-] = \log C$, see Eq. (3.30).

Correspondingly, at high pH,

$$[\mathrm{A}^-] = C \text{ and } \log[\mathrm{HA}] = pK_a - \mathrm{pH} + \log C$$

which implies that $\log[\mathrm{HA}]$ decreases with increasing pH, the slope being –1. This line also goes through $(\log C, pK_a)$.

At $\mathrm{pH} = pK_a$, $[\mathrm{A}^-] = [\mathrm{HA}] = C/2$ or $\log[\mathrm{A}^-] = \log[\mathrm{HA}] = \log C - 0.3$.

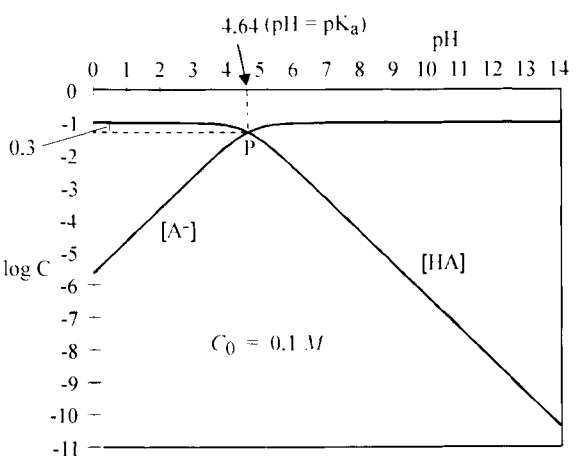

Fig. 3.29. Plot of values of the concentration of acid HA and A ion at different pH values.

3B.6 Adsorption and Ion Exchange

Adsorption is a partitioning or separation process whereby a species (adsorbate) is transferred from the dissolved phase in a fluid solution onto the surface of a solid substance (adsorbent); it is different from absorption, the process of interpenetrating within the solid of dissolved species. Adsorption may often be explained by an electrical attraction to the solid surface of components with a minor electrical charge and by minor free energy of adsorbate compared to the adsorbent one. The bonds formed are Van der Waals bonds according to the location of these sites on the surface or surface reaction between adsorbent and adsorbate. Adsorption results in the formation of a molecular layer of the adsorbate on the surface. Often an equilibrium concentration is rapidly formed on the surface and is sometimes followed by a slow diffusion into the particle of the adsorbent.

Pure adsorption is rarely observed in nature because it is usually coupled with ion exchange. Adsorption and ion exchange are significant processes in an environmental context and a description of the processes is often included in water quality modelling. Where water is in contact with suspended matter (organic or clay particles), sediment and biota, a significant transfer of matter by adsorption and ion exchange may take place.

A significant portion of pollutants of water is found in suspended matter, where the concentration of many pollutants is magnitudes higher than in water. Transport of pollutants in rivers and streams often takes place on suspended matter, either clay particles or organic matter.

Many organic compounds, including many pesticides, are adsorbed on suspended matter or sediment. Heavy metals ions are adsorbed and/or taken up by ion exchange by clay particles, which are often found to be major components of suspended matter in river and streams.

Clay, however, is often a significant part of river and lake sediment and its iron content may often play an important role in the ability of sediment to bind phosphate. The difference between adsorption and ion exchange ability under aerobic and anaerobic conditions may often be explained by the transformation of iron oxidation stage 3 to 2.

Equilibrium of Adsorption

Adsorption and *ion exchange* are fast processes, reaching equilibrium in minutes or hours, while the selected time step of water quality models is usually days or weeks. This implies that these processes can be described by means of equilibrium equations. Nevertheless, some particular water quality models can use a shorter time step and a dynamic model of these processes is requested. For this reason this chapter will also present a rate expression of adsorption.

The rate of adsorption is controlled by the transfer of species within the adsorbent particle because diffusion through solids is naturally slower than that in fluids

due to the mechanical obstruction, therefore the process continues until a characteristic equilibrium is attained at the adsorbent surface, between the adsorbate in the fluid phase and the adsorbate in the solid and adsorbed phase. Equilibrium begins to be attained when sorption time approaches the dosage of adsorbent required to remove a given amount of adsorbate from solution.

Equilibrium is mathematically described by an isotherm, which is specific for each adsorbate/adsorbent system.

An isotherm is a mathematical expression that describes adsorption equilibrium of the adsorbate between its fluid phase in solution and adsorbed phase onto the solid surface of adsorbent. Due to the wide presence of adsorption process in industrial chemistry, many models are available in the literature for this phenomenon. For environmental purposes we can consider a simple model at steady-state conditions. A general formula to correlate adsorption equilibrium has been presented as follows (Fritz and Schlunder, 1974)

$$q_e = \frac{kC_e}{\delta + hC_e^{\beta}} \tag{3.31}$$

where q_e (mg/g) and C_e (mg/l) are the solid and dissolved phase concentrations, respectively, k (l/g) is the equilibrium constant, h (l/g) is related to the heat of adsorption, β (dimensionless) is called the heterogeneity factor related to the surface properties of the adsorbent, and δ (dimensionless) is a generalization constant.

In practice, adsorption equilibria have been described by one or more simplifications of Eq. (3.31) according to the chemical and physical properties of the particular system. These properties lead to certain equilibrium patterns. The simplifications yield well-known relations, namely the *Redlich–Peterson*, *Langmuir* and *Freundlich* isotherms.

If $\delta = 1$, Eq. (3.31) takes the form of the Redlich–Peterson isotherm

$$q_e = \frac{kC_e}{1 + hC_e^{\beta}} \tag{3.32}$$

by linearization we can write

$$\ln\left(k\frac{C_e}{q_e}\right) = \beta \ln C_e + \ln h \tag{3.33}$$

provided that a value of k is fixed according to the adsorbate/adsorbent system, by regression with experimental data the slope β and the intercept $\ln(h)$ of Eq. (3.33) can be determined.

If $\delta = \beta = 1$, Eq. (3.31) takes the form of the Langmuir isotherm

$$q_e = \frac{kC_e}{1 + hC_e} \tag{3.34}$$

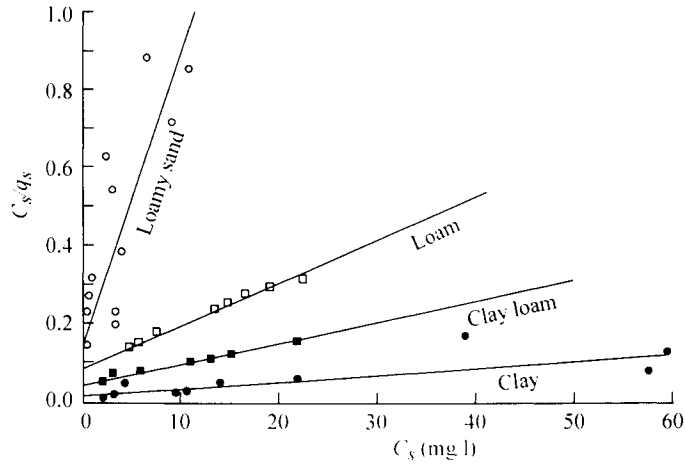

Fig. 3.30. Regression lines of Langmuir isotherms for phosphate adsorption in soils (after Novotny and Olem, 1994).

It assumes a heterogeneity factor of 1 implying an homogeneous adsorbent surface, which is a surface with identical and equally available adsorption sites that have equal energies of adsorption. It also assumes a monolayer adsorption, i.e. the adsorbent is saturated after one layer of adsorbate molecules on the surface. The ratio k/h is called the monolayer capacity.

By linearization of Eq. (3.34) we obtain

$$k(C_e/q_e) = hC_e + 1 \tag{3.35}$$

provided that a value for k is fixed according to adsorbate/adsorbent system, Eq. (3.35) gives different intercepts. An example of the application of the linear form of the Langmuir isotherm is shown in Fig. 3.30 for the adsorption of phosphate in soils with different characteristics.

If $\delta = 0$, Eq. (3.31) can be rearranged in the form

$$q_e = aC_e^{\gamma} \tag{3.36}$$

which is the well known Freundlich isotherm where $a = k/h$, the monolayer capacity, is proportional to the equilibrium constant and $\gamma = 1 - \beta$ is related to the heterogeneity factor related to the adsorbent capacity. The bigger their values the higher the adsorbent capacity (El-Dib et al., 1978; 1979). By linearization of Eq. (3.36) we get

$$\ln q_e = \gamma \ln C_e + \ln a \tag{3.37}$$

The Freundlich isotherm assumes a heterogeneous adsorbent with sorption sites that are energetically non-equivalent, i.e. sites that have different energies of ad-

Table 3.8. Freundlich constant a and γ for some compounds when adsorbed on activated carbon.

Compound	a (mg g)	γ
Aniline	25	0.322
Benzene sulphonic acid	7	0.169
Benzoic acid	7	0.237
Butanol	4.4	0.445
Butyraldehyde	3.3	0.570
Butyric acid	3.1	0.533
Chlorobenzene	40	0.406
Ethylacetate	0.6	0.833
Methyl ethyl ketone	24	0.183
Nitrobenzene	82	0.237
Phenol	24	0.271
TNT	270	0.111
Toluene	30	0.729
Vinyl chloride	0.37	1.088

sorption and that are not equally available. As an example, Table 3.8 reports the values of a and γ for some compounds on activated carbon, which is a common adsorbent used in water treatment.

Figure 3.31 compares the behaviour of the Redlich–Peterson, Langmuir and Freundlich isotherms for different values of the dissolved concentration C_s of phosphorus adsorbing on soil. The plate line of the Langmuir isotherm indicates the saturation of the single layer of adsorbate molecules, while the Freundlich isotherm is continuously growing as an effect of the possibility of adsorbing molecules with different energies. The steady-state condition of the Langmuir isotherm is reached

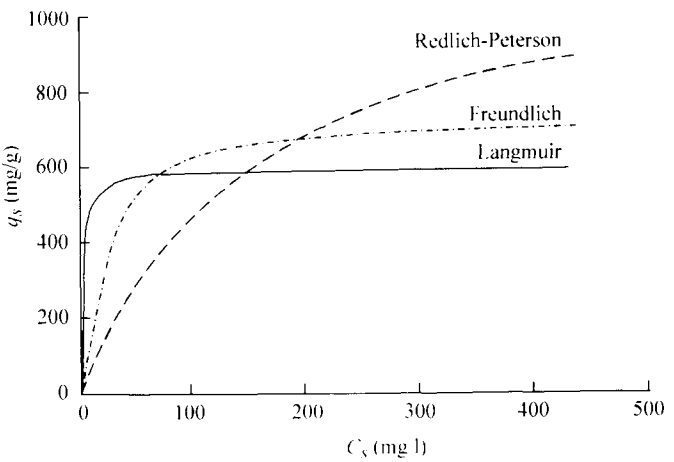

Fig. 3.31. Plot of some well known adsorption isotherms: values of the adsorbed concentration q_s versus the soluted one C_s.

when the adsorption velocity is equal to the desorption one. Compared with other environmental processes, adsorption is very fast, and the equilibrium between the solid and dissolved phase can be assumed in the models. This way a very used model for adsorption is usually written

$$q_s = kC_s$$

and k is called partition coefficient.

Partition of Ionic Organic Compounds

Many scientists have investigated the relation between the partition coefficient k and the properties of the chemical. And at least for the non-ionic organic chemicals, Karickoff et al. (1982) have discovered that it is a function of organic carbon content of the solid phase

$$k = f_{oc} k_{oc}$$

where f_{oc} is the weight fraction of total carbon in solid matter ($gC\ g^{-1}$) and k_{oc} is the organic carbon *partition coefficient* [$(mg\ gC^{-1})/(mg\ m^{-3})$]; in turn, k_{oc} can be estimated in terms of the contaminant's octanol–water partition coefficient k_{ow} [$(mg\ m^{-3}_{octanol})/(mg\ m^{-3}_{water})$]

$$k_{oc} = 6.17\ 10^{-7}\ k_{ow}$$

k_{ow} can be easily found in tables describing the characteristics of several substances or computed in terms of solubility in ($\mu moles\ l^{-1}$) S'_w, or in terms of solubility S_w ($mg\ l^{-1}$) of a given substance of molar weight M

$$\log k_{ow} = 5.00 - 0.670 \log S'_w = 5.00 - 0.670 \log(S_w/(M\ 10^{-3})).$$

The fraction of organic carbon in the solid phase, f_{oc}, is a key parameter of the model and has to be carefully estimated in aquatic systems with large amounts of autochthonous solid. This solid concentration can be of inorganic origin by resuspension but also of organic origin as a result of the decay of organic biomass, as usual in eutrophic water bodies. Such a case, Dissolved Organic Carbon (DOC), has to be considered as a third phase of adsorbing matter in addition to Particulate Organic Carbon (POC). Usually this third phase adsorbs toxicants more easily than POC and subtracts the substance to the sedimentation and volatilization processes and to the concentration in the pore water of the sediments. Adsorption onto DOC decreases the free substance concentration in the water and increases the feedback effect of sediment release to the water.

Figure 3.32 describes the partition in particulate and dissolved phases of organic toxicants as a function of their log k_{ow} and for different suspended solid con-

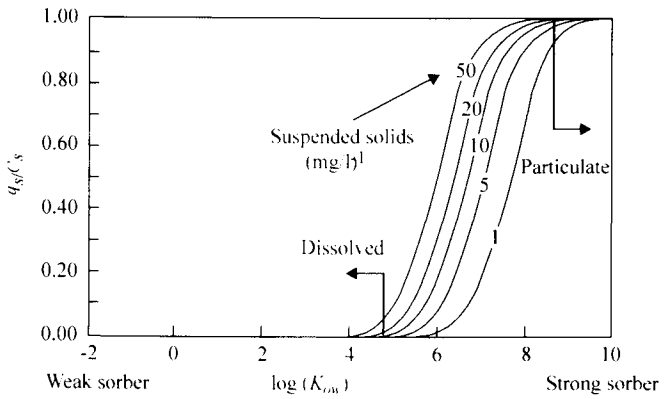

Fig. 3.32. Fraction (q_s/C_s) of a substance adsorbed on particulate matter as function of log(K_{ow}) at different suspended solids concentration.

Table 3.9. Range and average values of log k_{ow} for some organic toxicants.

Substance	log K_{ow}	
	Range	Average
PCB	3.30–6.53	5.60
Phthalate ethers	1.60–9.33	5.50
PAHs	2.67–7.73	5.50
Pesticides	0.53–6.93	3.60
α endosulfan	1.73	
β endosulfan	1.47	
Endosulfan sulphate	1.07	
MAHs	1.60–4.14	3.07
Hexachlorobenzene	6.27	
Phenols	0.93–3.60	2.14
Pentachlorophenol	5.6	
Nitrosamines	0.14–3.33	2.14
Alogenated aliphatics	0.93–2.80	2.00
Hexachloroethane	4.14	
Hexachlorobutadiene	4.80	
Hexachlorocyclopentadiene	5.07	
Ethers	0.14–5.07	1.60

centrations. Average values and ranges of log k_{ow} for some organic toxicants are reported in Table 3.9. According to the theory just presented, if the water body is eutrophic, the concentration of suspended solid would be substituted by the POC and DOC to have a better description of the partition.

Dynamics of Adsorption

The *adsorption rate* can be limited by diffusion in the fluid or inside in the solid phase, or by a combination of the two limitations. The first one controls the transfer of solute from the water to the boundary layer of fluid immediately adjacent to the external surface of the adsorbent and it is governed by molecular diffusion and by the eddy diffusion. The velocity of adsorption can be described by the following model

$$\frac{\partial C_s}{\partial t} = k_c (C_s - C_{s,eq})$$

where C_s and $C_{s,eq}$ are the actual concentration of the adsorbate in the fluid and that at the equilibrium between the two solute and adsorbed phases, respectively, and k_c is the external mass transfer coefficient.

The internal diffusion is modelled in a similar manner by

$$\frac{\partial q_s}{\partial t} = k_i \sigma \cdot (q_s - q_{s,eq})$$

where σ is the interparticle void ratio (porosity of adsorbent), and q_s and $q_{s,eq}$ are, respectively, the actual concentration of adsorbate in the solid phase and the concentration of adsorbate in the solid phase that is assumed to be in equilibrium with the coexisting liquid phase at concentration C_s, and k_i is the internal mass transfer coefficient.

The global mass transfer coefficient, as previously seen for the two film model, can be written

$$1/k = 1/k_c + 1/(k_i \sigma)$$

and the global dynamic model for adsorption is

$$\frac{\partial C_s}{\partial t} = k(C_s - q_s)$$

Equilibrium is reached when $C_s = q_s$, which means that for a particle of adsorbate leaving the solution to the adsorbent another one will be released from adsorbent to the solution.

Ion Exchange

Ion exchange is an exchange of ions between a liquid and a solid phase (matrix). The exchange takes place because the chemical energy at equilibrium after the exchange is lower than before. If a pure ion exchange process takes place, the number of ions released is equivalent to the number of ions taken up by the process.

Ion exchange is known to occur with a number of natural solids, such as soil, humus, metallic minerals and clay. Clay and, in some instances, other natural materials can even be used for ion exchange demineralization of drinking water.

The exchange reaction between ions in solution and ions attached to the matrix is generally reversible. The exchange can be treated as a simple stoichiometric reaction.

For cation exchange the equation is:

$$A^{n+} + n(R^-)B^+ = nB^+ + (R^-)_nA^{n+} \tag{3.38}$$

The ion exchange reaction is selective, so that the ions attached to the matrix will have a preference for one counter ion over another. Therefore the concentrations of different counter ions in the ion exchange will be different from the corresponding concentration ratio in the solution.

According to the law of mass action, the equilibrium relationship for reaction (3.38) will give for diluted solutions:

$$K_{AB} = \frac{[B]^n \cdot [(R^-)_n A^{n-}]}{[A] \cdot [RB]^n}$$

The *selectivity coefficient*, K_{AB}, is not actually constant, but is dependent upon experimental conditions. The plot in Fig. 3.33 is often used to illustrate the preference of an ion exchanger for a particular ion. As can be seen, the percentage in the matrix is plotted against the percentage in solution.

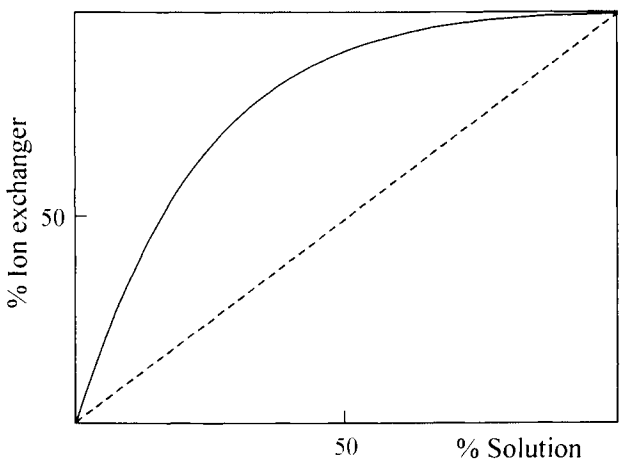

Fig. 3.33. Equilibrium plot between % of ions in solution and % in matrix. The dotted line indicates the case when the matrix has the same preference for the two competing ions.

A selectivity coefficient of 50% in solution is often used, and called $a_{50\%}$ when activities are considered. If we use concentration, when $n = 1$ in reaction (3.38)

$$[B] = [A];$$

and for low concentration of solute

$$a_{50\%} = K_{AB,50\%} = \frac{[RA]^-}{[RB]^-}$$

The plot in Fig. 3.33 can be used to read $a_{50\%}$.

The selectivity of the ion exchange material for the exchange of ions is dependent upon the ionic charge and the ionic size. An ion exchanger generally prefers counter ions of high valence. Thus, for a series of typical anions of interest, one would expect the following order of selectivity:

$$PO_4^{3-} > SO_4^{2-} > Cl^-.$$

Similarly for a series of cations:

$$Al^{3+} > Ca^{2+} > Na^+.$$

3B.7 Volatilization

From the two film theory we are able to calculate the transfer velocity of a substance from water to air and we can also do the same for turbulent flow accounting for a renewal time of water at the interface. The *volatilization model* can be transformed into a mass balance equation multiplying the flux by surface area to give

$$V\frac{dC_l}{dt} = vA_s\left(\frac{P_g}{He} - C_l\right)$$

where v is the velocity of volatilization and the other symbols take the usual meaning explained in the two film theory.

This general equation can be adapted according to the characteristics of the dissolved substance. If the gas is abundant in air as for nitrogen and oxygen the concentration of saturation in water will be accounted for. Otherwise, as for the case of toxicants, the partial pressure of the substance is negligible and the mass balance will be

$$V\frac{dC_l}{dt} = -vA_s C_l$$

The problem turns on estimating v, the formula for which is

$$v = \frac{K_l He}{He + RT\frac{K_l}{K_g}}$$

In other words, we have to estimate the Henry constant and the transfer coefficients for each single substance. For many toxic substances it is possible to find *He* in the specialized chemical literature and the transfer coefficients can also be estimated given the molar weight *M* of the substance

$$K_l = K_{l,O2}\,(32/M)^{1/4}, \quad K_g = 168\,u_w\,(18/M)^{1/4}$$

where u_w is the wind speed at the water surface in (m/s). With these definitions the coefficients K_l and K_g are expressed in (m/year).

Table 3.10. Range and average values of log *He* for different substances of environmental interest.

Substance	log *He*	
	Range	Average
Halogenated aliphatics	−3.41 – 0.29	−2.00
MAHs	−4.94 to −2.23	−2.70
PCBs	−5.06 to −2.82	−3.29
*Aroclor	−0.40	
Ethers	−6.70 to −3.76	−4.00
Pesticides	−8.94 to −2.82	−4.94
*Toxaphene	−0.71	
Dieldrin	−6.96 to −4.96	
Lindane	−5.50 to −6.45	
Aldrin	−4.92 to −4.56	
DDT	−4.45	
PAHs	−7.18 to −2.82	−5.29
Phenols	−6.53 to −4.47	−5.76
*2,4-Dinitrophenol	−9.29	
Nitrosamines	−8.59 to −3.29	−5.76
Phthalate esters	−6.82 to −4.59	−5.75
Methane (CH_4)	0.19	
Oxygen (O_2)	−0.11	
Nitrogen (N_2)	−0.16	
Carbon dioxide (CO_2)	−1.57	
Hydrogen sulphide (H_2S)	−2.03	
Sulphur dioxide (SO_2)	−3.16	
Ammonia (NH_3)	−4.86	

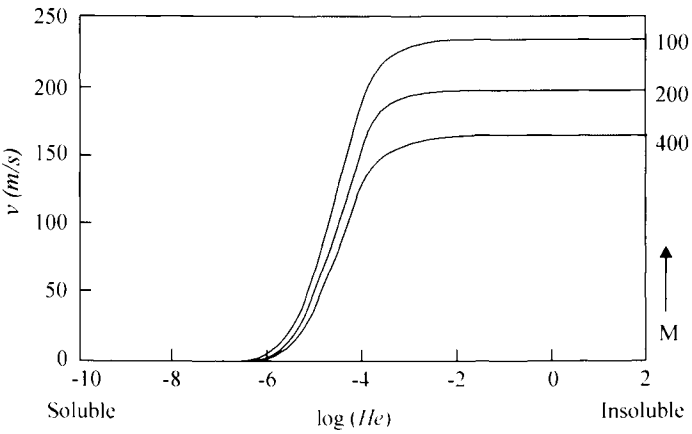

Fig. 3.34. Volatilization velocity at given molar weights and for a wind speed of 5 m/s as a function of log(*He*). Values of log(*He*) are reported in Table 3.10.

A simple idea of the volatilization velocity can be gained from Fig. 3.34 which presents the volatilization velocity at a given molar weight for different organic non-ionic substances in a log scale of *He*. The values are reported in Table 3.10. For a full list of *He* values for substances of importance in environmental chemistry, see http://www.mpch-mainz.mpg.de/~sander/res/henry.html

Part C. Biological Processes

Part 3 of this chapter deals with some complex processes of great interest for ecological modelling and includes a description of the modelling techniques of:

- biogeochemical cycles of the most important elements of an ecosystem;
- photosynthesis, because it is the process that accounts for the primary production which is at the basis of any ecosystem;
- growth of a single population of primary, secondary producers and of individuals.

Single and simple processes involved in these more complex processes are not always strictly biological because they also involve physical and chemical processes. We have included them in this part because they are usually strongly connected to those biological processes that cannot be listed under the previous parts.

3C.1 Biogeochemical Cycles in Aquatic Environments

The cycle of any chemical element in nature can pass through different macro-compartments of the ecosystem and change its chemical form, assuming an inorganic but also an organic form when it belongs to living individuals of the biotic compartment.

The *biogeochemical cycles* of macro constituents of organic matter, and in particular of nutrients such as carbon, oxygen, nitrogen, phosphorus and silicate, are of great interest for ecosystem modelling.

Usually, the cycles of nutrients are modelled calculating a mass balance of the single element appearing in different forms and flowing through different compartments.

For aquatic ecosystems a general figure of a minimum cycle is shown in Fig. 3.35; it includes the compartment of dissolved inorganic forms of nutrients, that of the organic forms, those of primary and secondary producers and finally the compartment of the storage of these elements in soil, water or air. Arrows in the figure indicate some of the processes that move a nutrient from one compartment to another.

Each nutrient listed has a typical cycle in which only some of the processes and some of the forms just shown become important.

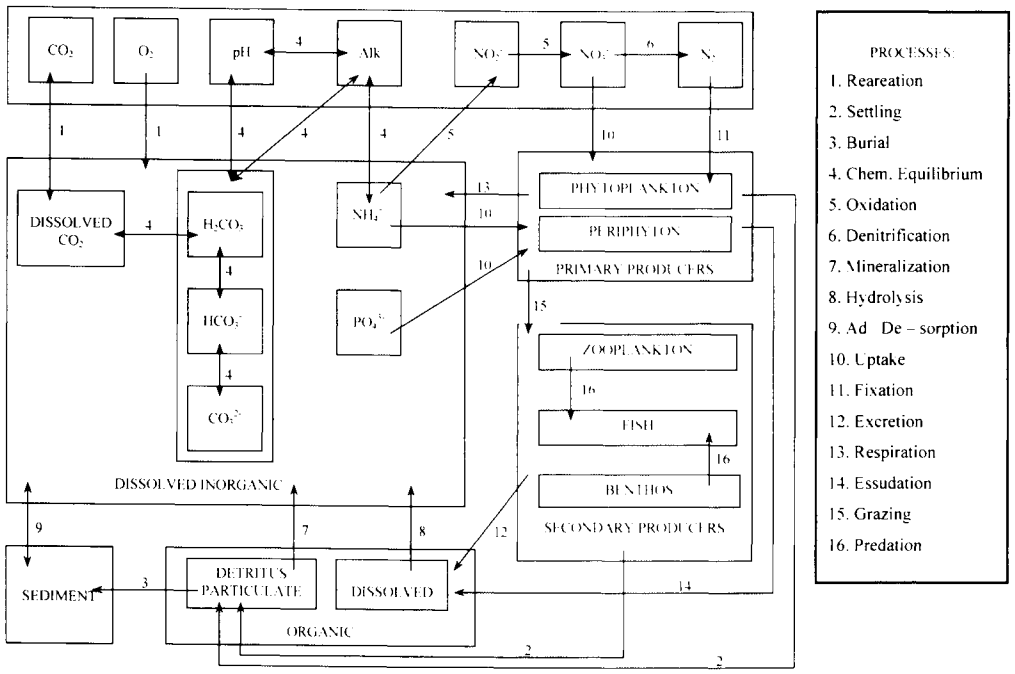

Fig. 3.35. General biogeochemical cycle of nutrients in an aquatic environment. Compartments are indicated by boxes. Arrows show some of the processes moving nutrients that are listed in the compartments.

For each of the macro-compartments, is possible to set up a model of the mass balance according to the equation:

$$\frac{dC}{dt} = \sum_i f_i$$

where C is the concentration of a nutrient in a given compartment, t is the time, and f_i are the input/output flows representing the processes shown in Fig. 3.35.

Some of these processes have been presented in previous parts of this chapter, others will be described in detail in this part. Most f_i are accounted for in modelling via a first-order decay.

Nitrogen Cycle

The nitrogen cycle is the most complex cycle of nutrients. Some processes like reaeration (the passage of N_2 from air to water) adsorption/desorption between sediment and water and settling of particulate nitrogen have been already presented in Part A: Physical Processes.

Chemical processes involving nitrogen account for *mineralization* of the organic form to the reduced inorganic form and include the decay of organic matter via ammonia transformation and hydrolysis of the dissolved ammonia. All these processes are accounted for in the model via a first-order decay:

$$C(t) = C_0 \cdot e^{-kt} \text{ and } k = k_{20} \cdot \theta^{(T-20)} \tag{3.39}$$

The values for k_{20} and θ used in the models for single reaction are listed in Table 3.11.

The equilibrium between NH_3 and ammonium ion NH^+_4 in the water depends on pH. NH_3 at high concentrations can be toxic for biota. Oxidation of ammonium NH^+_4 to nitrate, NO^-_3, is a two-step process using oxygen dissolved in the water. The first oxidation to nitrite, NO^-_2, involves *Nitrosomonas bacteria* which it is very slow compared to the second one which transforms NO^-_2 to NO^-_3 and involves *Nitrobacter bacteria*.

This difference in the velocities is the reason why the usual concentration of nitrite in surface water is lower than the nitrate one.

Different ranges of the k_{20} values for the two oxidation processes account for the reason why the first oxidation is the limiting step in the nitrogen cycle. Further chemical transformation of nitrate to nitrogen gas N_2 is a chemical reduction obtained by other bacteria in an anoxic environment. *Denitrification* is the only important way of removing nitrogen from water and of reducing the nutrient used for algal growth. This last process produces a minor quantity of NO_2, usually not considered in this cycle, but potentially harmful for the environment as a greenhouse-effect gas.

If suitable reducing conditions are coupled with the oxic conditions, denitrification can occur at a velocity comparable with the slower transformation step one, with a range of k_{20} values comparable with those of the limiting oxidation step. This means that denitrification is controlling the removal of mineralized nitrogen from water and justifies the usual large presence of nitrate in the water.

The values of k_{20} for mineralization of organic nitrogen to ammonium are one order of magnitude lower than the other chemical transformations of the nitrogen cycle. This justifies the fact that the pool of organic nitrogen is very high compared with that of dissolved nitrogen in the water and confirms the fact that mineralization is the real limiting process of the global nitrogen cycle.

Table 3.11. Values of k_{20} and of θ for processes of the nitrogen cycle.

Process	k_{20} (1/t)	θ
Mineralization of dissolved organic nitrogen DON → NH^+_4	0.002	1.02
Mineralization of particulate organic nitrogen PON → NH^+_4	0.01–0.03	1.02–1.08
Oxidation of ammonium to nitrite NH^+_4 → NO^-_2	0.1–0.5	1.047
Oxidation of nitrite to nitrate NO^-_2 → NO^-_3	0.5–2	1.047
Oxidation of ammonium to nitrate NH^+_4 → NO^-_3	0.1–0.2	1.08
Denitrification NO^-_3 → N_2	0.1	1.045
Release of ammonium from sediment	0.001–0.01	1.02 –1.08

A good example of these processes can be found in the wetlands where large amounts of aquatic plants settle in the wetlands to form organic detritus and a large pool of organic nitrogen. The most recalcitrant part of this organic nitrogen moves to deeper sediment and it is buried in the wetland forever. The upper layer of the sediment can exchange nitrogen with water and pore water. Anoxic conditions promote the mineralization of the most labile of organic nitrogen to ammonium ion. Aquatic plants are able to transfer through the plant, from leaves to roots, air and oxygen, forming a micro-environment around the roots where oxygen is present and sufficient to oxidize ammonium to nitrate. When nitrate is formed, it moves from the oxic micro-environment to the anoxic one and denitrification can occur. This particular environment of wetland can perform naturally the removal of nitrogen that is otherwise carried out in waste water treatment plants using sophisticated technology, thus justifying importance of wetlands for the conservation of the nitrogen cycle. A wetland model is presented in Chapter 7.

A biological process typical of the nutrient cycle is the uptake of plants: ammonium and nitrate are taken up by plants in order to grow. The molecule of ammonium passes through the cellular membrane more easily than that of nitrate because it is smaller. Consequently, during algal blooms, when a fast uptake of nutrients occurs, ammonium concentration decreases more rapidly than the nitrate one.

A dynamic model focusing on the nitrogen cycle would consider both the chemical forms (ammonium and nitrate) and could simulate the effect of the fast depletion of ammonium. In models where such a detail is not strictly required, nitrogen is accounted for without distinguishing between the chemical forms. This reduces the number of state variables and related parameters of the model and is recommended as a first approach in the dynamic simulation of aquatic ecosystems.

Nitrogen, as gas, can be taken up by some species of blue-green algae. This process is called nitrogen *fixation* and becomes important when blooms of blue-green algae occur, because it avoids the nitrogen limitation of growth. Fixation contributes to the blue-green algae growth when dissolved inorganic nitrogen is fully taken up. The uptake from aquatic pools is less energy-demanding than the transfer of N_2 from air to water and from water to the cell, and justifies the drop in inorganic dissolved nitrogen in aquatic environments, before the blue-green algae bloom.

The primary producers compartment of Fig. 3.35 interacts with the dissolved inorganic and organic one via *respiration* and *exudation*, while the secondary one interacts via *excretion*. These last three processes are usually simply accounted for in models of the nitrogen cycle and will be presented later.

Phosphorus Cycle

Phosphorus is a nutrient constituent of matter cycling through the abiotic and biotic compartment in a manner similar to that of nitrogen. The cycle of phosphorus is environmentally important because limitation of algal growth in fresh waters is often due to a lack of this element in a chemical form that can be taken up by algae.

Table 3.12. Values of k_{20} and θ for processes involved in the phosphorus cycle.

Process	k_{20} (1/t)	θ
Sediment release from organic pool Sediment → PO^{3-}_4	0.0004–0.001	1.02–1.08
Mineralization of particulate organic phosphorus POP → PO^{3-}_4	0.01–0. 1	1.02–1.14
Solution POP → DOP	0.22*	1.08
Mineralization DOP → PO^{3-}_4		

*Thomann and Fitzpatrick (1982) multiply this rate by an algal carbon limitation factor: $\frac{\text{Algae}-C}{k+\text{Algae}-C}$; where k = 10 mg C/l.

Fortunately, the chemical form of phosphorus of interest for primary producers is mostly the orthophosphate ion, PO^{3-}_4. Minor quantities of phosphorus can also be taken up directly as a second option in colloidal organic labile form and can contribute to reducing the orthophosphate limitation.

The most important processes in the phosphorus cycle are those connected with the adsorption–desorption equilibrium between phosphorus in the sediment and in the pore water, followed by the diffusion from pore water to the water column. This process has been already described previously.

In aquatic environments phosphorus is present as orthophosphate PO^{3-}_4 or as particulate organic phosphorus (POP) and dissolved organic phosphorus (DOP). Models account for the flows of this nutrient from organic to inorganic forms by the first-order kinetic. The values of k_{20} and those of θ for a single process are shown in Table 3.12. The limiting process in the cycle is clearly the release from organic pool of the sediment to the inorganic form. The velocity of this process is one to two orders of magnitude lower than the mineralization process of the dissolved organic forms.

As shown in the Table 3.13, this mineralization can be very fast (k_{20} = 0.22) but it is limited by a carbon availability (as far as for denitrification). For this reason, without considering the carbon limitation, the global effect of mineralization is usually accounted for with a k constant value one order of magnitude lower.

As for the nitrogen cycle, the biotic compartments close the cycle of phosphorus releasing the nutrient directly to the dissolved organic and inorganic pool via respiration, excretion and exudation.

Prediction of the Phosphorus Concentration in a Lake

Based on the nitrogen and phosphorus cycles, some models have been developed to predict the concentrations of nitrogen and phosphorus in lakes. This prediction is quite interesting for environmental reasons because, by applying the model, it is possible to understand the effect of an increase or decrease of nutrient loads on the trophic state of the lake.

As presented in detail in Chapter 5, Vollenweider (1968) assumed that the change in concentration of phosphorus in a lake is equal to the supply added per unit volume minus the loss through sedimentation and the loss by outflow:

$$\frac{dP}{dt} = \frac{L_{Pt} + L_{Pp} + L_{Pw}}{V} - s \cdot P - r \cdot P$$

where P represents the total phosphorus concentration (mg/l), V is the lake volume (l), L_{Pt} is the total amount of phosphorus supplied to the lake from diffuse sources (mg/y), L_{Pp} is the supply of phosphorus from precipitation (mg/y), L_{Pw} is the point sources supply of phosphorus to the lake (mg/y), s is the sedimentation rate, and r the flushing rate (y^{-1}); $r = Q/V$, where Q is the total volume of water flowing out per year (l/y).

The previous equation can be solved analytically:

$$P = \frac{L_P}{V \cdot (s+r)} + \left(P_0 - \frac{L_P}{V \cdot (s+r)} \right) \cdot e^{-(r+s)t}$$

where $L_P = L_{Pt} + L_{Pp} + L_{Pw}$.

The equations for nitrogen are parallel to those for phosphorus. The steady-state solution for phosphorus is:

$$P = \frac{L_P}{(s+r) \cdot V}$$

and for nitrogen:

$$N = \frac{L_N}{(s+r) \cdot V}$$

As can be seen, it is necessary to calculate or measure Q. In some cases the long-term average inflow, Q_{in}, can be calculated as:

$$Q_{in} = A_1 \cdot \sum p \cdot (1 - k')$$

where k' is the ratio of evapotranspiration to precipitation (p); k' is often known for a given geographical area, and Q can be found on the basis of a water balance, and A is the lake surface:

$$Q = Q_{in} + A \cdot p + A_S \cdot E_V$$

where E_V represents the evaporation ($mm/y \cdot m^2$). The only alternative to these calculations is to measure Q or Q_{in}.

It is rather difficult to determine the sedimentation rate s, although, for deep lakes, where resuspension is negligible, it can be done by sediment traps. However, an alternative retention coefficient, R (equal to the fraction of the loading that is not lost by the outflow) may be used. Dillon and Kirchner (1975) determined by multiple regression analysis that coefficient R was highly correlated with Q/A_S, the area water loading. The equation for the prediction of R is:

$$R = 0.426 \cdot e^{(-0.271 \cdot \frac{Q}{A_S})} + 0.574 \cdot e^{(-0.00949 \cdot \frac{Q}{A_S})}$$

If the lake has one or more lakes chained upstream that are sufficiently able to retain a significant amount of the total nutrient exported from their respective portion of the watershed, this can be taken into account by calculating the supply to the upstream lake, the lake's retention coefficient, R and multiplying the supply by $(1 - R)$, to give the fraction transferred to the downstream lake.

The above-mentioned retention coefficient was generated for phosphorus. Calculations carried out in 18 lake studies in Scandinavia have shown that R is relatively 10–20% lower (average 16%) for nitrogen than for phosphorus.

Imboden (1974) suggested a two-compartment model for phosphorus content. The model considers a stratified lake and includes input, output, and exchange between hypolimnion and epilimnion, as well as sediment exchange. Four coupled differential equations for dissolved and particulate phosphorus are applied. The model has been improved (Imboden and Gachter, 1978; Imboden, 1979) by describing nutrient and biomass concentrations as continuous functions of time and depth and by replacing the first-order kinetic by a Michaelis–Menten kinetics; O'Melia (1972) and Snodgrass and O'Melia (1975) developed a similar model, but did not include release of phosphorus from the sediment; however, depth-dependent rates of turbulent diffusion were considered.

Larsen et al. (1974) found that the models of Vollenweider (1968) and Snodgrass and O'Melia (1975) underestimated the actual amount of epilimnetic phosphorus, when applied to lake Shigawa in Minnesota. They then applied a slightly more complex model consisting of a three-compartment epilimnetic model, which includes algae as a sink for soluble reactive phosphorus and conversion of particulate phosphorus into the soluble form. The basic equations for this model are:

$$\frac{dP_A}{dt} = \mu_{max}(T) \cdot Light \cdot \frac{P_S}{k_p + P_S} \cdot P_A - (R_1 + S_1 + \rho_w) \cdot P_A$$

$$\frac{dP_S}{dt} = \frac{P_{SIN}}{V_E} - \mu_{max}(T) \cdot Light \cdot \frac{P_S}{k_p + P_S} \cdot P_A + R_2 \cdot P_P - \rho_w \cdot P_S$$

$$\frac{dP_P}{dt} = \frac{P_{PIN}}{V_E} + R_1 \cdot P_A - (R_2 + S_2 + \rho_w) \cdot P_P$$

where:

P_A is the concentration of algal phosphorus (mg/l)

μ_{max} (T) is the maximum specific growth rate of phytoplankton as a function of temperature (1/day)

T is the temperature

Light is the fractional reduction of μ_{max} in the epilimnion due to the availability of light

k_P is the half-saturation constant for phosphorus

R_1 is the rate constant for conversion of algal phosphorus to particulate phosphorus (1/day)

S_1 is the rate constant for settling of algal phosphorus (corresponding to a settling velocity of 0.02 m/day)

ρ_w is the hydraulic washout coefficient (1/day)

P_S is the concentration of soluble phosphorus (mg/l)

P_{SIN} is the rate of supply of soluble phosphorus to the epilimnion (mg/day)

V_E is the volume of the epilimnion (m^3)

R_2 is the rate constant for conversion of particulate phosphorus to soluble phosphorus (1/day)

P_P is the concentration of particulate (non-algal) phosphorus (mg/l)

P_{PIN} = is the rate of supply of particulate phosphorus to the epilimnion (mg/day)

S_2 = is the rate constant for settling of non-algal particulate phosphorus (corresponding to a settling velocity of 0.04 m/day).

Lorenzen et al. (1976) developed a model consisting of two differential equations only, one for soluble and one for exchangeable phosphorus in the sediment:

$$\frac{dP_S}{dt} = \frac{P_{S_{IN}}}{V_L} + \frac{k_2 \cdot A \cdot P_{sed}}{V_L} - \frac{k_1 \cdot A \cdot P_S}{V_L} - \frac{Q}{V_L} \cdot P_S$$

$$\frac{dP_{sed}}{dt} = -\frac{k_2 \cdot A \cdot P_{sed}}{V_S} + \frac{k_1 \cdot A \cdot P_S}{V_S} - \frac{k_1 \cdot k_3 \cdot A \cdot P_S}{V_S}$$

where:

P_S = concentration of soluble phosphorus

$P_{S_{IN}}$ = load of phosphorus

V_L = lake volume (m^3)

k_2 = rate transfer of phosphorus from the sediment (m/year)

A = lake surface (m^2)

P_{sed} = total concentration of exchangeable phosphorus in the sediment (mg/l)

k_1 = rate transfer of phosphorus to the sediment (m/year)

Q = outflow (m^3/day)

V_S = sediment volume (m^3)

k_3 = fraction of total phosphorus input to the sediment that is not available for exchange (m/day).

The purpose of the model is to predict long-term changes in lakes that have undergone significant changes in loading rates. The equations can be solved analytically and the steady-state solution of P_S is:

$$P_{S\infty} = \frac{P_{S_{IN}}}{Q + k_1 \cdot k_3 \cdot A}$$

A characteristic feature of this model, in spite of its simplicity, is that it considers the sediment-accumulated phosphorus and that only a fraction of the total phosphorus input to the sediment is available for the exchange process. More complex models do not include this important property of the phosphorus in the sediment, although it is of great importance for the long-term change in lakes because a substantial part of the phosphorus in a lake system is buried in the sediment.

The parameters of this model are estimated by the following procedure. When reasonably good data on loading rates and average aqueous and sediment concentrations are known:

1. k_3 is estimated;
2. Since $k_1 \cdot k_3 = \frac{P_{S_{IN}} - PS_\infty \cdot Q}{P_S \cdot A}$, k_1 can be calculated;
3. k_2 is calculated from: $k_2 = k_1 \cdot (1 - k_3)$. $\frac{P_{S\infty}}{P_{sed\infty}}$, as the ratio of steady-state aqueous to sediment phosphorus concentrations, is given by (analytical solution): $\frac{P_{S\infty}}{P_{sed\infty}} = \frac{k_2}{k_1} \cdot \frac{1}{(1 - k_3)}$

The model was used for Lake Washington by applying data from 1941–50 to calculate a consistent set of model constants, based on the assumption that $k_3 = 0.6$. k_3 can be found on the basis of sediment analysis (a method to examine sediment–water exchange of phosphorus was reported by Kamp-Nielsen 1975). The observations during 1955–70, which showed that the phosphorus loading increased up to 1964 and decreased thereafter, were well predicted by the model. However, $k_3 = 0.5$ gave a better result (Fig. 3.36).

Lappalainen (1975) improved Vollenweider's approach by considering the state of a lake as a function of lake volume, discharge and phosphorus input. In this model a regression equation that relates the net sedimentation of phosphorus and the oxygen concentration of the hypolimnion is determined.

The model includes a relationship between the sedimentation of phosphorus and volume, discharge, and phosphorus input. The sedimentation submodel and the regression expression were used to construct a model for the prognosis of the oxygen concentration in the hypolimnion, which is used to determine the boundary phosphorus input, comparable with loads given earlier in the literature.

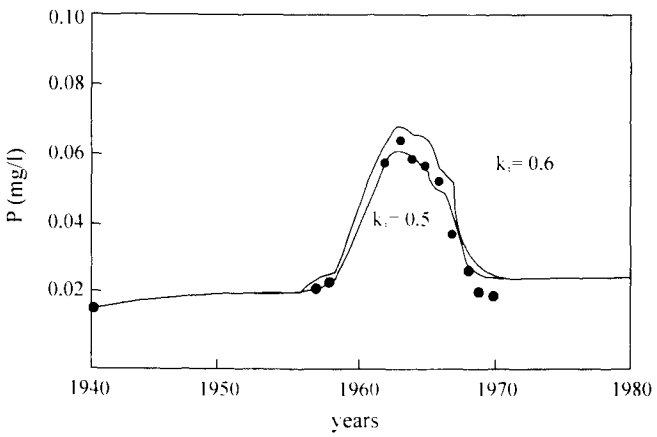

Fig. 3.36. Observed (filled circles) annual average total phosphorus concentrations (mg/l) in Lake Washington, and simulated values with two values of the k_s constant.

Oxygen Cycle

Oxygen is an important element for biotic life, it cycles in the environment as for the other elements and enters the processes of the other elements because of chemical reactions, respiration and production by photosynthesis.

Models of the aquatic environment account for oxygen with a mass balance in the water. The general approach is:

$$\frac{dC}{dt} = Reaeration - Consumption - Production$$

where C is the oxygen concentration dissolved in water as gas, t is time and the other terms are the main processes that contribute to the balance.

Reaeration is a consequence of different concentrations of oxygen in air and water. The flow can be oriented from air to water or *vice versa*, when the concentration of saturation in water is reached.

As shown in the two-film model, the model accounting for reaeration is:

$$\frac{dC}{dt} = k_R \cdot (C_S - C) \tag{3.40}$$

where C_S is the oxygen concentration in water when saturation is reached, and k_R is the transfer coefficient. C_S depends on temperature, pressure and salinity.

For distilled water the most common model accounting only for the dependence on temperature of oxygen concentration at saturation is Elmore and Hayes (1960) polynomial equation:

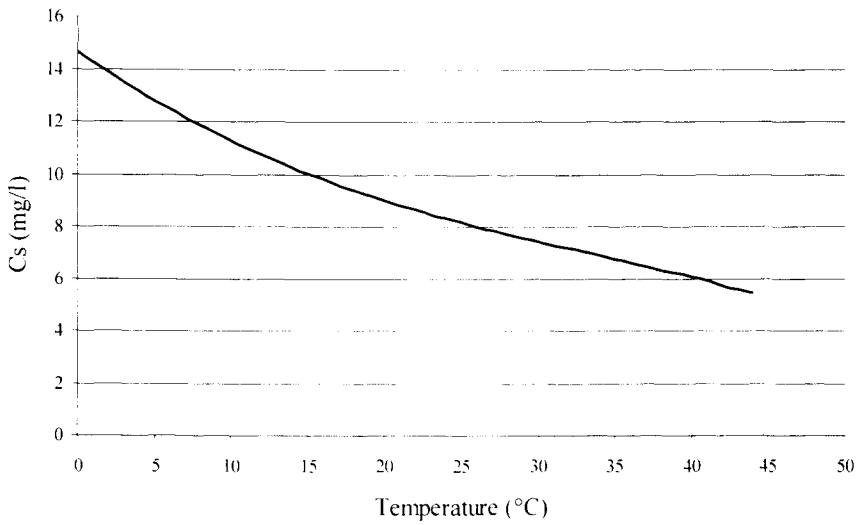

Fig. 3.37. Temperature effects on oxygen at concentration saturation in water.

$$C_S = 14.652 - (0.41022 \cdot T) + (0.007992 \cdot T^2) - (7.7774 \cdot 10^{-5} \cdot T^3)$$

where T is in Centigrade.

Figure 3.37 reports the effect of temperature on the concentration of dissolved oxygen at saturation. The importance of temperature in driving the oxygen content in the water is clear, particularly in the temperature range of 0–40°C, which is of environmental interest.

The oxygen concentration can reach very low values, which can become very harmful for biota if other conditions such as high salinity and low pressure are occurring contemporaneously.

Other models exist with slightly different coefficients, for instance: 14.62, 0.3898, 0.006969, $5.897 \cdot 10^{-5}$, because of some differences in the laboratory experiments carried out to determine them.

When, as is usual in environmental modelling, water is not distilled and it has a certain conductivity due to dissolved salts, or is seawater, the previous model cannot be used.

Salinity (in parts per thousand or g/l) is related to chlorinity (mg/l of Cl), by the following formula:

$$Salinity = 0.03 + 0.001805 \cdot Chlorinity$$

and to the specific conductance SC ($\mu\Omega$/cm) by the formula:

$$Salinity = 5.572 \cdot 10^{-4} \cdot SC + 2.02 \cdot 10^{-2} \cdot SC^2$$

The Benson and Krause (1984) model put together the dependence on temperature and salinity at 1 atmosphere of pressure to describe oxygen concentration at saturation. The model, empirically set up, is:

$$\ln C_S = -139.34411 + \left(\frac{1.575701 \cdot 10^5}{T}\right) - \left(\frac{6.642308 \cdot 10^7}{T^2}\right) + \left(\frac{1.243800 \cdot 10^{10}}{T^3}\right) - \left(\frac{8.621949 \cdot 10^{11}}{T^4}\right) - Chl \cdot \left[(3.1929 \cdot 10^{-2}) - \left(\frac{1.9428 \cdot 10}{T}\right) + \left(\frac{1.8673 \cdot 10^3}{T^2}\right)\right]$$

where T in Kelvin can range between 273.15 and 313.15 and chlorinity between 0 and 28 g/l.

The non-standard pressure conditions for oxygen saturation, C'_S, are described by the formula:

$$C'_S = C_S \cdot P \cdot \frac{\left(1 - \frac{P_{wv}}{P}\right) \cdot (1 - \theta \cdot P)}{(1 - P_{wv}) \cdot (1 - \theta)}$$

where C_S is the standard (1 atm) concentration at saturation, P is the pressure of the environment ranging between 1 and 2 atm, and P_{wv} is the partial pressure of the water vapour (atm):

$$\ln P_{wv} = 11.8571 - \left(\frac{3840.70}{T}\right) - \left(\frac{216961}{T^2}\right)$$

with T in Kelvin, and θ is accounted for by:

$$\theta = 0.000975 - (1.426 \cdot 10^{-5} \cdot T) + (6.436 \cdot 10^{-8} \cdot T^2)$$

with T in Centigrade.

The last problem to solve to calculate reaeration by the formula 3.40 is the estimation of the value of the transfer coefficient or rate of transfer, k_R. This rate depends on the type of the water body.

In the literature, some formulations of k_R ($1/t$) for rivers are reported assuming a temperature of 20°C and no wind at the interface between air and water. One of these for small rivers, validated by experiments with radioactive processes, assumes the form:

$$k_R = \alpha \cdot \frac{\Delta h}{t}$$

where Δh is variation in elevation, t is time and $\Delta h/t$ is an energy dissipation, α (l^{-1}) depends on the characteristic of the river.

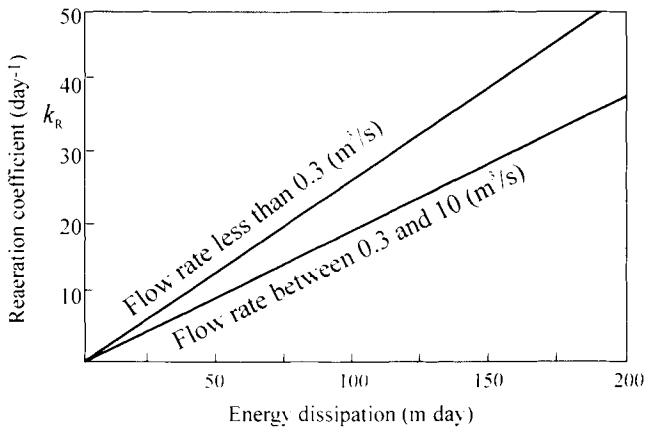

Fig. 3.38. Reaeration coefficient versus energy dissipation for different flow rates.

Experimental data and linear regression used to estimate k_R are reported in Fig. 3.38.

A more general formulation of the k_R is given by the formula:

$$k_R = \alpha \cdot v^{\beta} \cdot h^{-\gamma}$$

where v (m/s) is the velocity of the water and h is the water depth (m) and the values of the coefficient are given in Table 3.13. As usual the dependence on temperature of k_R is accounted for by the Arrhenius equation:

$$k_R(T) = k_R(20) \cdot e^{\theta(T-20)}$$

where θ assumes the value of $0.024°C^{-1}$ for T ranging between 5 and 25°C.

If we assume that wind blows at the interface between air and water, we have to account for this effect because it greatly increases the reaeration. The wind effect on reaeration assumes a greater importance compared with the turbulence effect, when the current in the river is slow and it becomes almost the only process for reaeration in lakes.

Table 3.13. Values of the coefficients in the k_R formula $k_R = \alpha \cdot v^{\beta} \cdot h^{-\gamma}$, used by different authors.

Authors	α	β	γ
Streeter and Phelps (1925)	1.0	0.57–5.40	2.0
O'Connor and Dobbins (1956)	1.7	0.5	1.5
Isaacs and Gaudy (1968)	1.35–2.22	1	1.5
Negulescu and Rojanski (1969)	4.74	0.85	0.85
Bennet and Rathburn (1972)	2.33	0.674	1.865
Owens et al. (1964)	2.13–3.0	0.67–0.73	1.75–1.85

The effect of wind on the values of the reaeration coefficients estimated for rivers has been empirically investigated and a simple model has been set up to calculate the wind effect:

$$\frac{k_R}{(k_R)_0} = 1 + 0.2395 \cdot v_w^{1.043}$$

where k_R is the coefficient under wind conditions, $(k_R)_0$ is that without the wind condition, and v_w is the wind velocity above the boundary layer between air and water.

Figure 3.39 reports the effect of the wind on the reaeration coefficient for rivers with different, but low, water velocities where the turbulence effect would be negligible and it clearly points out how k_R values increase with the wind velocity.

A general formulation for the reaeration velocity for lakes k_L (m/day) is:

$$k_L = \alpha \cdot v^b$$

where v is the wind velocity, α (dimensionless) assumes an average value of 0.0276 and β (dimensionless) depends on the wind conditions:

$$\beta = \begin{cases} 1/2 & 0 < v < 5.5 \text{ m/s} \\ 1 & \text{average value} \\ 2 & v > 5.5 \text{ m/s} \end{cases}$$

Notice that it is a different unit from the one which is usually applied for streams. For lakes, reservoirs and open bays, the effect of wind may be significant for the rate or

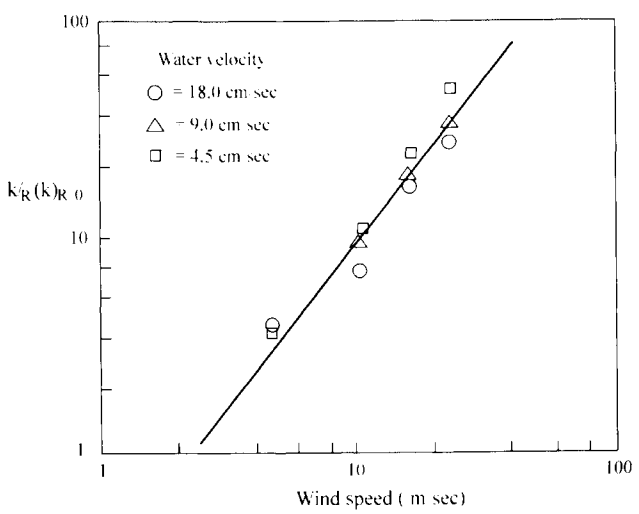

Fig. 3.39. Ratio of the reaeration coefficient under windy conditions to the reaeration coefficient without wind, as a function of wind speed (based on laboratory studies).

Table 3.14. Average fresh-water plant composition on wet basis.

Element	Plant content (%)	Element	Plant content (%)
Oxygen	80.5	Chlorine	0.06
Hydrogen	9.7	Sodium	0.04
Carbon	6.5	Iron	0.02
Silicon	1.3	Boron	0.001
Nitrogen	0.7	Manganese	0.0007
Calcium	0.4	Zinc	0.0003
Potassium	0.3	Copper	0.0001
Phosphorus	0.08	Molybdenum	0.00005
Magnesium	0.07	Cobalt	0.000002
Sulphur	0.06		

reaeration. Banks (1975) and Bank and Herrera (1977) suggest using the following equation to estimate the reaeration in these cases:

$$k_L = 0.782 \cdot v^{1.5} - 0.317 \cdot v + 0.0372 \cdot v^2$$

where v is the wind speed (m/s), 10 m above the water surface. The amount of oxygen expressed in g/(day·m^2), transferred by reaeration, is found from k_L by multiplication with the difference in concentration at saturation and in the water. To find the change in concentration, it is therefore necessary to divide by the depth of the lake.

Consumption is the second main process entering the oxygen cycle. It accounts for the microbial degradation of organic matter, which requires oxygen to oxidize all the reduced compounds that are the products of the general reaction of organic matter degradation.

The biochemistry of all organisms on earth are surprisingly similar. The main components of organic matter are carbohydrates, lipids and proteins, supplied by a wide spectrum of other components, such as DNA (the genetic material), ATP (adenosine triphosphate), hormones, haemoglobin, inorganic ions (sodium, calcium, magnesium, chloride, sulphate, potassium, hydrogen carbonate and so on). It implies that the elementary composition of organic matter is also very similar; Table 3.14 gives a typical example for freshwater plants. Notice, furthermore, that the dry matter is only 10–20% of the total biomass. This means that except for hydrogen and oxygen, which are mainly in the wet part of the organic matter, the dry matter percentage is 5–10 times higher than the wet one.

If we assume that a simplified stoichiometric composition of organic matter is given by $C_{106}H_{263}O_{110}N_{16}P_1S_1$, the general reaction of organic matter decomposition can be written as:

$$C_{106}H_{263}O_{110}N_{16}P_1S_1 + R(O) + \text{Decomposers} \longrightarrow$$
$$\longrightarrow aCO_2 + bNH_4^+ + cHPO_4^{2-} = dHS^- + eH_2O + fH^+ + \text{Energy} \qquad (3.41)$$

Table 3.15. Yields of kJ and ATPs per mole of electrons, corresponding to 0.25 moles of CH_2O oxidized. The released energy is available to build ATP for various oxidation processes of organic matter at pH = 7.0 and $T = 25°C$.

Reaction	kJ·mole e^-	ATPs/mole e^-
$CH_2O + O_2 \rightarrow CO_2 + H_2O$	125	2.98
$CH_2O + 0.8\ NO_3^- + 0.8\ H^+ \rightarrow CO_2 + 0.4\ N_2 + 1.4\ H_2O$	119	2.83
$CH_2O + 2MnO_2 + 4H^+ \rightarrow CO_2 + 2Mn^{2+} + 3\ H_2O$	85	2.02
$CH_2O + 4FeOOH + 8\ H^+ \rightarrow CO_2 + 7\ H_2O + 4Fe^{2+}$	27	0.64
$CH_2O + 0.5\ SO_4^{2-} + 0.5\ H^+ \rightarrow CO_2 + 0.5\ HS^- + H_2O$	26	0.62
$CH_2O + 0.5\ CO_2 \rightarrow CO_2 + 0.5CH_4$	23	0.55

The decomposition of organic matter is a redox process, a reaction in which one or more electrons are transferred. The organic matter delivers electrons to an oxidizing agent, which takes up the electron. This means that mainly carbon in the organic matter has a higher oxidation state by formation of carbon dioxide, while the oxidizing agent has a lower oxidation state. If oxygen is used as the oxidizing agent the process is called respiration.

Various oxidizing agent can oxidize organic matter, as shown in Table 3.15, but the one that gives the highest amount of stored energy (most ATPs, most energy) will always win, which is in accordance with the ecosystem theory based on exergy (see Chapter 9). Therefore, if oxygen is present, oxygen will be used. When the oxygen is used up, nitrate will be used and so on.

In aquatic environments some of the inorganic compounds, resulting from organic matter decomposition (3.41), are in equilibrium with other chemical forms of the same element according to the oxygen availability and pH of the water.

The consumption of oxygen in aquatic environment is mainly due to:

- Degradation of dissolved and suspended organic matter known as Biological Oxygen Demand (BOD);
- Oxidation of chemical compounds dissolved in water (COD);
- Oxidation of Nitrogen (NOD) according to the cycle of nitrogen;
- Sediment Oxygen Demand (SOD) including oxidation of settled organic matter and respiration of benthic biota.
- Respiration of primary and secondary producers living in the water.

Almost all water quality models use a first-order kinetic to account for variation of the *Biological Oxygen Demand (BOD)* in a water body:

$$\frac{dL}{dt} = -k_d \cdot L$$

where L is the concentration of organic matter measured as BOD, usually expressed as O_2 mg/l required by the decomposer bacteria to oxidize organic matter, t is time, and k_d is the rate coefficient (1/day).

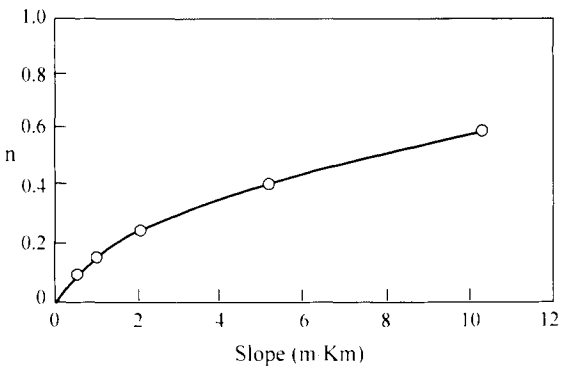

Fig. 3.40. Coefficient of bed activity n as a function of stream slope (Bosko, 1966).

BOD_5 indicates the oxygen required by the process in 5 days and is extensively used in environmental science and practice to evaluate the state of a water body. As usual, the problem of the first-order kinetic is the estimation of the rate coefficient. For rivers it can be simply estimated by the Bosko (1966) model:

$$k_e = k_c + n \cdot \frac{v}{h}$$

where k_1 is the rate constant for calm water, v is the stream velocity, h the water depth, and n is a dimensionless coefficient related to the river bed activity dependent on the slope, according to the values of Fig. 3.40.

Values of k_1 depend on the type of water, as shown in Table 3.16, and on temperature according to the formula:

$$k_1(T) = k_1(20) \cdot \theta^{(T-20)}$$

where $\theta = 1.05$ and T is the temperature in Celsius.

While for rivers the main effect of oxidation is due to the characteristics of flow and river bed, for lakes the autochthonous sources of organic matter (i.e. phytoplankton and zooplankton dead biomass) demand a lot of oxygen to be mineralized.

Table 3.16. Ranges of value of k_1 and of BOD_5 concentration for different types of water.

Water type	k_1 (1/day)	BOD_5 (mg/l)
Municipal waste water	0.35–0.40	150–250
Mechanically treated municipal waste waters	0.35	75–150
Biologically treated municipal waste waters	0.10–0.25	10–80
Drinking water	0.05–0.10	0–1
River water	0.05–0.15	0–5

The basic first-order kinetic assumes, for lakes, the following formulation:

$$\frac{dL}{dt} = -k_d \cdot L + \alpha \cdot (F_P \cdot P + F_Z \cdot Z)$$

where $\alpha = 2.67$ is a stoichiometric coefficient mg O_2/mg C accounting for degradation of organic matter expressed as carbon concentration to CO_2; F_P and F_Z are the death rate of phytoplankton and zooplankton due to grazing and predation (1/day); and P and Z are the concentration of phytoplankton and zooplankton (mg C/l).

The *Chemical Oxygen Demand (COD)* is driven by the stoichiometry of the reactions. The global reaction transfers each carbon atom of organic matter in a molecule of CO_2, with the rate just seen of 2.67.

Nitrogen Oxygen Demand (NOD) is a more complex process already seen in the nitrogen cycle.

The global process can be written as follow:

$$\text{OrgN} \xrightarrow[a]{} NH_4^+ \xrightarrow[b]{} NO_2^- \xrightarrow[c]{} NO_3^-$$

- Process *a*, the hydrolysis of organic nitrogen of organic matter to ammonia, does not consume oxygen;
- Process *b*, the oxidation of ammonium to nitrite by the action of *Nitrosomonas bacteria*, is given by:

$$NH_4^+ + 1.5O_2 \rightarrow NO_2^- + H_2O + 2H^+$$

and it consumes 3.43 g of O_2 per gram of nitrogen as ammonium;

- Process *c*, the oxidation of nitrite to nitrate by the action of *Nitrobacter bacteria*, is given by:

$$NO_2^- + 0.5O_2 \rightarrow NO_3^-$$

and it consumes 1.14 g O_2 per gram of nitrogen as nitrite.
The global process (*b*+*c*) is given by:

$$NH_4^+ + 2O_2 \rightarrow NO_3^- + H_2O + 2H^+$$

and it consumes 4.57 g of oxygen per gram of nitrogen as ammonium; 4.57 is the stoichiometric coefficient α for the global process, but due to bacterial assimilation of ammonia, this coefficient is usually corrected to 4.3 g O_2/g($N\text{–}NH_4^+$).
In practice the first-order kinetic for this process can be written as:

$$\frac{dO}{dt} = \alpha \cdot k_N (N - NH_4^-).$$

Table 3.17. Range of values of k_N and ammonium concentration for different types of waters.

Water type	k_N (1/day)	$N\text{-}NH_4^+$ (mg/l)
Municipal waste water	0.15–0.20	80–130
Mechanically treated municipal waste waters	0.10–0.25	70–120
Biologically treated municipal waste waters	0.05–0.20	60–120
Drinking water	0.050	0–1
River water	0.05–0.10	0–2

k_N assumes different values according to the quality of organic matter dissolved in the water, as shown in Table 3.17, and it depends on temperature according to the formula:

$$k_N(T) = k_N(20) \cdot \theta^{(T-20)}$$

where θ values range from 1.0586 (typical for oxidation of $N\text{-}NO_2^-$) to 1.0850 (typical for oxidation of $N\text{-}NO_4^+$) and T is the temperature in Centigrade.

k_N values also depend on the pH of the water, as shown in Fig. 3.41.

It is clear that a good range of pH for such an oxidation is from 8 to 9, with an optimum for both processes of around 8.5.

The oxygen demand by benthic sediments and organisms, usually called *Sediment Oxygen Demand (SOD)* (g O_2/m^2 day), can represent a large fraction of oxygen consumption in surface water bodies.

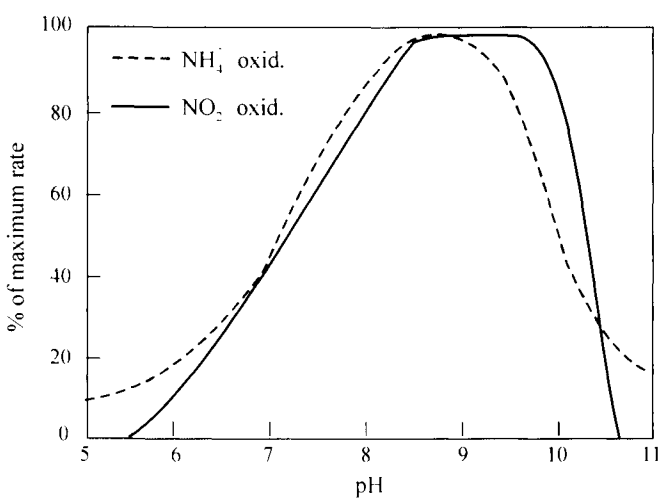

Fig. 3.41. Dependence of the rate of oxidation of NH_4^+ and NO_2^- on pH.

The two main sources of SOD are:

- the degradation of organic matter settled on the bottom of the water body and coming from allocthonous sources like river inlet or waste discharge, or from endogenous sources like phytoplankton and zooplankton growing in the water body;
- the respiration of benthic biota.

The degradation process of organic matter in sediments is strongly influenced by the diffusion of dissolved oxygen from the water column to pore water and the diffusion of mineralized reduced forms of organic matter from pore water to water column.

Bioturbation of sediment by benthic organisms increases the interface exchanges and it is usually accounted for in the model as an increment of the active exchange surface. To give an idea of the importance of bioturbation, it is useful to mention that the labyrinth of small tubes created by worms in the sediment of the Lagoon of Venice (Italy) has an exchange surface four times larger than the related horizontal surface of the bottom.

The model that accounts for the SOD process is:

$$\frac{dC}{dt} = -\frac{1}{h} \cdot k_S$$

where C (mg/l) is the oxygen concentration at the water–sediment interface; t is the time, h the water depth (m) and k_S (g O_2/m^2 day) is the specific rate of oxygen consumption. k_S can either be measured by benthic chamber or estimated from values given in Table 3.18 (Thomann, 1972).

Some models to estimate SOD have been proposed in the literature to account for the dependence on oxygen concentration in water:

- SOD = $k_S \cdot C^b$, where the constant b has to be empirically determined and C^b is dimensionless;
- SOD = $k_S \cdot \frac{C}{k_{O_2} + C}$, where k_S is multiplied by a Michaelis–Menten limitation, with a value of the semisaturation constant k_{O_2} ranging from 0.7 to 1.4 mg O_2/l;

Table 3.18. Ranges and average values of specific rate k_S (g O_2 m^2 day) of oxygen consumption for different types of substrate.

Bottom type	Range	Average
Filamentous bacteria (10 g dry wt./m^2)	5–10	7
Municipal sewage sludge outfall vicinity	2–10	4
Municipal sewage sludge downstream of outfall	1–2	1.5
Estuarine mud	1–2	1.5
Sandy bottom	0.2–1.0	0.5
Mineral soils	0.05–0.1	0.07

- or a two-fractions model resulting from the combination of the previous two models, and accounting for the different behaviour of the chemical and biological fractions of SOD:

$$\text{for the chemical fraction, CSOD} = k_{CS} \cdot C$$

$$\text{for the biological fraction, BSOD} = k_{BS} \cdot \frac{C}{k_{O_2} + C}$$

Other assumptions have been proposed in the literature to account for the variability of the substrate. The first assumes that the decay of the substrate is balanced by a continuous settling, resulting in a steady-state sediment concentration of oxygen demanding substrate:

$$\frac{dC}{dt} = -\frac{1}{h} \cdot k_S$$

while a second assumption assumes a variable settling rate:

$$\frac{dC}{dt} = k_S \cdot \text{SED}$$

where SED is a function of the sediment concentration of oxygen demanding substrate varying as a consequence of loads and water turbulence.

Illustration 3.1

To give an idea of the effects of the processes of reaeration and consumption it may be useful to illustrate the oxygen profile measured in a small lake and shown in Fig. 3.42.

The water of the lake is fresh and the temperature at the surface is around 25°C. According to the theory of the oxygen concentration at saturation, the expected concentration is around 8 mg/l as shown in Fig. 3.42. The slightly higher concentration in the epilimnion is due to a photosynthetic production of phytoplankton and in this case the lake surface is releasing oxygen to the atmosphere. The oxygen concentration is constant along the water column until the thermocline depth, which is at a depth of 5 metres. In the hypolimnion the oxygen concentration drops quickly to low values (about 2 mg/l) and at the water–sediment interface (depth = 7 m), it is almost zero. This strong depletion of the oxygen concentration is due to the SOD of anoxic sediments.

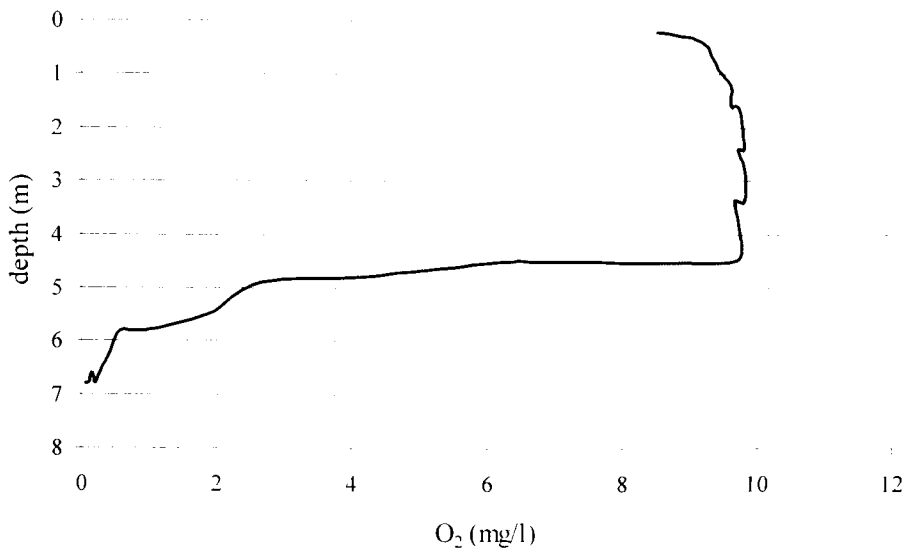

Fig. 3.42. Oxygen profile measured in a small lake.

Oxygen Dynamics in a River

The dynamics of oxygen in a river due to the reaeration and organic matter degradation was initially investigated by Streeter and Phelps (1925). The model is based on the following assumptions:

1. only one source of pollutants exists;
2. a constant load of pollutants is discharged at a single point;
3. there is no tributary inflow;
4. flow rate is constant;
5. the cross section of the river is uniform;
6. the turbulence is sufficient to allow the concentration of BOD and DO to be uniform throughout the cross section;
7. biodegradation and reaeration are first-order reactions and they are the only processes to be considered.

Under the previous assumptions, the following differential equation can be set up:

$$\frac{dD}{dt} = -k_R \cdot D + k_1 \cdot L_t \tag{3.42}$$

where $D = C_S - C_t$, oxygen at saturation minus oxygen concentration at time t; L_t = organic matter concentration at time t; k_R = reaeration rate; k_1 = degradation rate.

According to assumption 7, $L_t = L_0 \cdot e^{-k_1 \cdot t}$, where L_0 is the initial value of BOD at the point of the discharge.

As seen before, numerical values of k_R can be calculated by:

$$k_R(T) = \frac{2.26 \cdot v}{h^{\frac{3}{2}}} \cdot 0.024^{(T-20)}$$

and for k_1 by $k_1(T) = k_1(20) \cdot 1.05^{(T-20)}$, and the model 3.42 can be consequently written:

$$\frac{dD}{dt} = -k_R \cdot D + k_1 \cdot L_0 \cdot e^{-k_1 \cdot t} \tag{3.43}$$

If $k_R \neq k_1$, it takes the form of a first-order differential equation:

$$\frac{dx}{dt} = \alpha(t) \cdot x + \beta(t)$$

for which the general solution is:

$$x(t) = e^{\int \alpha(t)dt} \cdot \left(\int \beta(t) \cdot e^{\int \alpha(t)dt} dt + c \right)$$

If we apply this solution to our model, we get:

$$\begin{aligned} D &= e^{-k_R t} \cdot \int k_1 \cdot L_0 \cdot e^{-k_1 t} \cdot e^{+k_R t} dt + c \\ &= e^{-k_R t} \cdot \int k_1 \cdot L_0 \cdot e^{(k_R - k_1)t} dt + c \\ &= k_1 \cdot L_0 \cdot e^{-k_R t} \cdot \frac{e^{(k_R - k_1)t}}{k_R - k_1} + c \\ &= \frac{k_1 \cdot L_0}{k_R - k_1} \cdot e^{-k_R t} + c_1 \cdot e^{-k_R t} + c \end{aligned}$$

at $t = 0, D = D_0$ and $c_1 = D_0 - \frac{k_1 \cdot L_0}{k_R - k_1}$.

$$D = \frac{k_1 \cdot L_0}{k_R - k_1} \cdot (e^{-k_1 t} - e^{-k_R t}) + D_0 \cdot e^{-k_R t} \tag{3.44}$$

If we plot C_t, instead of D versus time, we obtain the so-called oxygen sag curve of Fig. 3.43.

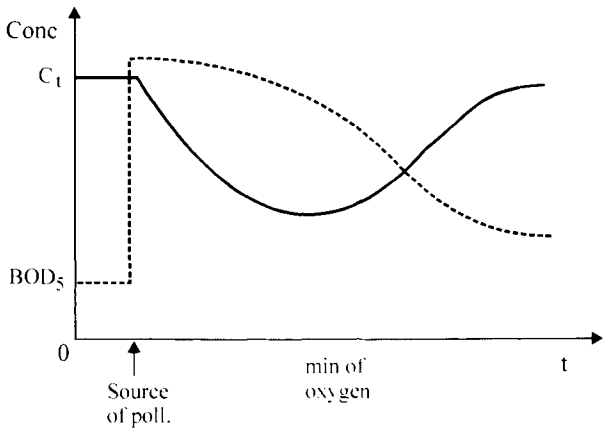

Fig. 3.43. Concentration of oxygen and BOD_5 along a river according to the Streeter and Phelps model.

The minimum value of C_t is occurring at the critical time t_c for oxygen depletion; we can get t_c because if $t = t_c$, $\frac{dD}{dt} = 0$ and $\frac{d^2D}{dt^2} < 0$ and from 3.43 we get:

$$0 = -k_R \cdot D + k_1 \cdot L_0 \cdot e^{-k_1 \cdot t}$$

$$\Rightarrow t_c = \frac{1}{k_R - k_1} \cdot \ln \frac{k_R}{k_1} \cdot \left(1 - \frac{D_0 \cdot (k_R - k_1)}{L_0 \cdot k_1}\right)$$

by substitution of t_c in 3.44 we get the minimum value of C_t and the maximum value of D:

$$D_0 = \frac{k_1}{k_R} \cdot L_0 \cdot e^{-k_1 \cdot t_c}.$$

According to assumption 4, the flow velocity v is constant and the distance x from the discharge point can be calculated by $x = v \cdot t$.

Assumption 7 of the model formulation can be changed by adding a source of ammonium–nitrogen. Provided that it can be modelled with a first-order kinetic too, $N_t = N_0 e^{-k_N \cdot t}$, it does not change the model (3.42) too much, which becomes:

$$\frac{dD}{dt} = -k_R \cdot D + k_1 \cdot L_t + \alpha \cdot k_N \cdot N_t$$

where α is the stoichiometric coefficient, k_N the rate constant for ammonium–nitrogen oxidation and N_t is the ammonium–nitrogen concentration. Its solution is:

$$D = \frac{k_1 \cdot L_0}{k_R - k_1} \cdot (e^{-k_1 t} - e^{-k_R t}) + \frac{\alpha \cdot k_N \cdot N_0}{k_R - \alpha \cdot k_N} \cdot (e^{-k_N t} - e^{-k_R t}) + D_0 \cdot e^{-k_R t}$$

The last process in the oxygen cycle is the biological *production* of this element due to the living algae in the water body.

Because algae produce oxygen when they grow by photosynthesis (P) and they consume oxygen by respiration (R), the model has to account for the net production which is the algebraic sum of the two processes.

Photosynthesis (mg O_2/l day) is simply accounted for in many models as $P = \alpha_1 \cdot \mu \cdot A$, where α_1 is the ratio (mg O_2/mg Chl-a) of oxygen per chlorophyll-a content in the algae A; α_1 is ranging between 0.1 and 0.3 with an average value of 0.18; and μ is the growth rate (1/day) of phytoplankton. The model for μ, explained in the following section, depends on many factors such as nutrient availability, water temperature and light.

Respiration (mg O_2/l day) is also accounted for in a simple way as: $R = \alpha_2 \cdot \rho \cdot A$, where α_2 is the ratio (mg O_2/mg Chl-a) of oxygen per chlorophyll-a content in the algae A; α_2 is about one tenth of α_1; ρ is the respiration rate (1/day) which mainly accounts for the temperature dependence by the usual Arrhenius formula: $\rho = \rho_{20} \cdot 1.08^{(T-20)}$.

The net production model can be finally written as:

$$\frac{dC}{dt} = (\alpha_1 \cdot \mu - \alpha_2 \cdot \rho) \cdot A$$

3C.2 Photosynthesis

Photosynthesis plays a key role in closing the cycles of oxygen and carbon, in reducing the oxidized form of carbon (CO_2) and in producing oxygen (O_2). The photosynthetic process is of great importance in ecological modelling because it represents the production of the biomass at the basic level of an ecosystem. It may be divided into the following independent series of reactions: the light absorption producing energy (known as the light reaction), and the reductive reaction of carbon dioxide fixation (known as the dark reaction). The light reaction transforms the energy of sunlight into the two biochemical energy sources ATP and $NADPH_2$ via the two main photochemical pathways. Chlorophyll-a is an essential substance in this process. This photosynthetic pigment of vegetal cells captures the energy of photon and concentrates it in the chloroplasts. In these particular parts of the cell, photolysis of water produces H^+ which reduces (via enzymatic reaction) NADP to $NADPH_2$ and results in a net production of O_2.

$$2H_2O + \text{oxidized chlorophyll-a} + \text{energy} \rightarrow$$
$$\text{reduced chlorophyll-a} + O_2 + 4H^+ \rightarrow$$
$$4H^+ + 2NADP \rightarrow 2NADPH_2$$

The dark reaction uses the biochemical energy sources ATP and $NADPH_2$ to reduce carbon dioxide to organic carbon.

The overall reaction of photosynthesis can be simply written:

$$6CO_2 + 6H_2O + h\nu \rightarrow C_6H_{12}O_6 + 6O_2$$

Obviously, photosynthesis involves two sets of external limiting factors: the availability of energy and of inorganic elements (CO_2). These two elements govern the rates of the light and the dark reactions.

In addition, internal limiting factors are involved since transport mechanisms provide the nutrients essential for the synthesis of organic matter. Besides this, organisms need time to adapt to fluctuations in environment conditions (e.g., a change in radiant intensity), and so both internal pools of nutrients (C, N, P, H_2O, S, etc.) and the "reaction tools" (enzymes, transport mechanisms, respiration, leaf index, reproductive stage, etc.) may limit the rate of photosynthesis.

The common mathematical description of photosynthesis involves a coupling of light and nutrient dependency, and this may be categorized as an empiric model. If no change in adaptation occurs, then photosynthesis may be quoted as:

$$\text{PHOTO} = k \cdot f\,(\text{maximum requirement of limiting factors})$$

where PHOTO is the photosynthesis measured as uptake of CO_2, production of O_2, increased organic energy, or similar units, and f represents the optimal yield of the maximum limiting nutrients, external as well internal. Figure 3.44 gives some basic experimental results to illustrate different types of limiting factors and adaptation cases.

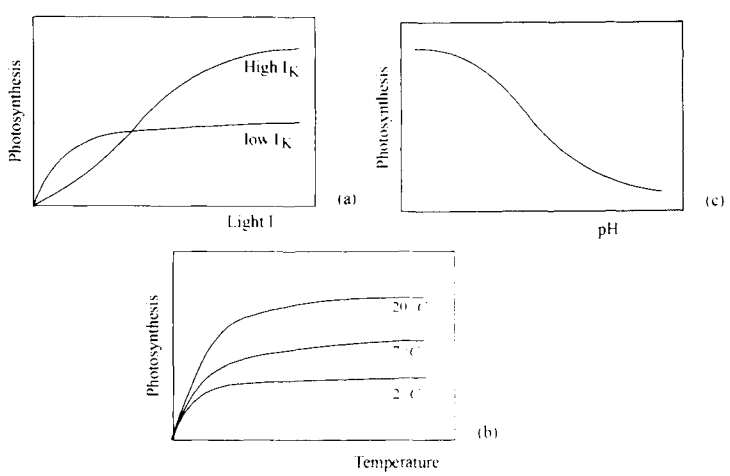

Fig. 3.44. Rate of photosynthesis as a function of: (a) radiation energy at different values of I_k adaptation at high intensity; (b) temperature at different values of environmental temperature; (c) pH values.

Photosynthetic Rate

Only a part of global incident radiation may be used for the photosynthetic reaction, this is usually called *Photosynthetical Active Radiation (PAR)* and it is almost 56% of the total incident radiation I_0 at the air–water interface.

As shown in Part A of this chapter, in aquatic ecosystems the incident radiation is reduced by the turbidity of the water. The quantity of light I that can be used by algae to photosynthesize is finally:

$$I = \alpha \cdot I_0 \cdot e^{-\gamma h}$$

where I_0 is the incident light at the water surface; α is a coefficient that accounts for the photosynthetic activity, namely $\alpha = 0.56$; γ is the extinction coefficient in water body; and h is the water depth.

The photosynthetic rate P (mg O_2/g·h) can be expressed by a saturation process depending on light, according to the following equation:

$$P = P_{max} \cdot \frac{\frac{I}{I_k}}{\sqrt{1+\left(\frac{I}{I_k}\right)^2}} \tag{3.45}$$

where P_{max} (mg O_2/g·h) is the maximum rate in optimal conditions and I_k is a parameter accounting for light adaptation. Low values of I_k are typical of algae adapted to low light intensity and will ensure the maximum photosynthetic rate is reached with low values of I. On the other hand, high values of I_k will provide the maximum P with higher values of I, as shown in Fig. 3.44a. P_{max} also depends on environmental factors such as temperature and pH.

As discussed in Part B, temperature influences photosynthesis because it is an enzymatic reaction and pH influences photosynthesis because of the role that it plays in the equilibrium of carbonates. High values of pH move the equilibrium towards the CO_3^{2-} ion and reduce the availability of CO_2 in the water to almost zero at pH = 8.5. Equations that account for those effects are:

$$P_{max}(T) = P_{max}(20) \cdot \frac{1}{1+\alpha \cdot e^{-\beta(T-20)}} \tag{3.46}$$

$$P_{max}(\text{pH}) = P_{max}(6.5) \cdot e^{-\gamma(\text{pH}-6.5)^2} \tag{3.47}$$

where the usual values of the parameters for an aquatic plant such as *Ceratophyllum demersum* are: P_{max} (100 W/m^2, 20°C, 6.5 pH) = 13.267 (mg O_2/g·h); $\alpha = 0.273$; $\beta = -0.169$; $\gamma = -0.438$.

3C.3 Algal Growth

As has been seen, photosynthesis is the process that provides the growth of plants. This process is related to the total system and to simulate it, demographic equations are used. In aquatic environments, equations treating algal growth can be based on the average biomass of one or more species, or of a few dominant functional groups (e.g., diatoms, green algae, blue-green algae, etc.). A general model for the *algae A growth* is:

$$\frac{dA}{dt} = (\mu - r - es - m - s) \cdot A - G \tag{3.48}$$

where A is the algal biomass or concentration expressed as dry weight biomass, chlorophyll-a concentration, or equivalent mass or concentration of the most important nutrients (C, N, P, Si); μ is the gross growth rate ($1/t$); r is the respiration rate ($1/t$); es is the essudation rate ($1/t$); m is the non-predatory mortality rate ($1/t$); s is the settling rate ($1/t$); and G is the loss due to grazing.

Sometimes algae such as phytoplankton is expressed in terms of number of cells. In this case r and es rates are not meaningful and Eq. (3.48) is consequently rearranged. *Algal gross growth rate* μ is usually modelled by the equation:

$$\mu = \mu_{max}(T_{ref}) \cdot (f_1(T), f_2(L), f_3(\text{C,N,P,Si})) \tag{3.49}$$

where $\mu_{max}(T_{ref})$ is the maximum growth rate at a reference temperature; T_{ref} under optimal, non-limiting, light and nutrients availability; $f_1(T)$ accounts for temperature variations; $f_2(I)$ accounts for light limitation; f_3(C, N, P, Si) accounts for nutrient limitations.

As discussed later in this section, some nutrients may play a non-limiting role and can be ignored in the formulation of the model. The function $f_1(T)$ adjusts the maximum growth rate at the reference temperature $\mu_{max}(T_{ref})$ to the water temperature. Three major models are reported in the literature for this function;

the linear model:

$$f_1(T) = \frac{T - T_{min}}{T_{ref} - T_{min}}$$

the usual Arrhenius exponential model

$$f_1(T) = \vartheta^{(T - T_{ref})}$$

and the skewed normal distribution around an optimum temperature:

$$f_1(T) = e^{\left[-2.3\left(\frac{T - T_{opt}}{T_L - T_{opt}}\right)^2\right]}$$

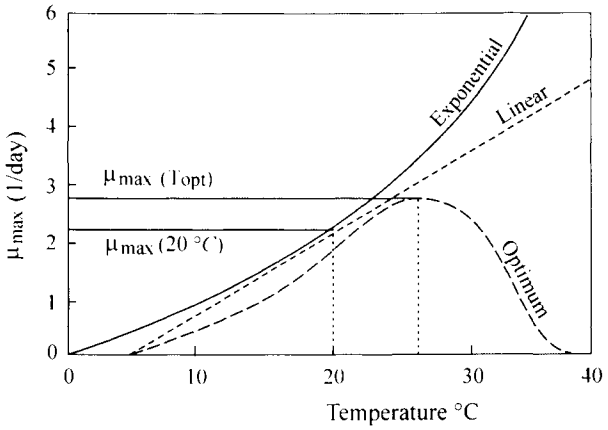

Fig. 3.45. Plots of different functions of the temperature adjustments. Optimum temperatures vary according to different algal species.

where T_{ref} assumes the usual value of 20°C: T_{min} is the minimum temperature under which the growth is zero; T_{max} is the maximum temperature giving a non-zero growth; T_{opt} is the optimum temperature for the growth: $T_x = T_{min}$ if $T \leq T_{opt}$; $T_x = T_{max}$ if $T \geq T_{opt}$.

Minimum, maximum and optimum values of the temperature vary according to algal species and adaptation to environmental factors. The application of this model is shown in Fig. 3.45.

The light limitation $f_2(I)$ is usually accounted for in the model by two functions. The first is a Michaelis–Menten equation which simulates a saturation effect of light similar to that shown for photosynthesis in Eq. (3.45).

$$f_2(I) = \frac{I}{k_L + I} \tag{3.50}$$

where I is the light intensity useful for photosynthesis at time t and depth h, and k_L is the semisaturation constant. $f_2(I)$ has to be integrated over the photoperiod and over the light depth penetration to obtain the total daily light active for the photosynthetic process in a day.

The second light limitation model is an optimum curve, or *Steel formulation*,

$$f_2(I) = \frac{I}{I_{opt}} \cdot e^{\left\{1 - \frac{I}{I_{opt}}\right\}}$$

If necessary, I_{opt} has to be adapted according to the adaptation of algae to light variation over a year. Also, this formulation has to be integrated over the photoperiod and the light depth to obtain the total daily light photosynthetically active.

Limitation by nutrient availability, f_3, has been modelled in the literature by two approaches: the *Monod* or *Michaelis–Menten kinetics* in which the maximum growth rate μ_{max} is limited by the external concentration, C_N, of the nutrient under constant nutrient composition of the algae, also known as the fixed stoichiometry model:

$$f_3(C_N) = \frac{C_N}{k_C + C_N},$$

a two-step process simulating firstly the nutrient uptake by the cell and secondly all the growth. The uptake process depends on the external concentration, C_N, as well as on the internal concentration q of the cell, and can be formulated as:

$$f_3(q, C_N) = (q_{max} - q) \cdot \left(\frac{C_N}{k_C + C_N} \right)$$

or as

$$f_3(q, C_N) = \frac{q_{max} - q}{q_{max} - q_{min}} \cdot \left(\frac{C_N}{k_C + C_N} \right)$$

where q is the internal concentration of the *nutrient cell quota*, and q_{min} and q_{max} are the minimum and maximum possible concentration of the nutrient in the cell, respectively.

Cell growth depends only on the internal quota, q, and may assume several forms:

1. $f_3(q) = \frac{q}{k_1 + q}$ Michaelis–Menten (q);

2. $f_3(q) = \frac{(q - q_{min})}{k_2 + (q - q_{min})}$ Michaelis–Menten ($q - q_{min}$);

3. $f_3(q) = 1 - \frac{q_{min}}{q}$ like (2) where $k_2 = q_{min}$;

4. $f_3(q) = \frac{q - q_{min}}{q_{max} - q_{min}}$ linear;

5. $f_3(q) = \frac{k_3 - (q_{max} - q_{min})}{(q_{max} - q_{min})} \cdot \frac{(q - q_{min})}{k_3 + (q - q_{min})}$

If more than one nutrient is limiting the growth, the model can account for this fact in a number of ways. Four major ways are reported in the literature. Theoretically, according to Liebig's law of minimum, f_3 would be written as:

$$f_3 = \min[f(\mathrm{C}), f(\mathrm{N}), f(\mathrm{P}), f(\mathrm{Si})]$$

the formulation of the single nutrient limiting function f_3 ranging between 0 and 1, will be presented later. A second way of accounting for the general limitation, is the so-called multiplicative limitation, where:

$$f_3 = f(\mathrm{C}) \cdot f(\mathrm{N}) \cdot f(\mathrm{P}) \cdot f(\mathrm{Si})$$

This function is usually limiting the growth too strongly because it multiplies factors all ranging between 0 and 1.

A third way is represented by the arithmetic mean of the single limitation functions and a fourth by their harmonic mean. Usually, the arithmetic mean does not limit the growth enough, while the harmonic one results in an effect similar to the first formulation of Liebig's law.

One of these combinations of the single limiting function can be selected and applied to the model according to the specific case and the best fit of the experimental data.

With reference to the general model for algal growth (3.48), respiration, essudation and natural mortality rates are usually accounted for with the same formula:

$$x = x(T_{\mathrm{ref}}) \cdot f_x(T)$$

where x is one of the processes listed above, and f_x is the usual Arrhenius function.

Finally, settling of algae follows the model shown in the section on settling in Part A of this chapter, and grazing G is proportional to the zooplankton grazer and fishes biomass.

Values for the parameters used in the model in this section can be found in Jorgensen et al. (1991).

Nutrient Limitation

The growth of a population is always limited by the availability of the resources in the environment: food, solar energy and even space can be some of the factors limiting the potential growth. The various resources are, of course, never available in exactly the proportions needed for growth (see, for instance, Table 3.14 which shows the composition of freshwater plants). Figure 3.46 shows the ideal growth of a single population of bacteria feeding on a limited amount of substrate. Initially, the large availability of all types of resources allows an exponential growth of the population, but as a consequence of the declining amount of substrate, the population growth starts to be limited. The population declines to a steady-state value which corresponds with a balance between use and regeneration of the resource.

The basic theory of growth limitation was described Liebig (1840). It assumes that the composition of an organism is (almost) constant. The growth requires

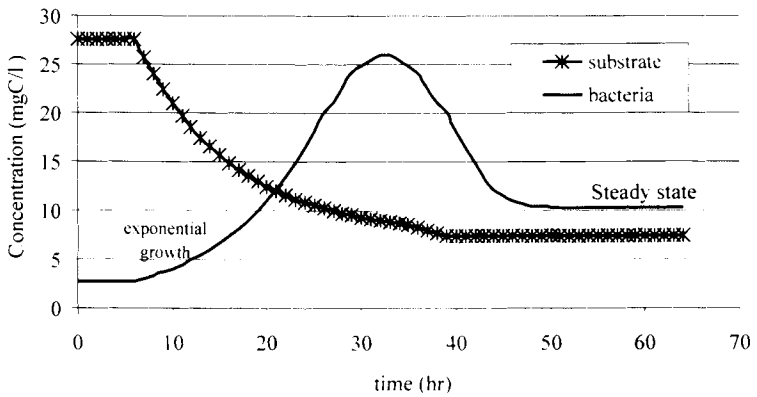

Fig. 3.46. Ideal growth of a single population of bacteria feeding on a limited amount of substrate of organic matter.

nutrients available in a balanced quantity. According to Table 3.14, phytoplankton consists mainly of C, H, O, N, P, Si and S. The ratio C:N:P = 40:7:1 by weight, called the *Redfield ratio*, is often used to indicate the three most important nutrients for phytoplankton growth of plants in general. If the N:P ratio is more than 7, P will be limiting. If the ratio is less than 7, N is limiting. C is only very rarely the limiting nutrient.

The ratio total nitrogen to total phosphorus is often applied to indicate whether nitrogen or phosphorus is limiting, but this is a simplification that can hardly be justified in modelling or in practical environmental management. The following complications should therefore be considered in our model development:

1. Not all forms of nitrogen and phosphorus are directly available for growth.
2. The growth of phytoplankton is a two-step process: first uptake of nutrients, which determine the intracellular concentration. Second, a growth determined by the intercellular nutrient concentration. This is the basis for the more complex eutrophication model presented in Section 7.4.
3. Even if the concentration of soluble available nitrogen or phosphorus is very low, it does not necessarily imply that nitrogen or phosphorus is limiting, if the uptake rate is currently balanced with a regeneration rate. Phosphorus and nitrogen can, for instance, be released rapidly from the sediment, which can therefore supply the phosphorus and nitrogen needed for growth, although the concentrations in the water phase are low.
4. In environmental management, the core question is not which nutrient is limiting, but which nutrient can we most easily play on as limiting? Phosphorus is often not limiting in lakes with a high waste water loading, because the ratio nitrogen to phosphorus in waste water is about 4:1, less than 7:1. As phosphorus is more easily removed from waste water and present in drainage water from

non-point sources in much lower concentrations than nitrogen, it is often the best environmental strategy to remove phosphorus from the waste water with a high efficiency.

The considerations behind the these four complications are illustrated in Fig. 3.47.

Whereas the dissolved inorganic forms NO_x and NH_4 seem to provide a fairly reliable indicator of nitrogen available for phytoplankton growth, phosphorus speciation is much more difficult because of its reactivity with particles of different size in the water. Phosphorus as orthophosphate and as colloids in labile forms is available for growth, while phosphorus associated with very fine particles and colloids in more recalcitrant forms is not available for algal uptake, but usually accounted for in inorganic phosphorus analysis. Conversely, phosphorus adsorbed on particles and sediments may be available to buffer dissolved phosphorus concentration.

Figure 3.48 shows the dynamics of phytoplankton, assimilable nitrogen and orthophosphate in *Lake Belau* during the year 1991: nutrient decrease anticipates the end of the bloom, which is sustained in its final stage by the internal quota of nutrients and not by their lack of external concentrations. Following Liebig's law, a ratio between assimilable nitrogen and orthophosphate concentration in the water of 7:1 is balanced, a larger ratio indicates a phosphorus limitation, a lower one a nitrogen lack. Data reported in Fig. 3.48 show an initial limitation due to nitrogen (ratio 5:1); at the end of the bloom the concentrations show a system limited by phosphorus (ratio 9:1).

If we consider the internal quota at the end of the bloom, we discover that, in spite of this change in the external concentrations, internally the cells constantly show a nitrogen limitation; furthermore, nitrogen reaches the bottom concentration for survival (10 μg/l) very soon, while phosphorus does so only in the final stage of the bloom.

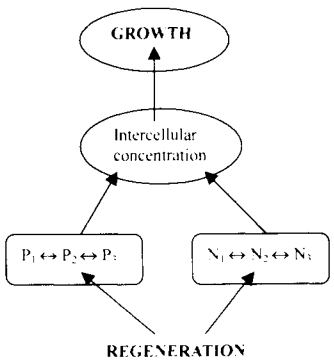

Fig. 3.47. Complications associated with the concept of the limiting nutrient. The growth is determined by the intracellular concentration, not by the concentration in the water phase. Some of the forms symbolized by P_1,P_2,P_3 and N_1,N_2,N_3, are not directly available. Furthermore, current regeneration will be able to balance the consumption. Moreover, in practical environmental management the problem is more related to which nutrient can we most easily make limiting, rather than which nutrient is limiting.

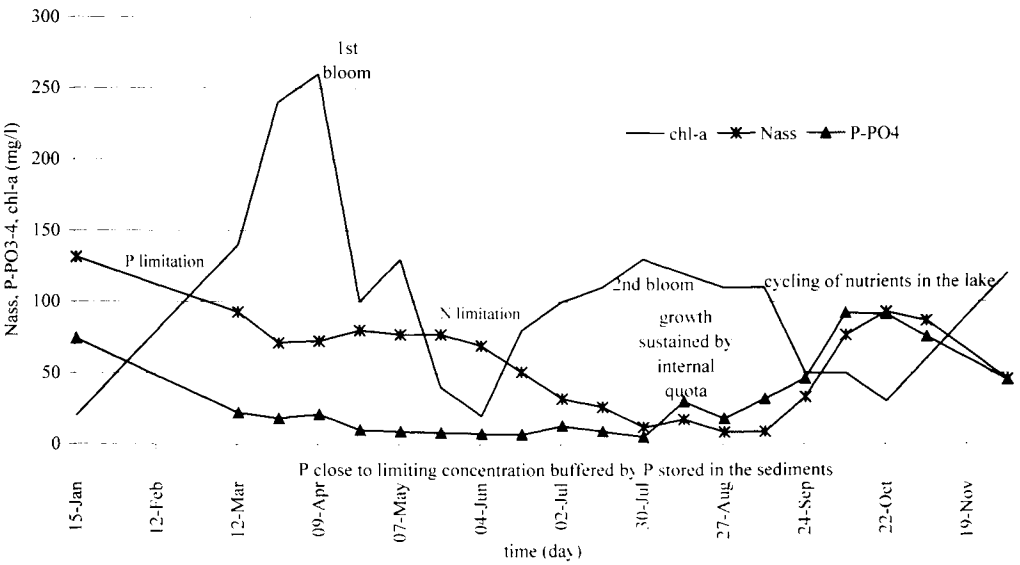

Fig. 3.48. Dynamic of phytoplankton, assimilable nitrogen and orthophosphate in lake Belau during 1991. The values of chlorophyll-a concentration are multiplied for 10^{-4}.

3C.4 Zooplankton Growth

Ecosystems are complex systems in which a food web can be identified. The compartment of primary producers of aquatic ecosystems includes algae that are grazed by the upper levels of the web. In the previous section we presented a way to model algal growth. In this section we present a model for *zooplankton growth* which is the basic component of the secondary producers. Many ecological models deal with primary producers and this is the reason why we can find in the literature a large number of them that simulate algal growth. But only a few models include zooplankton growth because it is necessary only to simulate the long-term behaviour of the ecosystem.

The basic conceptual model including zooplankton growth is represented in Fig. 3.49, where grazing and excretion close the biogeochemical cycle between nutrients, algae and zooplankton. However, such a simple model does not include other processes such as respiration (r), mortality (m), and settling (s) that transfer dead biomass to detritus, and the feedback of decomposition that completes the biogeochemical cycle.

As for algae, zooplankton biomass can also be simulated in a global way without differentiation between groups of zooplankton or making any distinctions according to feeding types (herbivores, omnivores, carnivores, selective and non-selective filters) or taxonomic groups (*Cladocerans*, *Copepods*, *Rotifers*, etc.).

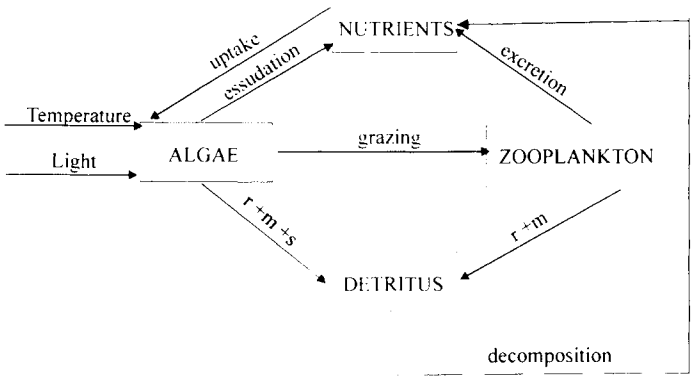

Fig 3.49. Conceptual model of a basic ecosystem including zooplankton. If the focus of the model is on the long-term ecosystem behaviour, the detritus compartment and the related processes of respiration, mortality, settling and decomposition can be omitted.

The growth of zooplankton Z is usually modelled with the following equation:

$$\frac{dZ}{dt} = (g - r - ex - m) \cdot Z - G \tag{3.50}$$

where g is the gross growth rate ($1/t$); r is the respiration rate ($1/t$); ex is the excretion rate ($1/t$); m is the non predatory mortality rate ($1/t$); and G is the loss velocity for predation exerted by other groups of zooplankton or fishes.

Settling is not included in the model, because zooplankton is mobile and can swim in the water. Equation (3.50) does not account for partition into age cohorts which can be included in more complex models.

The growth rate of zooplankton usually simulates the reproduction of the population and the individual biomass growth. They depend on the ingested and on the assimilated food. The efficiencies of these two processes vary according to:

- zooplankton factors such as: species, age, size, sex, reproductive state;
- food factors such as: concentration, type, quality, desirability;
- temperature.

In spite of the number and complexity of the processes and factors that regulate zooplankton growth rate, even a simple model such as the following, may be a good model:

$$g = C \cdot E$$

where C is the ingestion rate (mass of food ingested per mass of zooplankton in time); and E is a dimensionless parameter accounting for assimilation of food. This

model requires few data for its calibration. The ingestion rate is usually modified for filtering zooplankton groups in this way:

$$C = C_f \cdot F \tag{3.51}$$

where C_f accounts for filtration process (volume of water filtered per mass of zooplankton in time), and F is food concentration (mass of food per volume of water).

A slightly more complex version of the model (3.51) introduces the dependence on temperature, $f_1(T)$, and that for food, $f_2(F)$ without distinction between different types of available food:

$$C = C_{max}(T_{ref}) \cdot E_{max}(T_{ref}) \cdot f_1(T) \cdot f_2(F) \tag{3.52}$$

where $C_{max}(T_{ref})$ and $E_{max}(T_{ref})$ are the maximum ingestion rate and the maximum assimilation efficiency at the reference temperature, respectively; $f_1(T)$ is the temperature function; and $f_2(F)$ is the function that accounts for the food availability.

Temperature affects not only the growth but also the reproduction of these animals. It is accounted for in the model as an optimum function, $f_1(T)$, similar to that used for algae.

The food limitation processes are different for predators and filter feeders. For the zooplankton groups of predator, at low concentrations of food, ingestion rate is proportional to the prey density, since less energy and time are required to find and capture the prey. At very low food concentrations, zooplankton no longer feeds and F can be modified into $F - F_0$ where F_0 is the food concentration below which feeding does not occur.

At abundant food concentrations, the ingestion rate reaches a saturation level. This can be modelled, either with a Michaelis–Menten equation, or with the *Ivlev function*:

$$f_2(F) = 1 - e^{-k \cdot F}$$

For the zooplankton group of filter feeders, the limitation of the growth rate generally decreases with an increase in the food concentration, and the following model is used to account for this process:

$$f_2(F) = 1 - \frac{F}{k+F} = \frac{k}{k+F}$$

If more than one food type F_i is considered, for feeding, the $f_2(F)$ function in model (3.52) accounts for them putting $F = \sum_i p_i \cdot F_i \cdot E_i$; where zooplankton preference for each type of food is included in the model by a dimensionless preference parameter p_i, and by an assimilation efficiency E_i, typical of the food type.

As for the algal growth model, respiration, excretion and natural mortality are usually accounted for in the model with a function:

Table 3.19. Summary of the most common values of the parameters used in the zooplankton model.

Zooplankton group	Ingestion (1/day)	Filtration (1/(mg C·day))	Growth (1 day)	Assimilation efficiency	Ingestion half saturation constant (mg/l)
Total	0.3–0.8	0.1–1.0	0.1–0.3	0.6	0.5–2.0
Omnivores	0.4–1.4	–	–	0.6	0.3
Herbivores	–	0.7–1.4	–	0.6	0.01–0.015 mg Chl-a/l
Carnivores	0.7–1.6	1.0–3.9	–	–	0.02–0.2
Copepods	1.7–1.8	0.1–6.0	0.5	–	1
Rotifer	1.8–2.2	0.6–1.5	0.4–0.7	0.5	0.5
Mysidis	1.0–1.2	–	0.1	0.5	0.5
Cladocerans	1.6–1.9	0.2–1.6 1/(mg DW·day)	0.3–0.7	0.5	0.5–1.8

$$x = x(T_{ref}) \cdot f_t(T)$$

The loss velocity for predation, G, in model (3.50) is set constant if zooplankton is the top level of the modelled food web. Otherwise it can be simulated by the usual function:

$$G = \gamma \cdot Z$$

where γ is the predation rate (mass of zooplankton per mass of predators over time) and Z is the predator biomass feeding on zooplankton. Table 3.19 summarizes the values of the parameters used in this section: more details can also be found in Jorgensen et al. (1991).

3C.5 Fish Growth

Fish is a component of ecosystems that are very rarely included in the most complex models of ecosystems. Fishes feed on algae or on zooplankton, or both, and their growth depends on other environmental factors. The models presented in this section describe a simple case that does not account for the structure or age of the fish population. The models are able to simulate a single species of fish and can be adapted either to an individual fish or to a population of fishes. The body size is an important parameter of the model because no realistic growth model can ignore the influence of body size on the growth processes. A growth model stressing the fate of food items is of the metabolic type.

Earlier growth models have been more or less empirical equations fitting a course of growth in relation to time or age, e.g. the *logistic*-, the *Gompertz*-, the *Johnson*-, and the *Richard-growth curve*. These models are all discussed by Ricker

(1979). Their purpose was to get the best fit without considering the meaning of the parameters.

It was also generally observed that the growth curve, in temperate climates, varies seasonally with changes in temperature and food availability. It generally follows a *sigmoid course* of growth when the fish approached the so-called asymptotic body size. Changes in the environment to more favourable conditions increase the growth of fish to a new and higher asymptotic body size. These distinctive patterns of growth in the life of a fish were called growth stanzas, separated by physiological and ecological thresholds (Parker and Larkin, 1959).

A growth model ought to consider all the factors that might influence growth. These factors are:

- intrinsic: fish species and race, fish size, swimming activity, maturity, age;
- extrinsic: which can be subdivided into:
  —abiotic: photoperiod, temperature, oxygen content of the water, pH, carbon dioxide, various toxic substances such as ammonia, nitrite, heavy metals etc., salinity, light intensity
  —biotic: diets, ration, feeding frequency, care, diseases, and social hierarchy.

To incorporate all these factors in a growth model will demand an enormous amount of experimentation. Any growth model must include at least the three factors: ration, fish size and temperature, as variables having a great influence on the growth for a given species and diet. The basis for animal life and for growth is food consumption. Hence, a growth model will partly be a description of the fate of the food consumed. This fate can be written in the following way:

$$B = C - F - U - R$$

where B is the total change in energy value of body (growth); C is the energy value of food consumed; F is the energy value of faeces; U is the energy value of materials excreted in the urine or through the gills or skin; R is the total energy of metabolism which can be subdivided as follows: $R = R_s + R_d + R_a$, where R_s is the energy equivalent to that released in the course of metabolism by an unfed and resting fish (standard conditions); R_d is the additional energy released in the course of digestion, assimilation and storage of materials consumed (including specific dynamic action); and R_a is the additional energy released in the course of swimming and other activities.

If we consider the body weight, w, instead of its energy content, the previous equation can be written in a continuous way:

$$\frac{dw}{dt} = \xi(t) + in - out$$

where *in* and *out* stand for the quantity of energy matter entering the fish and leaving the fish respectively during the time dt. As a unit for w, *in* and *out* we shall use wet

weight but the following derivation would still hold if another unit such as dry weight or caloric content was applied. A basic and tacit assumption of the model is that the food (*in*) and the fishes are assumed to have approximately equal chemical composition; $\xi(t)$ designates total accumulated food intake of a fish at age t, in other words, the quantity of food consumed during the time period dt. The term *out* comprises *fasting catabolism*, non-digested food and *feeding catabolism*. Fasting catabolism $w(t)_{\text{fasting}}$, which will be quantified below, represents losses due to the metabolic processes that take places independent of feeding at time t.

When feeding, only a constant fraction β of the food consumed is assumed to be digested. Feeding catabolism represents losses due to the process of feeding and the subsequent activities of assimilation and is assumed to amount to a constant fraction α of the digested food $\beta \cdot \xi$. Thus we can write:

$$out = w(t)_{\text{fasting}} + (1 - \beta) \cdot \xi(t) + \alpha \cdot \beta \cdot \xi(t)$$

where $(1 - \beta) \cdot \xi(t)$ is the undigested part of the food and $\alpha \cdot \beta \cdot \xi(t)$ is the energy food quantity necessitated by feeding. $\frac{dw}{dt}$ may now be rewritten as:

$$\frac{dw}{dt} = \xi(t) - (1-\beta) \cdot \xi(t) - \alpha \cdot \beta \cdot \xi(t) - w(t)_{\text{fasting}}$$

or, rearranging the equation, as:

$$\frac{dw}{dt} = \beta(1-\alpha) \cdot \xi(t) - w(t)_{\text{fasting}}$$

The terms for fasting catabolism, $w(t)_{\text{fasting}}$, give the weight loss of a fish fasting in the period dt. The magnitude of this weight loss depends on the weight of the fish and on the duration of the fasting period, because even in a fasting fish every cell must continue to metabolize in order to remain alive. From respiration experiments there is evidence that fasting catabolism is not proportional to the weight proper. To account for this fact the following model is used:

$$w(t)_{\text{fasting}} = k \cdot w(t)^n$$

where k is the coefficient of fasting catabolism and n is the exponent of fasting catabolism.

The food intake $\xi(t)$ is assumed to be proportional to the length of the time period dt. $\xi(t)$ is also assumed to be proportional to the body weight w to the power m, i.e. the food-absorbing surface is assumed proportional to w^m. The interaction with the environment is described by a factor called the *feeding level*, which is a real number between 0 and 1. A fish is said to obtain feeding level 0 under starvation ($\xi = 0$) and a fish eating all the food it possibly can ($\xi = h \cdot w^m$) is said to have reached feeding level 1. A fish eating the fraction f of its maximum intake is said to have feeding level f. Thus:

$$\xi(t) = f \cdot h \cdot w(t)^m$$

We can now write the model as:

$$\frac{dw}{dt} = \beta(1-\alpha) \cdot f \cdot h \cdot w(t)^m - k \cdot w(t)^n$$

This is also known as the Ursin *metabolic growth* model (Ursin 1967, 1979; Andersen and Ursin, 1977), with no account of spawning losses where: $w(t)$ weight of a fish aged t (years) (g); β = fraction absorbed of food eaten; α = fraction of assimilated food lost in feeding catabolism; f = feeding level ($0 \leq f \leq 1$); h = coefficient of food consumption (g^{1-m} $year^{-1}$); m = exponent of food consumption; k = coefficient of fasting catabolism (g^{1-n} $year^{-1}$); n = exponent of fasting catabolism.

The parameters of the metabolic growth model are usually assumed to remain approximately constant in time and the Ursin metabolic model is given in the form:

$$\frac{dw}{dt} = H \cdot w(t)^m - k \cdot w(t)^n$$

where

$$H = \beta \cdot (1-\alpha) \cdot f \cdot h$$

The shape of the growth curves depends on m and n. If $m < n$, the characteristic shape will be as shown in Fig. 3.50a with an asymptote of

$$W_\infty = \left(\frac{H}{k}\right)^{\frac{1}{(n-m)}}$$

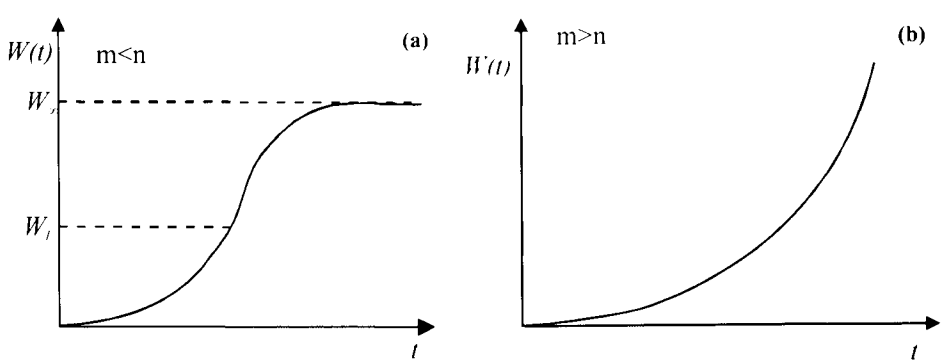

Fig. 3.50. Growth curve characteristics of the metabolic growth model with constant parameters.

and a point of inflection (i.e. maximum growth rate) occurring at

$$W_I = W_\infty = \left(\frac{m}{n}\right)^{\frac{1}{(n-m)}}$$

If $m \geq n$, the shape will be as shown in Fig. 3.50b.

3C.6 Single Population Growth

The models presented in Sections 3C.3, 3C.4 and 3C.5 refer to specific populations or individuals of primary and secondary producers and give a detailed description of the influence on growth of external forcing functions and of specific mechanisms. If we refer to a single population of a given species and we are interested in simulating the dynamics of growth of this population, we can refer to a set of models with different degrees of sophistication

The *linear growth* is the most simple type of model for population dynamics. It is not very diffused because it simulates a growth limited by values of a factor, e.g. a gene essential for the growth of the cell, passed only to one of the two new cells, with the consequence that the cell with the gene can further reproduce and the other is sterile.

The model can be written in this way:

$$\frac{dx}{dt} = C$$

where x is the population and C is the constant factor.

If we consider a population in which each individual is able to reproduce, we obtain an *exponential growth*. This model can be written:

$$\frac{dx}{dt} = r \cdot x$$

where r is the specific growth rate. Its solution is

$$x(t) = x_0 \cdot e^{rt}$$

where x_0 is the initial value of the population.

An exponential growth is not sustainable in the long period because of the limited resources of the environment that can support the growth. After an initial phase of exponential growth, the population density approaches a certain value and, over a long period, tends to stabilize around this value, which is usually called the *carrying capacity* of the ecosystem for the given population.

This type of single population growth is known as *logistic growth*. Its model is:

$$\frac{dx}{dt} = r \cdot x \cdot \left(1 - \frac{x}{k}\right)$$

The previous exponential model is multiplied by a term accounting for the decrease of the growth rate as the population approaches the carrying capacity, k.

At this value, the population growth is zero and it reaches a stable steady state. The solution of the logistic model is:

$$x(t) = \frac{k \cdot x \cdot e^{r \cdot t}}{k - x_0 \cdot (1 - e^{r \cdot t})}$$

the maximum growth rate of the population is reached where $x = \frac{k}{2}$, which is the flex point of the symmetric curve (see Fig. 3.51). The logistic model belongs to the more general class of models of *sigmoidal curves*

$$x(t) = \frac{A}{1 + e^{\phi(t)}}$$

where $\phi(t)$ is a generic function of the growth rate.

In this class can be included other classical models used in the literature to simulate the single population dynamic. For instance the *von Bertalanffy* and the *Ursin models*, already seen for the fish growth simulation, can be applied to a population:

$$\frac{dx}{dt} = r \cdot x^n - k \cdot x^m$$

where the growth of the population is the effect of an anabolic process $r \cdot x^n$, proportional to a power $2/3 \leq n \leq 1$ of the population, and of a catabolic one proportional to the population too.

Almost two centuries ago, Gompertz proposed the following sigmoidal model to simulate the growth of a population:

$$\frac{dx}{dt} = r \cdot x \cdot (\ln k - \ln x)$$

where the specific growth rate

$$R = \frac{1}{x}\frac{dx}{dt} = r \cdot (\ln k - \ln x)$$

accounts for the senescence of a population decreasing in time its growth rate. Another model of this class is represented by *Richard's model*:

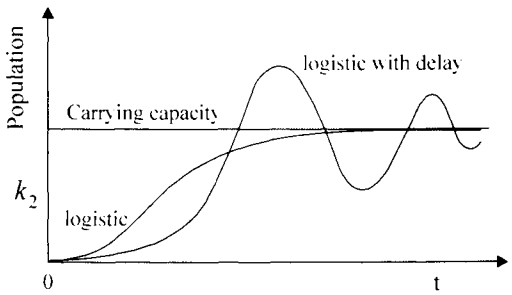

Fig. 3.51. Plot of the logistic model compared with the same one, in which a delay time in reproduction has been introduced.

$$\frac{dx}{dt} = x \cdot \frac{r}{n} \cdot \left(1 - \frac{x^n}{k^n}\right)$$

which is a general form of the logistic one to which it can be reduced if $n = 1$. This model has been applied extensively to the growth of plants.

All the previous models consider that the reproduction of an individual may occur immediately after it is born. This is a simplification of the reality because reproduction usually occurs after the maturity time t_M, which is a delay in reproduction time.

Such a delay can be inserted in the logistic curve in this way:

$$\frac{dx}{dt} = r \cdot x(t) \cdot \left(1 - \frac{x \cdot (t - t_M)}{k}\right)$$

The introduction of the delay induces oscillations in the population dynamic, shown in Fig. 3.51, which may result in values of x higher than the carrying capacity.

In the long period, according to different values of t_M, fluctuations may tend to decrease and to set up around the carrying capacity y, or they may result in a limit cycle and the population may totally collapse too.

3C.7 Ecotoxicological Processes

Biodegradation

We can distinguish between primary and ultimate biodegradation: primary biodegradation is any biologically induced transformation that changes the molecular integrity; ultimate biodegradation is the biologically mediated conversion of organic compounds to inorganic compounds and products associated with complete and normal metabolic decomposition.

The biodegradation rate is expressed by application of a wide range of units:

- as a first order rate constant (1/24 h);
- as half life time (days or hours);
- mg per g sludge per 24 h (mg/g 24 h);
- mg per g bacteria per 24 h (mg/g 24 h);
- ml of substrate per bacterial cell per 24 h (ml/24 h cells);
- mg COD per g biomass per 24 h (mg/g 24 h);
- ml of substrate per gram of volatile solids inclusive microorganisms (ml/g 24 h);
- BOD_x/BOD, i.e., the biological oxygen demand in x days compared with complete degradation, called the BOD coefficient;
- BOD_x/COD, i.e., the biological oxygen demand in x days compared with complete degradation, expressed by means of COD.

The biodegradation rate in water or soil is difficult to estimate because the number of microorganisms varies by several orders of magnitudes from one type of aquatic ecosystem to the next and from one type of soil to the next.

Biodegradation rates may be expressed in several ways; microbiological degradation may, with good approximation, be described as a Michaelis–Menten equation:

$$\frac{dC}{dt} = -\frac{dB}{Y \cdot dt} = -\mu_{max} \cdot \frac{B}{Y} \cdot \frac{C}{k_m + C} \tag{3.53}$$

where C is the concentration of the compound considered, Y is the yield of microorganism biomass B per unit of C, μ_{max} is the maximum specific growth rate and k_m is the half saturation constant. If $C << k_m$, the expression is reduced to a first-order reaction model:

$$\frac{dC}{dt} = -k_1 \cdot B \cdot C \tag{3.54}$$

where

$$k_1 = \frac{\mu_{max}}{Y \cdot k_m}$$

B is, in nature, determined by the environmental conditions. In aquatic ecosystems B is, for instance, highly dependent on the presence of suspended matter. B may therefore, under certain conditions, be considered a constant which reduces the rate expression to:

$$\frac{dC}{dt} = -k \cdot C \tag{3.55}$$

An indication of the values of k ($1/t$) can therefore be used to describe the rate of biodegradation. If the biological half life time is denoted by $t_{1/2}$, we get the following relation:

$$\ln 2 = 0.693 = k \cdot t_{1/2}$$

This implies that the biological half life time can also be used to indicate the biodegradation rate.

In some cases, however, the biodegradation is very dependent on the concentration of microorganisms as expressed in Eqs. (3.53) and (3.54). Therefore, k_1 indicated in the unit mg/(g · d.wt. · 24 h) will in many cases be more informative and correct.

In the microbiological decomposition of xenobiotic compounds an acclimatization period from a few days to 1–2 months should be foreseen before the optimum biodegradation rate can be achieved.

The Equilibrium between Spheres

An increase or decrease in the concentration of components or elements in ecosystems is of vital interest, but the observation of trends in global changes of concentrations might be even more important as they may cause changes in life conditions on earth.

Concentrations in the four spheres, atmosphere, lithosphere, hydrosphere and biosphere, are of importance in this context. They are determined by the transfer processes and the equilibrium concentrations among the four spheres. As shown in Part A of this chapter, the solubility of a gas at a given concentration in the atmosphere can be expressed by means of *Henry's law* which determines the distribution between the atmosphere and the hydrosphere.

If we consider only two components in the hydrosphere: a tracer h and water, and we assume that $C_h << C_w$, we can replace C_w with the concentration of water in water = 1000/18 = 55.56 mol/l. According to these approximations, we obtain the following equation:

$$\frac{C_a}{C_h} = \frac{He}{R \cdot T \cdot C_w}$$

where C_a is the molar concentration in the atmosphere of component h, expressed in (mol/l) and C_h is the concentration in the hydrosphere expressed also in (mol/l) and C_w is the (mol/l) of water (and other possible components).

The soil–water distribution may be expressed by one of the *adsorption isotherms*, presented in Part B of this chapter, for compounds of ecotoxicological interest, the exponent γ in *Freundlich's adsorption isotherm* (3.36) is often close to 1 and for most environmental problems C is small. This implies that

$$a = \frac{q_s}{C_s}$$

becomes a distribution coefficient, usually indicated by k. As shown in Section 3B.6 for 100% organic carbon, k is denoted by k_{oc}, may be estimated from k_{ow}. Several estimation equations have been published in the literature; see for instance Jørgensen et al. (1997a). The following log–log relationships between k_{oc} (100% organic carbon presumed) and k_{ow} are typical examples (Brown and Flagg, 1981):

$$\log k_{oc} = -0.006 + 0.937 \cdot \log k_{ow} \tag{3.56a}$$

or (Leeuwen and Hermens, 1995):

$$\log k_{oc} = -0.35 + 0.99 \cdot \log k_{ow} \tag{3.56b}$$

Several other estimation equations of importance for ecotoxicological modelling can be found in Section 8.5.

In the case where the carbon fraction of organic carbon in soil is f, the distribution coefficient (k_D) for the ratio of the concentration in soil and in water can be found as $k_D = k_{oc} \cdot f$. If the solid is activated sludge (from a biological treatment plant) instead of soil, Matter-Müller et al. (1980) have found the following relationship:

$$\log FAS = 0.39 + 0.67 \log k_{ow}$$

where FAS (fraction of the activated sludge) is the ratio between the equilibrium concentrations in activated sludge and in water.

k_{ow} can be found for many compounds in the literature, but if the solubility in water is known it is possible to estimate the partition coefficient n-octanol–water at room temperature by the use of a correlation between the water solubility (in μmol/l) and k_{ow}. A graph of this relationship is shown Fig. 8.10.

Bioaccumulation

The distribution between the biosphere and the hydrosphere is also of importance. BCF (bioaccumulation factor) is the ratio between the concentrations in an organism and in water. It is used to describe the bioconcentration. It can be found for many compounds and for some organisms in the literature. BCF may also be estimated (see Fig. 8.11) where two log–log plots between BCF and k_{ow} are shown for mussels and fish (length 20–30 cm).

H_e, k_{oc}, k_D and BCF all express a ratio between two equilibrium concentrations in two different spheres. A transfer of a compound from one sphere to another will take

place until the equilibrium concentrations have been attained. The rate of transfer will usually be proportional to the distance from equilibrium, and dependent on the diffusion coefficient of the compounds and of the resistance at the boundary layer between the two spheres. The resistance at the boundary layer and the influence of the diffusion coefficient are usually covered by an empirical expression which is dependent on the temperature (the diffusion is strongly dependent on the temperature), the surface exposed to the atmosphere relative to the water volume and the rate of the water flow.

The uptake from water can often be expressed in the same simple manner for both animals and plants. A good approximation is:

$$BCF = \frac{C_b}{C_w} \tag{3.57}$$

where BCF = a concentration factor; C_b = the biotic concentration (g/kg); C_w = the concentration in water (g/l).

There is a correlation between BCF and k_{ow} as previously presented in Section 2.5.

Equation (3.57) may be modified to account for the lipid phase in the organism. This is of importance particularly when we are using allometric principles to extrapolate the BCF value from one or a few organisms to many organisms. The allometric principles presented in Section 2.3 are strictly valid only for hydrophilic compounds ($\log k_{ow} \leq 1.5$) or for organisms with the same percentage of fat tissue.

Generally we can state (see, for instance, Connell, 1997) that:

$$\log BCF = \log f_{lipid} + b \cdot \log k_{ow} \tag{3.58}$$

where f_{lipid} is the lipid fraction in the organisms; b is usually close to 1 (often indicated to be 1.03). If C_L is the concentration of the lipophilic organic compound in the fat tissue, we have:

$$C_L = \frac{C_b}{f_{lipid}}$$

As $k_{ow} = C_L/C_w$, provided that we can consider the solubility in the fat tissue to be close to the solubility in octanol, we get:

$$\log BCF = \log f_{lipid} + \log k_{ow} \tag{3.59}$$

which is Eq. (3.58) with $b = 1.0$.

This equation implies that the allometric principle can be used only for the same lipid fraction. However, Eq. (3.59) can be used to convert from one lipid fraction to

another. Many fish contain about 5% lipid, or $\log f_{\text{lipid}} = -1.3$. If we know *BCF* values for fish with a lipid concentration of 5% and we want to know the *BCF* value for a fish of another size and with 10% lipid, we can use the allometric principles to find the *BCF* for the right fish size but with 5% lipid and then add 0.3 to the log *BCF* value to account for the higher lipid content.

The bioaccumulation factor *BCF* for the relationship between soil or sediment and biota is: C_b/q_s, completely parallel to Eq. (3.57). If the concentration in the pore water is denoted by C_w, we obtain the following expression:

$$BCF = \left(\frac{C_b \cdot C_w}{q_s \cdot C_w} \right) = \frac{BCF_{\text{org-water}}}{k_D} \tag{3.60}$$

By using Eq. (3.58) and the partition coefficient k defined in Section 3B.6 and remembering the correlation of $BCF_{\text{org-water}}$ and k to k_{ow}, we get:

$$BCF = \frac{f_{\text{lipid}} \cdot k_{ow}^{b}}{x \cdot f_{oc} \cdot k_{ow}^{a}}$$

where x is a proportionality constant, and f_{oc} is the fraction of organic carbon in the soil, as shown in Section 3B.6.

If we use the above-mentioned b value of 1.03, the value corresponding to x, the proportionality constant in Eq. (3.56a) which is antilog $(-0.006) \approx 0.99$ and the a value in Eq. (3.56a) which is 0.937, we get the following expression for the *BCF* for the bioaccumulation factor soil or sediment–organism:

$$BCF = \left(1.01 \cdot \frac{f_{\text{lipid}}}{f_{oc}} \right) \cdot k_{ow}^{0.09}$$

This implies that *BCF* soil or sediment–organism has only a small dependence on k_{ow} and other properties of the soil. It depends more on the properties of the soil and the biota, particularly the ratio of lipid in the biota to the organic carbon content of the soil.

The *retention of toxic substances* is determined by the excretion rate, which can be approximated by means of the following first-order equation:

$$r_e = k_e \cdot C_b$$

where r_e = excretion rate (g/day·body weight); k_e = excretion rate coefficient (1/day); C_b = concentration of toxic substances (g/body weight).

The excretion rate coefficient, k_e, can be approximated as:

$$k_e = a \cdot m^{b}$$

where a and b are constants (b is close to 0.75), and m is the body weight. The retention can now be calculated as:

$$\frac{dC_b}{dt} = U - r_e$$

where U = (uptake from food + uptake from air + uptake from water + uptake from soil).

This model of the concentration of toxic substances in plants and animals is extremely simple and should only be used to give a first rough estimate. For a more comprehensive treatment of this problem, see Butler (1972), ICRP (1977), de Freitas and Hart (1975), Mortimer and Kundo (1975), Seip (1979), Jørgensen et al. (1991) and Jørgensen (1994). Tables 3.20 and 3.21 give some characteristic excretion rates and uptake efficiencies. Note that the uptake efficiency is dependent on the chemical form of the component and on the composition of the food.

A wide variety of terms is used in an inconsistent and confusing manner to describe uptake and retention of xenobiotics by organisms using different paths and mechanisms. However, three terms are now widely applied and accepted for these processes:

Table 3.20. Excretion rates with the urine of some metals for some animals.

Species	Component	Excretion rate (% abs. amount/day)
Rat	Cd	1.25
Homo sapiens	Hg	0.01
Rat	Hg	1.0
Sheep	Pb	0.5–1.0
Homo sapiens	Zn	8.0

Table 3.21. Uptake efficiencies of some toxicants for some animals.

Species	Component	Uptake efficiency
Homo sapiens	DDT	14.4% (dairy product)
Homo sapiens	DDT	40.8% (meat product)
Homo sapiens	DDT	9.9% (fruit)
Monkey	Hg	90.0% (methyl-Hg)
Rat	Hg	90.0% (methyl-Hg)
Rat	Hg	20.0% (Hg-acetate)
Rabbit	Pb	0.8–1.0% (in food)
Sheep	Pb	1.3% (in food)
Pinfish	Zn	19.0% (in food)

1. *Bioaccumulation* is the uptake and retention of pollutants by organisms via *any* mechanism or pathway. It implies that both direct uptake from air and water and uptake from food are included.
2. *Bioconcentration* is uptake and retention of pollutants by organisms directly from water through gills or epithelial tissue. This process is often described by means of a concentration factor.
3. *Biomagnification* is the process whereby pollutants are passed from one trophic level to another and it exhibits increasing concentrations in organisms related to their trophic level.

An enormous amount of data has been published on chemical analyses of plants and animals, but much is of doubtful scientific value. The precise questions to be answered through a given examination need to be clearly formulated at the initial stage. Again, the problem is very complex. It is not sufficient to set up computations for the retention of toxic substances; it is necessary to ascertain the distribution in the organism, the lethal concentration, the effect of sublethal exposure and the effects on populations over several generations (Moriarty, 1972; Schüürmann and Markert, 1998). Our knowledge in the field of ecotoxicology is rather limited and further research in the area is urgently needed.

PROBLEMS

1. A well mixed lake of 10^7 m^3 of volume is loaded with 300 kg of $N\text{-}NH_4^+$.
   - How much oxygen is consumed to oxidize completely this load?
   - How much time is needed if the water temperature is 15°C?
   - Suppose that the lake water is initially oxygen saturated, which oxygen concentration will be reached at the end of the oxidation process?
2. A shallow lake with a surface of 10^6 m^2, an average depth of 2 m, an affluent inflow of 3 m/s and a initial value of the phosphorus concentration of 0.1 mg/l, is loaded with 100 kg/y of phosphorus.
   - What will be the concentration at the steady state condition?
   - Which is the order of magnitude of the phosphorus settled in the lake?
3. BOD_5 is 25 mg/l at 25°C. Find the BOD_5 at 20°C.
4. The reaeration ratio of a river is 0.8 (1/day) at 15°C. Find the rate at 20°C.
5. A municipal waste water treatment discharges secondary effluent to a surface stream. The waste water has a flow of 100 l/s, a BOD_5 concentration of 30 mg/l at 20°C, an O_2 concentration of 2 mg/l and a temperature of 25°C. The stream has a summer minimum

flow of 1 m^3/s, BOD_5 of 3 mg/l a temperature of 22°C and an oxygen saturation concentration. Complete mixing is almost instantaneous. The velocity of river water is 0.2 m/s, and the depth of 0.8 m.

- Find the critical oxygen concentration and the distance from the treatment plant where the situation is most critical.
- Suppose a winter condition and evaluate the effect in this condition.

6. Consider a completely mixed shallow lake with an inflow of 40 l/s, an average depth of 3 m and an area of 150,000 m^2. The average wind speed on the area is approximately 5 m/s. The inflow water is characterized by an oxygen concentration of 8 mg/l and no BOD. The lake is impacted by a waste water discharge that produces 120 kg/day of BOD. The bottom of the lake is sandy and the Secchi depth is 2.25 m. The fraction of daylight is 0.5 while μ_{max} for dominant species of phytoplankton is 2 1/day. Due to the nutrient limitation μ can be estimated to 1 1/day, by using the model portrayed in Section 3C.3. The chlorophyll-a concentration is found to be 20 μg/l on average for the period considered. The O_2/chl-a ratio α_1 is estimated to be 0.2. A value of $k_1 = 0.2$ 1/day can be used. Assuming a temperature of $T = 20$°C determine the BOD_5 and the oxygen concentration in the lake.

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CHAPTER 4

Conceptual Models

4.1 Introduction

Nine different methods of *conceptualization* are presented in this chapter, along with their advantages and disadvantages. A general recommendation as to which method to use is not given. This is not possible, because, as will become clear from the discussion, the problem, the ecosystem, the application of the model and the habits of the modeller will determine the preference of the conceptualization method.

A conceptual model has a function of its own. If flows and storage are given by numbers, the diagram gives an excellent survey of a steady-state situation. It can be applied to get a picture of the changes in flows and storage if one or more forcing functions are changed and another steady-state situation emerges. If first-order reactions are assumed, it is even easy to compute other steady-state situations that might prevail under other combinations of forcing functions (see also Chapter 5). Two illustrations of this application of conceptual models are included in Section 4.4 to give the reader an idea of these possibilities.

4.2 Application of Conceptual Diagrams

Conceptualization is one of the early steps in the modelling procedure (see Section 2.3), but it can also have a function of its own, as will be illustrated in this chapter.

A conceptual model can not only be considered as a list of state variables and forcing functions of importance to the ecosystem and the problem in focus, but it will also show how these components are connected by processes. It is employed as a tool to create abstractions of reality in ecosystems and to delineate the level of organization that best meets the objectives of the model. A *wide spectrum* of conceptualization approaches is available and will be presented here. Some give only the components and the connections, others imply mathematical descriptions.

It is almost impossible to model without a conceptual diagram to visualize the modeller's concepts and the system. The modeller will usually play with the idea of constructing various models of different complexity at this stage in the modelling procedure, making the first assumptions and selecting the complexity of the initial model or alternative models. It will require intuition to extract the applicable parts of the knowledge about the ecosystem and the problem involved. It is therefore not possible to give general lines on how a conceptual diagram is constructed, except that it is often better at this stage to use a slightly too complex model than a too simple approach. At the later stage of modelling it will easily be possible to exclude redundant components and processes. On the other hand, if a too complex model is used even at this initial stage, the modelling will be too cumbersome.

Generally, good knowledge about the system and the problem will facilitate the conceptualization step and increase the chance of finding close to the right complexity for the initial model. The questions to be answered are:

- What components and processes of the real system are essential to the model and the problem?
- Why?
- How?

In this process a suitable balance is sought between elegant simplicity and realistic detail.

Identifying the level of organization and selecting the correct complexity of the model are not trivial problems. Miller (1978) indicates 19 hierarchical levels of living systems, but to include all of them in an ecological model is of course an impossible task, mainly due to the lack of data and a general understanding of nature. Usually, it is not difficult to select the focal level, where the problem is, or where the components of interest operate. The level one step lower than the focal level is often relevant to a good description of the processes. For instance, *photosynthesis* is determined by the processes going on in the individual plants. The level one step higher than the focal level determines many of the constraints (see the discussion in Section 2.12). These considerations are visualized in Fig. 4.1.

However, it is not necessary, in most cases, to *include more than a few or even only one hierarchical level* to understand a particular behaviour of an ecosystem at a particular level; see Pattee (1973), Weinberg (1975), Miller (1978) and Allen and Star (1982). Figure 4.2 illustrates a model with three hierarchical levels, which might be needed if a multi-goal model is constructed. The first level could, for instance, be a hydrological model, the next level a *eutrophication* model and the third a model of phytoplankton growth, considering the intracellular nutrients concentrations.

Each *submodel* will have its own conceptual diagram; see, e.g., the conceptual diagram of the phosphorus flows in a eutrophication model, Fig. 2.9 and 2.10. In this latter submodel there is a sub-submodel considering the growth of phytoplankton by use of intracellular nutrient concentrations (see Chapter 3C), which is conceptualized in Figs. 3.47 and 4.3. The nutrients are taken up by phytoplankton at a

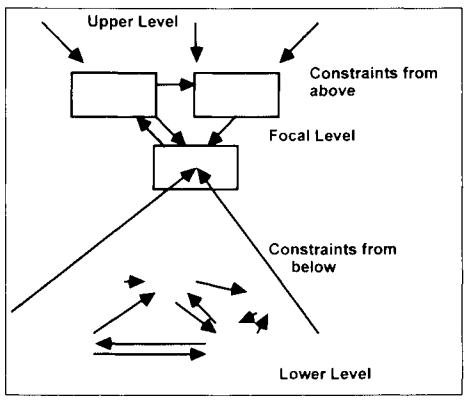


Fig. 4.1. The focal level has constraints from both lower and upper levels. The lower level determines, to a great extent, the processes and the upper level determines many of the constraints on the ecosystem.

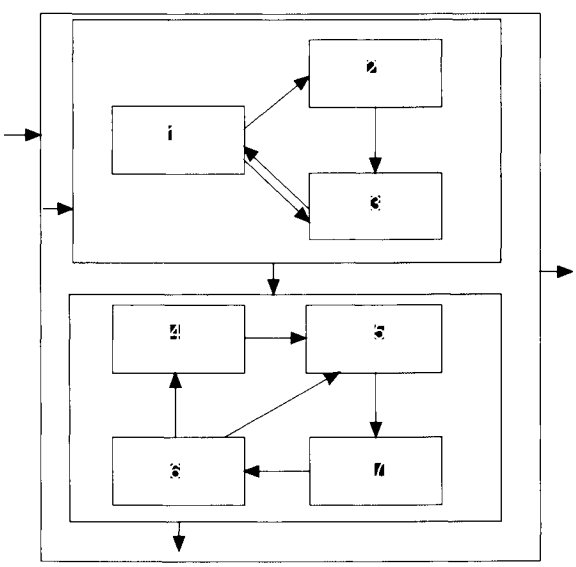


Fig. 4.2. Conceptualization of a model with three levels of *hierarchical organization*.

rate that is determined by the temperature, nutrient concentration in the cells and in the water. The closer the nutrient concentration in the cells is to the minimum, the faster is the uptake. The growth, on the other hand, is determined by solar radiation, temperature and the concentration of nutrients in the cell. The closer the nutrient concentration is to the maximum concentration, the faster is the growth. This description is according to phytoplankton physiology and a *eutrophication model* based on this description of phytoplankton growth (production) is presented in Chapter 7.

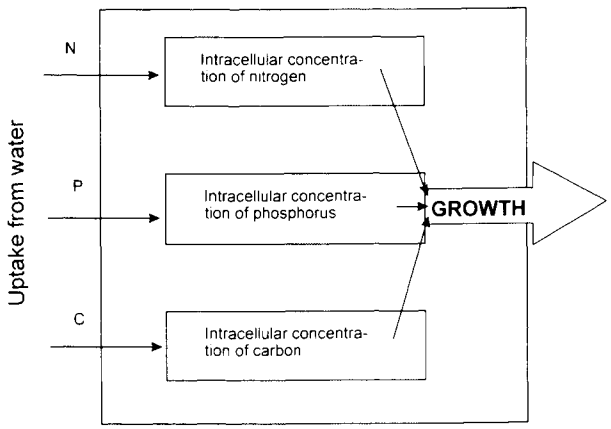


Fig. 4.3. A phytoplankton *growth model* with two hierarchical levels: the cells which determine the uptake of nutrients, and the phytoplankton population, the production (growth) of which is determined by the intracellular nutrient concentrations.

Models that also consider the distribution and effects of toxic substances might often require three *hierarchical levels*: one for the hydrodynamics or aerodynamics to account for the distribution, one for the chemical and biochemical processes of the toxic substances in the environment, and the third for the effect on the organism level.

4.3 Types of Conceptual Diagrams

Nine types of conceptual diagrams are presented and reviewed.

1. *Word models* use a verbal description of model components and structure. Language is the tool of conceptualization in this case. Sentences can be used to describe a model briefly and precisely. However, word models of large complex ecosystems quickly become unwieldy and are therefore only used for very simple models. The saying "One picture is worth a thousand words" explains why the modeller needs to use other types of conceptual diagrams to visualize the model.

2. *Picture models* use components seen in nature and place them within a framework of spatial relationships. Figure 4.4 gives a simple example.

3. *Box models* are simple and commonly used conceptual designs for ecosystem models. Each box represents a component in the model and arrows between boxes indicate processes. Figures 2.1, 2.9 and 2.10 show examples of this model type. The conceptual diagrams show the nutrient flows (nitrogen and phosphorus) in a lake. The arrows indicate mass flows caused by processes. Figure

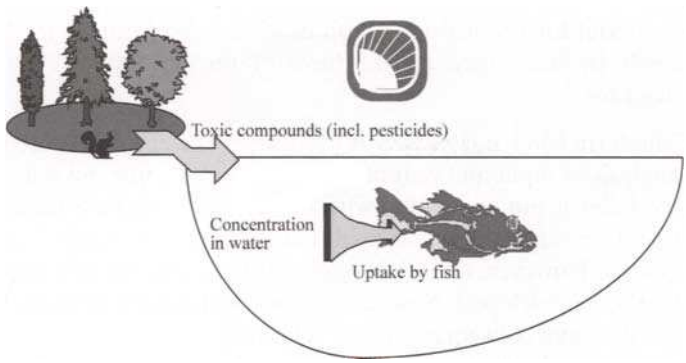


Fig. 4.4. Example of a picture model: pesticides from the littoral zone result in a certain concentration in the water. Fish take up the toxic compounds directly from the water. The model attempts to answer the crucial question: what would be the concentration in the fish of the toxic substance?

4.5 gives a conceptual diagram of a global carbon model, used as the basis for predicting the climatic consequences of increasing concentrations of carbon dioxide in the atmosphere. The numbers in the boxes indicate the amount of carbon on a global basis, while the arrows give information on the amount of carbon transferred from one box to another per annum. Some modellers prefer other geometric shapes, for example, Wheeler et al. (1978) prefer circles to boxes in their conceptualization of a lead model. This results in no principal difference in the construction and use of the diagram.

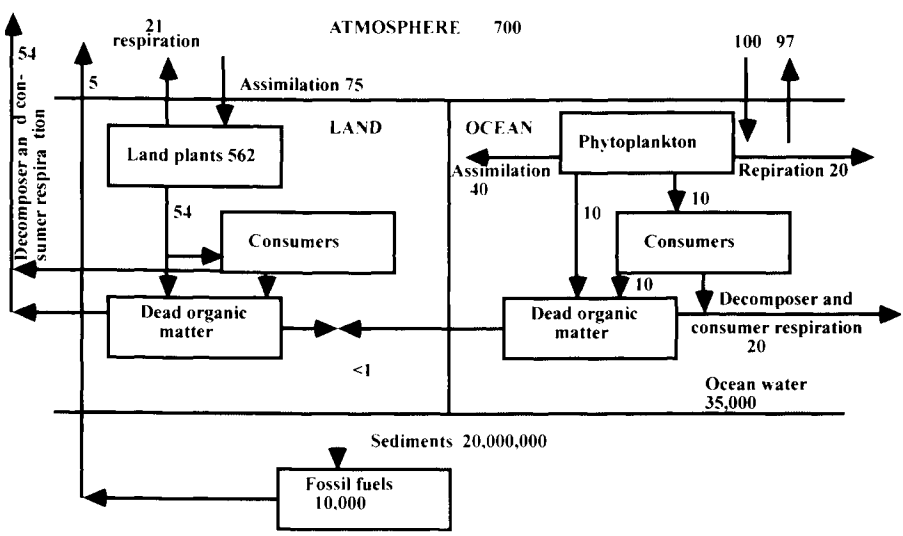


Fig. 4.5. Carbon cycle, global. Values in compartments are in 10^{9} tons and in fluxes 10^{9} tons/year. All fluxes balance each other with the exception of the transfer of carbon dioxide from fossil fuel to the atmosphere. Fortunately, 60% of this flux is absorbed by the ocean.

A model for predicting carbon dioxide concentration in the atmosphere can easily be developed on the basis of the mass conservation applied in the diagram.

The term *black box models* is used when the equations are set up based on an analysis of input and output relations, for example, by statistical methods. The modeller is not concerned with the causality of these relations. Such a model might be very useful, provided that the input and output data are of sufficient quality. However, the model can only be applied to the case study for which it has been developed. New case studies will require new data, a new analysis of the data and consequently new relations.

White box models are constructed based on causality for all processes. This does not imply that they can be applied to all similar case studies, because, as discussed in Sections 2.3 and 2.5, a model always reflects ecosystem characteristics. In general, however, a white box model will be applicable to other case studies with some modification.

In practice most models are *grey*, as they contain some *causalities* but also apply empirical expressions to account for some of the processes.

4. *Input/output models* differ only slightly from box models, as they can be considered as box models with indications of inputs and outputs. The global carbon model (see Fig. 4.5) can be considered an input/output model as all inputs and outputs of the boxes are indicated with numbers. Another example is shown in Fig. 4.6: this is an oyster community model, developed by Patten (1985). The same model is illustrated by use of matrix conceptualization (see item 5 below).

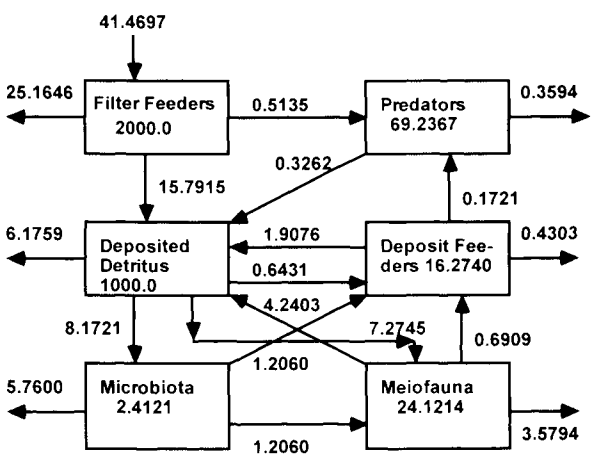


Fig. 4.6. *Input/output model* for energy flow (cal m^{-2} d^{-1}) and storage (kcal m^{-2}) in an oyster reef community, (reproduced from Patten, 1985). In the matrix representation is the sequence: (1) filter feeders; (2) deposited detritus; (3) microbiota; (4) meiofauna; (5) deposit feeders; (6) predators.

COMPARTMENTS

(a)

From / To	1	2	3	4	5	6	Row Sum
1	1	0	0	0	0	0	1
2	1	1	0	1	1	1	5
3	0	1	1	0	0	0	2
4	0	1	1	1	1	0	3
5	0	1	1	1	1	0	4
6	1	0	0	0	1	1	3
Column Sum	3	4	3	3	3	2	18

(b)

From / To	1	2	3	4	5	6	Row Sum
1	9.948^{-1}	0	0	0	0	0	9.948^{-1}
2	1.974^{-3}	9.944^{-1}	0	1.395^{-2}	2.930^{-2}	1.178^{-3}	1.071
3	0	2.043^{-3}	1.530^{-1}	0	0	0	1.551^{-1}
4	0	1.818^{-3}	1.250^{-1}	9.121^{-1}	0	0	1.039
5	0	1.608^{-4}	1.250^{-1}	6.850^{-1}	9.614^{-1}	0	1.093
6	6.419^{-5}	0	0	0	2.644^{-3}	8.975^{-1}	1.000
Column Sum	9.969^{-1}	9.985^{-1}	4.030^{-1}	9.629^{-1}	9.934^{-1}	9.987^{-1}	5.353

Fig. 4.7. Oyster reef model first-order matrices (a) A for paths, and (b) P for causality. Example entry in P: $9.948^{-1} = 9.948 \times 10^{-1}$. See text for explanation of numbers. The time unit applied in the matrix representation is 6 hours, not 24 hours as used in Fig. 4.6.

5. *Matrix conceptualization* is illustrated in Fig. 4.7. The first upper matrix is a so-called *adjacency matrix*, that shows the connectivity of the system. This matrix has $a_{ji} = 1$ if a direct causal flow (or interaction) exists from compartment j (column) to compartment i (row), and $a_{ji} = 0$ otherwise. The lower matrix, called a flow or in/output matrix, represents the direct effects of compartment j on compartment i. The number expresses the probability that a substance in j will be transferred to i in one unit of time. P is a one step transition matrix in Markov chain theory and can be computed readily from storage and flow information. Notice that Fig. 4.6 uses the units cal/m^2 and cal/(m^2 day), while the flow matrix in Fig. 4.7 uses six hours as the time unit. The number for a_{12} is therefore found as $15.7915/(4 \cdot 2000) = 0.1974 \times 10^{-2}$ indicated in the matrix as 1.974^{-3}.

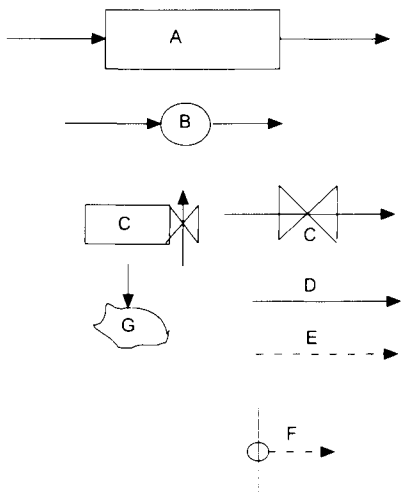


Fig. 4.8. Symbolic language introduced by Forrester (Jeffers, 1978). (A) State variable; (B) auxiliary variable; (C) rate equations; (D) mass flow; (E) information; (F) parameter; (G) sink.

The two matrices provide a survey of the possible interactions and their quantitative role.

6. The *feedback dynamics* diagrams use a symbolic language introduced by Forrester (1961) (see Fig. 4.8). Rectangles represent state variables. Parameters or constants are small circles. Sinks and sources are cloud-like symbols, flows are arrows and rate equations are the pyramids that connect *state variables* to the flows.

   A modification has been developed by Park et al. (1979). It differs from the *Forrester diagrams* mainly by giving more information on the processes.

7. A *computer flow chart* might be used as a conceptual model. The sequence of events shown in the flow chart can be considered a conceptualization of the ordering of important ecological processes. An example is given in Fig. 4.9, which is a swamp model developed by Phipps (1979). The model subjects each of the three species in the swamp to the same sequence of events with specific parameters as a function of species. Trees are born, grow and die off due to old age (KILL), lumbering (CUT) or environmental forces (FLOOD). Birth depends on another process. This type of model is very useful for setting up computer programs, but does not give information on the interactions. For example, it is not possible to read on Fig. 4.9 that GROW is a subroutine, which considers the effects of interactions between the water table and crowding on the individual tree species.

   A subcategory of computer flow charts is analog computer diagrams. Analog symbols are used to represent storage and flows. An amplifier is used to sum

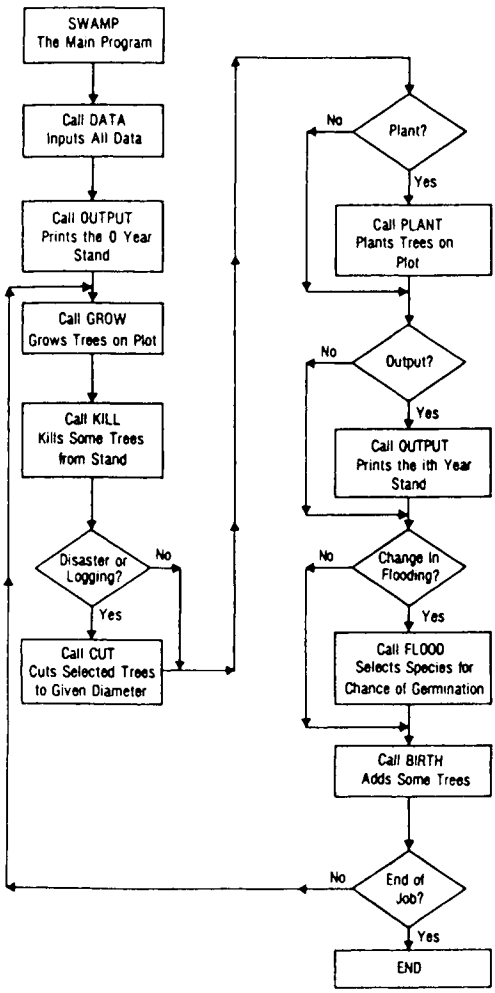
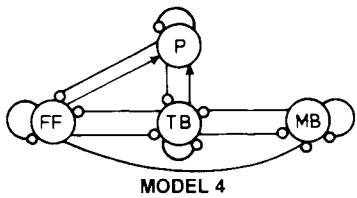


Fig. 4.9. Flow chart of SWAMP (modified from Phipps, 1979).

and invert one or more inputs. By adding a capacitor to an amplifier, we get an integrator. Analog computers have found only a limited use in ecological modelling. For descriptions see Patten (1971–1976).

8. *Signed digraph models* extend the adjacency concept. Plus and minus signs are used to denote positive and negative interactions between the system components in the matrix and the same information is given in a box diagram; see Fig. 4.10 which shows a general benthic model (Puccia, 1983). Lines connecting the components represent the causal effects. Positive effects are indicated by arrows; lines with a small circle head show a negative effect.



MODEL 4

Parameter input to	Change in equilibrium FF	TB	MB	P
FF	+	-	+	-
TB	-	+	-	-
MB	+	-	+	+
P	+	+	+	+

Fig. 4.10. A *general signed digraph model* for the east coast (USA). Benthic organisms from a sandy environment (from Puccia, 1983).

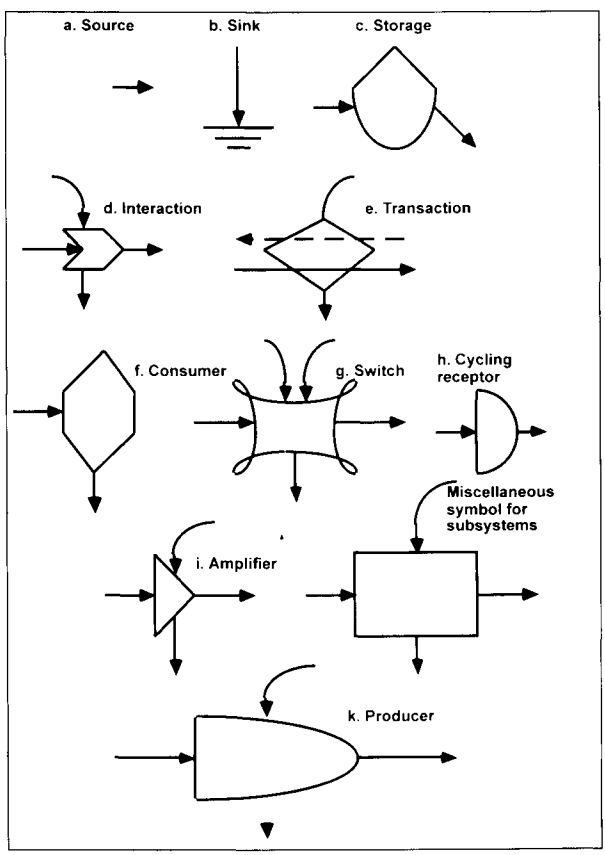


Fig. 4.11. Diagrammatic *energy circuit language* of Odum (1983) developed for ecological conceptualization and simulation applications.

9. *Energy circuit diagrams*, developed by Odum (see Odum 1983), are designed to give information on thermodynamic constraints, feedback mechanisms and energy flows. The most commonly used symbols in this language are shown Fig. 4.11. As the symbols have an implicit mathematical meaning, much information is given about the mathematics of the model. It is, furthermore, rich in conceptual information and hierarchical levels can easily be displayed. Numerous other examples can be found in the literature; see, for example, Odum (1983). A review of these examples will reveal that energy circuit diagrams are very informative, but they are difficult to read and survey, when the models are a little more complicated. On the other hand, it is easy to set up energy models from energy circuit diagrams. Sometimes it is even sufficient to use the energy circuit diagrams directly as energy models. These diagrams have found a wide application in the development of ecological/economic models, where the energy is used as the translation from economy to ecology and *vice versa*. In this context, H.T. Odum has used the approach for developing models for entire countries. As mass carries energy, it is possible to use the energy circuit diagram for *biogeochemical models*, too, although it is sometimes more cumbersome and causes unnecessary complications.

4.4. The Conceptual Diagram as Modelling Tool

The *word models*, *picture models* and *box models* all give a description of the relationship between the problem and the ecosystem. They are very useful as a first step in modelling, but their application as a modelling tool on their own is limited. Additional information is needed to answer even semi-quantitative questions. This is, however, possible using many of the other conceptual approaches demonstrated in this section.

Illustration 4.1

In Fig. 4.5 the *global C-cycle* is shown. It is seen that the input of carbon dioxide due to the use of fossil fuels increases the atmospheric carbon dioxide concentration by (5/700) per annum or (5/7%). If the amount of carbon dioxide dissolved in the sea is deducted, the increase will only amount to (2/7%). As the carbon dioxide concentration in 1970 was 0.032% on a volume–volume basis, it is easy to see that at the present rate of fossil fuel combustion, the concentration will reach 0.040% in 2003–04. It is, of course, also possible to compute the concentration at year x, when a certain trend in the use of fossil fuels is given, or the time it will take with a certain global energy policy to reach a given threshold concentration. These computations assume that the percentage of carbon dioxide transferred to the sea is constant or at least given as function of time. A far more complex computation is, of course,

required to find the carbon dioxide concentration in the atmosphere if we want to incorporate the actual mechanisms for these transfer processes from the atmosphere to the sea, but as seen by this illustration it is possible to get some first approximations by using a conceptual diagram with indication of storage, input and output flows.

Illustration 4.2

Patten (1991) uses the *matrix representation* directly to compute what he calls the indirect effects. If the adjacency matrix is multiplied by itself, the product A^2 indicates the number of indirect paths of the length 2 from one compartment to another. In general the product of the matrix A^n will represent the number of length n paths from compartment j to compartment i. Figure 4.12a shows the tenth-order matrix of the model. As can be seen, the number of paths of length 10 is incredibly

	COMPARTMENTS						
	(a)						
From / To	1	2	3	4	5	6	Row Sum
1	1	0	0	0	0	0	1
2	23696	34729	23697	27201	23696	16168	149187
3	11033	16168	11032	12664	11033	7528	69458
4	16169	23696	16168	18560	16169	11033	101795
5	23695	34729	23696	27201	23696	16169	149186
6	11032	16]69	11033	12664	11032	7527	69457
Column Sum	85626	125491	85626	98290	85626	58425	539084
	(b)						
From / To	1	2	3	4	5	6	Row Sum
1	9.491–1	0	0	0	0	0	4.494–1
2	1.883–2	9.494–1	7.290–2	2.988–1	2.410–1	1.137–2	1.592
3	4.029–5	2.303–3	1.581–4	6.662–4	5.254–4	2.430–5	3.718–3
4	1.416–4	1.396–2	6.616–2	4.011–1	1.915–3	8.512–5	4.833–1
5	3.353–5	4.009–3	1.089–1	3.899–2	6.753–1	2.014–5	8.282–1
6	6.203–4	4.520–5	3.003–2	5.831–4	2.203–2	9.755–1	1.002
Column Sum	9.690–1	9.697–1	2.521–1	7.401–1	9.408–1	9.870–1	4.859

Fig. 4.12. Oyster reef model tenth-order matrices. (a) A^{10} for paths, and (b) P^{10} for influences. Smaller values than corresponding non-diagonal entries in P^5 are underlined. Note: 1.883–2 is shorthand for 1.883×10^{-2}.

high. There are more than 500 000 length 10 paths in the model. The reason is that the length of a cyclic path is infinite. Matter, energy and information may pass around such a path until it either dissipates from or leaves the cycle.

The P^{10} for influences is shown in Fig. 4.12b. Smaller values than corresponding non-diagonal entries in P^3 are underlined. Thus indirect effects are generally still tending to grow at the 10th order level due to the enormous number of paths. Patten demonstrates, by this simple analysis, the importance of indirect effects. These aspects will be discussed further in Section 5.3.

PROBLEMS

1. Draw a Forrester and energy circuit diagram for Fig. 2.8.
2. Set up a matrix representation of the model in Fig. 2.5.
3. Set up a matrix representation of the global carbon cycle Fig. 4.5.
4. Make a STELLA diagram of the picture model in Fig. 4.4. Set up an adjacency matrix for the model.
5. What will the probable carbon dioxide concentration in the atmosphere be in year 2025? It is presumed that 0.00032 volume/volume % increase will cause a temperature increase of 0.02°C. Which temperature increase relatively to 1900 (the concentration was 0.028 volume/volume %) and 1970 should be expected in the year 2004 and year 2025?
6. Set up an adjacency for the model of Illustration 5.1.

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CHAPTER 5

Static Models

5.1 Introduction

A model resulting from a purely phenomenological description of the flows through the components of an ecosystem is of static type as long as no equations related to the dynamics of the variables appear in the model. This means that time is not a variable of static models and they may be viewed as a "snapshot" of an ecosystem at a particular moment.

The state variables of static models assume values averaged over a certain time period during which the ecosystem can be assumed to be in a steady-state condition and its dynamic behaviour may be forgotten. Usually, static models consider a steady-state condition of an ecosystem averaged over a season or a full biological cycle of the year. Static models are used to construct a trophic web or network, representing the complex of relations between organisms (biotic factors) and/or between organisms and the environment (abiotic factors).

These relationships represent the processes related to feeding and growth of individuals, amongst them being the production of new biomass, consumption, excretion, respiration, and mortality.

Static models are also used to simulate the response of an ecosystem when forced by external factors. Static models account for zero dimensional systems where values of the variables, besides the time average, are also averaged over the entire space occupied by the ecosystem.

Under steady-state conditions, the state variables of a web model, represented by the biomass of organisms that compose the nodes of the web, do not vary in time, and the flows entering and exiting each node are balanced. Such a hypothesis is not as strict as it seems; in fact the value of a variable associated with a node is often the result of the mean of values obtained during a particular time interval. Steady states are good representations of an average situation and it is easy to compare different steady states resulting from different sets of forcing functions.

The hypothesis of a steady-state condition for an ecosystem provides several advantages from a computational point of view in the static network model, since for each node the quantity of energy entering must be equal to the amount leaving the node, yielding an equation useful to calculate unknown parameters.

Static models offer some advantages:

- Static models give important information on flows and storages in an ecosystem.
- In a static model differential equations will be reduced to algebraic equations, which are a more simple mathematical representation to use as a model. An analytical solution might be provided, usually fewer data are needed, a parameterization is most often easier, and the computations are carried out more easily.
- Static models need a more limited dataset than dynamic models and they are less time consuming to develop.
- Static models give good pictures of average situations and it is easy to compare different steady states resulting from different sets of forcing functions.
- A large number of system elements can be included in static models.
- A response mode is a type of a static model using simple statistical methods to elaborate data referring to a system.

But static models have also some limitations:

- A system performing dynamic behaviour cannot be simulated by a static model.
- A time factor is not included; therefore, transitions cannot be described.
- The results of a static model are valid only for the simulated system in the given state; they cannot be extrapolated to systems other than that used for the development of the model, nor to other states of systems.

5.2 Network Models

A network is a collection of elements called *nodes*, pairs of which are joined to one another by a (usually larger) set of elements called edges. The nodes are arranged in some sequence, and an edge is identified by the names of the two nodes that it joins.

A trophic network or web ecosystem describes the complex of relations between organisms and/or between organisms and their environment. These relationshups are determined by the processes of feeding and growth of individuals inside the ecosystem and by interactions of the system with the outside

The translation of this set of relationships into quantitative terms is a difficult task due to: the high number of variables involved: the variations that these variables

experience during a certain time span (such as abundance of organisms, physical and metabolic features of the single species, qualities of abiotic factors); and eventual spatial differences inside the same system.

The classical approach of the models of the reductionist type describes a system in the form of differential equations where each equation represents the dynamics of the state variables (organisms or groups of organisms, organic matter, nutrients) in time. Such a dynamic is determined by the combined effect of the single processes in which the variable is participating, described as the relation of cause and effect with the other variables and with the respective forcing functions. Such an approach proves inadequate for the construction of a trophic web, because the number and complexity of the relationships involved are too large to be described in detail.

The static representation of an ecosystem can be easier to build up but it can also present some difficulties. The first difficulty consists in the appropriate selection of the compartments or nodes, or in other words the selection of the state variables of the network. The second difficulty consists in the construction of an adequate data base. Experimental campaigns must be realized simultaneously and with the appropriate and coherent methodologies. Very often, the costs and difficulties of organization do not allow a work of this kind, since it is quite unlikely to create a data base that is sufficient for the realization of a static model including all organisms of the ecosystem. The gaps in the data base render the calibration of parameters of single processes more difficult and the uncertainty about the outcome may provide unrealistic results, or at least results of reduced reliability. The complexity of the tasks may be reduced by decreasing the number of state variables to be treated. Such a decrease is obtained by means of an adequate aggregation of organisms present in the system. The criteria of aggregation may follow diverse philosophies, depending on the aim of the research and on the interest to characterize organisms with respect to size, habitat or trophic role, etc.

The problem of spatial variability of the data may be faced by selecting areas presenting sufficient homogeneity. The level of homogeneity may be judged according to the purpose of the analysis and/or on the necessity of comparison with other ecosystems. Nevertheless, the most important simplification is imposed on the time factor. To represent a trophic web by means of a quantitative model it is necessary to renounce the research of the dynamic of state variables, to content with "mean" values, representative of the situation in the defined time span. Therefore, the data necessary to describe the trophic web are the mean biomasses of the state variables and the flows associated with these variables.

The flows associated with a compartment of a trophic network or web may be classified into two categories: incoming flows and outgoing flows. As the compartments (or nodes) of a trophic network represent a community of individuals, there can also exist flows representing exchanges with the exterior of the system, such as *immigration* and *emigration*. Among the processes that determine incoming flows are *feeding* and *immigration*. Among those that determine outgoing flows are *predation mortality*, *natural mortality*, *respiration*, *excretion*, and *emigration*. Feeding is determined by the need for energy of an organism and is limited by resource availability.

In the following, the flow associated with the feeding process will be called *consumption*.

The incoming flow to a compartment by migration of organisms refers to the immigration process. In the following, *import* refers to the total amount of an eventual flow of immigration and to the flow associated with the consumption of resources not included in the model, i.e., resources which are not present in any node forming the web.

The process of natural mortality (due to aging, illness and all causes that cannot be attributed to predation by other individuals) and the process of excretion generate a flow of organic matter towards the compartment of *detritus*. Such a compartment represents the pool of dead organic matter being decomposed by associated micro-organisms.

An eventual emigration of organisms out of the system and the predation by organisms not included in the model are represented by a unique flow called *export*. For instance, the flows associated with fishing or harvesting are also classified as an export.

Another flow out of the system is that associated with *respiration*. This metabolic end product can no longer be used for production of biomass and is exported out of the system as dissipative flow (always present in a system that is in a state far from thermodynamic equilibrium, such as the ecosystems).

The complex of flows related to a compartment in a trophic network may be graphically indicated by a figure whose nodes represent the biomass of various biological groups and whose arrows represent flows of matter or energy, usually called "*currency*", that belong to one of the processes listed above.

Figure 5.1 shows how such flows may occur. T_{ij}, T_{ji} = between compartments; I_i = from outside to a compartment (import); E_i = out of the system in form of currency that is still usable (export); R_i = out of the system in form of non-usable currency (dissipation of energy also called "costs of maintenance", a synonym for respiration in an environmental system).

The law that allows us to quantify the flows in a trophic network is the law of conservation of mass and energy. The amount of matter or energy entering a compartment via consumption can partly be transformed into new biomass, partly be

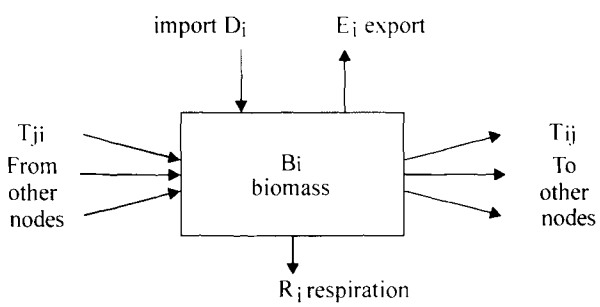

Fig. 5.1. Flows related to the i'th node of the trophic web.

used ("burned") to support vital functions (this quantity is generally defined as respiration) and partly be lost as a non-assimilated part of the food:

$$Q = P + R + NA \tag{5.1}$$

where Q = consumption, P = net production, R = respiration, NA = non-assimilated part of the food.

Under steady-state conditions, i.e. when everything that enters a compartment equals everything that exits, the newly produced biomass is then consumed by predators or is lost as natural mortality or emigrates out of the system. Therefore, the mass (or energy) balance equation will be as follows:

$$D + P = M + M_2 + E \tag{5.2}$$

where: D = import[1]; M = natural mortality; M_2 = predation mortality; E = export. The flow to detritus is given by the sum of natural mortality and the unassimilated part of the food; thus, considering the topological aspect of a trophic web, the structure of the flows can be represented by a figure in which the size of flows gives a measure of the importance of the connections. Such a figure can be substituted by a square matrix T, called flow matrix or "exchange matrix" T, whose dimension is equal to the number n of compartments of the trophic web and whose elements are T_{ij} (where the flows go from rows to columns). Three column vectors of the dimension n, [Import (D), export (E), and respiration (R)], can be added to the matrix T to describe the flows not originating from other nodes and not directed to any node.

The balancing equation written in function of the elements of these matrices, then becomes:

$$D_i + \sum_{j=1}^{n} T_{ji} = \sum_{k=1}^{n} T_{ki} + E_i + R_i, \quad i = 1, \ldots, n \tag{5.3}$$

The entire trophic web is condensed in these four components from which one is able to gain an important global property of the system, i.e., the total flow going through the system or *Total System Throughput* (*TST*) or *Total System throughFlow* (*TSF*).

It is defined as the sum of all flows present:

$$TST = \sum_{j=1}^{n} \sum_{i=1}^{n} T_{ji} + \sum_{i=1}^{n} (E_i + R_i) + \sum_{i=1}^{n} D_i \tag{5.4}$$

TST is an extensive index of the size of the system and can be used for intersystem comparison.

1 The notation of the input vector has been modified to avoid confusion with the identity matrix I which will be defined further below. In the section describing the Ecopath software, the input vector was defined as I to adjust it to all the terminology related to that software

5.3 Network Analysis

The mathematical description of a trophic network by means of the instruments provided by matrix calculation has great advantages, particularly concerning the analysis and interpretation of the results. The relationship between the elements of the diet matrix and associated flows is obtained by dividing each entering flow to a compartment by the total amount of entering flows to the same compartment, i.e.:

$$g_{ij} = \frac{T_{ij}}{T\text{in}_j} \tag{5.5}$$

Having defined the amount of the flows entering the compartment $T\text{in}_j$ as:

$$T\text{in}_j = D_i + \sum_i^n T_{ij} \tag{5.6}$$

where the element D_i, represents the i'th element of import vector D.

The element g_{ij} of the matrix G represents the fraction of everything entering j coming directly from i. This matrix is usually called the diet matrix because it describes how much food is entering a compartment and where it is coming from. Analogously, the matrix F can be defined whose elements are determined dividing each outgoing flow by the total of outgoing flows, i.e.:

$$f_{ij} = \frac{T_{ij}}{T\text{out}_i} \tag{5.7}$$

where the amount of outgoing flows from node i is given by:

$$T\text{out}_i = \sum_i T_{ij} + E_i + R_i \tag{5.8}$$

The element f_{ij} of the matrix F represents the fraction of everything that exits from i and goes directly into j. Those matrices are particularly important for the analysis of *indirect effects* occurring in a system having multiple interconnections and different cycles of the flows; thus, it might occur that the indirect influence exerted by one compartment over another could surmount the direct effect exerted by a third one. In this context an indirect relation indicates a flow of mass or energy along a pathway higher than one, defining the length of the path by the number of connections of which it is composed (or of the number of nodes touched before joining the final one. Note that this definition of F is different from that given for P by Patten and shown in Illustration 4.2.

The matrices G and F are a fundamental part of a method called "*input–output analysis*" (Ulanowicz, 1986; Kay et al., 1989), initially introduced in the economic

field by Leontief (1936) and Augustinovics (1970), and for the first time applied to ecological webs by Hannon (1973).

Leontief and Augustinovics have faced the problem of connecting input and output of a web starting from two opposite points of view. Leontief had to cope with the problem of determining the productive activity required in any compartment of the web to sustain a determined amount of external uses and internal consumptions; therefore, the problem consisted of going back to inputs starting from conditions imposed on the outputs of the system (i.e. export and dissipation). The relation, written in vector form, that connects the total flow through a node and the outputs of the system is as follows:

$$T\text{out} = \frac{(E+R)}{[I-G]} \tag{5.9}$$

where I is the identity matrix.

The matrix $[I-G]$ is the matrix of Leontief (1951), while the inverse of the matrix of Leontief is the *input structure matrix*. (Hannon, 1973).

In the same way, Augustinovics treated the problem of determining the destination of each input to the system. The relation that connects entering flows with the nodes to the input from outside is given by:

$$T\text{in} = \frac{D}{[I-F]} \tag{5.10}$$

where the matrix $[I-F]^{-1}$ is the inverse matrix of Augustinovics' matrix and it is defined as output structure matrix.

An important result for applications in ecology was obtained by Levine (1980) when he showed that the sum of elements in the columns of the input structure matrix provides the equivalent trophic level of the organism corresponding to the column.

The synthesis of the calculation procedure at the equivalent trophic level consists in distributing the trophic levels among the compartments; analogously it is possible to carry out the inverse procedure of distributing a compartment over several trophic levels (Ulanowicz and Kemp, 1979; Ulanowicz, 1995). The result is a mapping of the web into a sequence of energetic transfers occurring between the discrete trophic levels *sensu* Lindeman.

To understand this procedure of mapping, it is recommended to look at the meaning of the exponents of the matrices G and F. Matrix G represents the direct transfers (i.e. the pathways of length 1) from the indicated element in the row to the element in the column (as a fraction of the amount of entering flows). Matrix G^2 represents then the transfers among compartments through all the pathways of length 2.

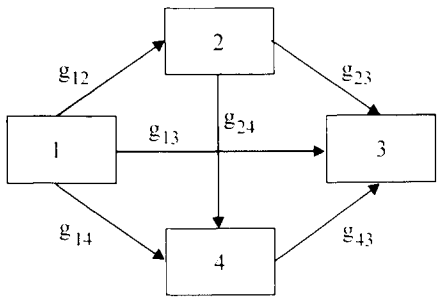

Fig. 5.2. Examples of a web of flows (adapted from Ulanowicz, 1986).

If, for instance, the web in Fig. 5.2 is observed, matrix G is given by (5.11):

$$G = \begin{bmatrix} 0 & g_{12} & g_{13} & g_{14} \\ 0 & 0 & g_{23} & g_{24} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & g_{43} & 0 \end{bmatrix} \tag{5.11}$$

while matrix G^2 results in:

$$G^2 = \begin{bmatrix} 0 & 0 & g_{12}g_{23} + g_{14}g_{43} & g_{12}g_{24} \\ 0 & 0 & g_{24}g_{43} & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \tag{5.12}$$

which, considering the four pathways of length 2 present in the web, quantifies the fraction of currency entering flows in each node through all the pathways of that length. Matrix G^3 is given by:

$$G^3 = \begin{bmatrix} 0 & 0 & g_{12}g_{24}g_{43} & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \tag{5.13}$$

which shows that it is possible to quantify the fraction of currency entering in each node through a pathway of a length equal to the exponent of the matrix.

In general, elements of the matrix G^m represent the fraction of currency that enters a node coming from a pathway formed by m transfers of energy. Analogously,

matrix F^m stands for the giving node, or else the element ij gives the fraction of all the energy coming out of the i'th node that reaches node j through a path of length m.

If we define a row vector L, whose elements are equal to 1 when corresponding to primary producers and equal to 0 if the corresponding group consists of consumers, and we multiply vector L to the left by matrix G, we obtain a linear vector (LG), whose elements provide the fraction that enters each node from a single internal transfer from primary producers. This quantity identifies the percentage of this node that belongs to the second trophic level. In the same way (LG^{m-1}) provides the fraction entering in each node after m internal transfers, i.e. the percentage belonging to the m'th trophic level. If cycles are not present in the web, the resulting linear vector is the zero vector after a maximum of n steps, where n is the number of nodes.

The matrix whose rows are the vectors obtained through successive multiplications of L, by the exponents of G is the *matrix of trophic transformation* by Lindeman. This matrix is peculiar because of the fact that the i'th row gives the amount of activity of each organism at the i'th trophic level and consequently the composition of these levels. This information is used to calculate the aggregation of flows in relation to trophic level. When a mean of the elements of the j'th column is calculated, weighed by the row index (corresponding to the trophic level), the organism's equivalent trophic level j is obtained.

In most ecological systems cycles are present, but these almost always comprise a share of non-living matter, such as detritus or nutrients. Since the concept of trophic level makes sense in the first place for living organisms, the Lindeman matrix is constructed by just considering the nodes related to these organisms and leaving aside eventual flows associated with cycling pathways between living organisms.

Nevertheless, the quantity of currency flowing through the recycling pathways in the non-living compartments is anything but insignificant. Therefore, using the hypothesis that assigns the trophic level 1 to these compartments, the extended matrix of transformation of Lindeman is constructed, obtained by adding as many rows and columns as there are compartments. The elements of these columns will be 0 but for one of a value 1.

Knowing the matrix of trophic transformation, it is possible to discriminate between the flows by trophic level and to distinguish between the contributions of primary producers and of detritus, determining the corresponding trophic chain of primary producers and that of detritus.

Apart from being an instrument for the analysis of the trophic state of a system, the web analysis is also useful to estimate the importance of indirect effects. Patten (1985) demonstrated that it is possible to quantify the influence of a compartment on another one, by calculating the total flow from the first to the second one via all possible pathways, depurated for the influence of the second compartment on the first one by the effect of recycling. In this way two analogous matrices to G and F may be defined, the matrix of the coefficients of total dependence, T_d and the matrix of the coefficients of total contribution, T_c. The element ij of the matrix T_d represents the fraction of all that is entering j coming from i through all possible pathways, while

the element ij of the matrix T_c represents the fraction of all that is leaving from i and arriving at j considering all possible pathways.

Very interesting results may emerge from a comparison of the matrix of "direct" diets G and the matrix of the coefficients of total dependence, which takes into account the indirect dependence of the receiving compartments with respect to the donor. The column j of the matrix T_d provides the extended diet of the compartment j, and this information can reveal and explain important phenomena not evidenced by the analysis of the "direct" diet.

A successfully operated historical example of this kind is that of the Chesapeake Bay in Maryland (Baird and Ulanowicz, 1989). On this occasion it was attempted to explain why two species of fish, both predators and piscivorous (*Morone saxatilis*, striped bass, and *Pomatomus saltatrix*, bluefish, green-house fish), had different levels of residues of the pesticide Kepone after a contamination of the sediment in the 1970s. Analysing the "extended" diets, i.e. the pathways along which the food had passed before arriving in the final consumer it was discovered that while the food of the bluefish (or better the dietary web of the prey organisms that are later consumed by the fish) was principally based on detritus, the food of the striped bass consisted of fish whose food was mainly sustained by the planktonic chain. In particular, 63% of the diet of the bluefish had passed through the compartment of benthic bacteria and 48% had passed through the compartment of polychaetes (obviously a quantity of food may pass through more than one compartment before arriving at the final user, therefore, the amount of the relative percentage of the diet may surpass 100%). On the other hand, the diet of the striped bass depends mainly on the three components of the plankton community: phytoplankton 64%, microzooplankton 12%, and mesozooplankton 66%; no benthic compartment surpassed 18% of the total of the "extended" diet of this fish. The higher levels of toxic substance found in the bluefish could be explained by the closer link with the polluted sediment revealed by the analysis of the extended diets.

The last analysis to be carried out on indirect effects using the web analysis is provided by the matrix of total trophic impacts M (Ulanowicz and Puccia, 1990). Defining as mixed trophic impact of the compartment i on the compartment j the difference between the benefit of j having i as prey and the relative loss by being prey of i, the matrix of mixed trophic impacts Q may be constructed, whose elements are given by:

$$q_{ij} = g_{ij} - f_{ji} \tag{5.14}$$

Since the elements of F and G are all between 0 and 1, $|q_{ij}| \leq 1$. Analogously to what has been shown for the exponents of the matrix G, Ulanowicz and Puccia (1990) could demonstrate that the amount of the sum of the integer powers of the matrix Q gives the total trophic impact of i on j via all possible direct and indirect pathways. On the other hand, the exponents of Q are convergent since $|q_{ij}| \leq 1$, therefore it could be written:

$$M = \sum_{h=1}^{\infty} Q^h \tag{5.15}$$

This analysis may evidence typical indirect effects, such as the benefit that some predators may bring to their prey and the virtuous cycles of mutual benefit. The matrix of total trophic impacts can also give indications on organisms having the largest positive or negative impacts, identifying organisms that may be key elements for the ecosystem.

Illustration 5.1

Figure 5.3a illustrates a model of water balance within the watershed of Okefenokee Swamp (Patten and Matis, 1982) and introduces another concept of network analysis: the environment. The four compartments represent water storages in the

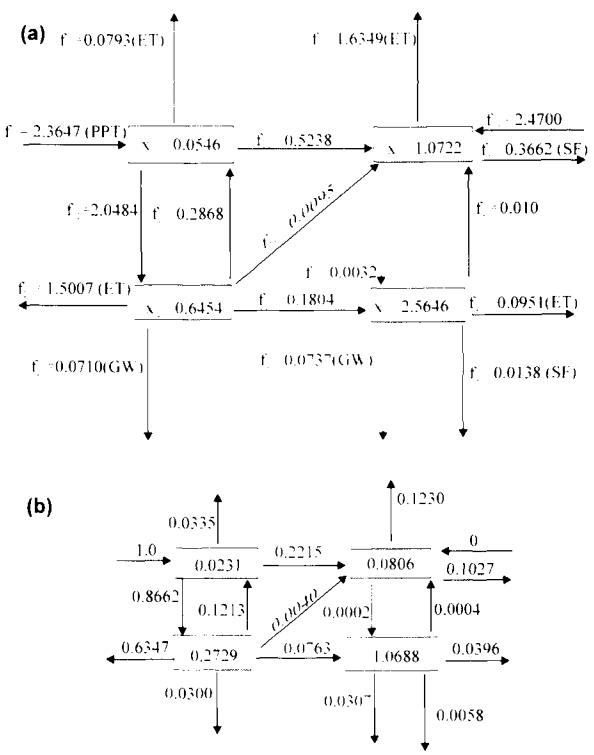

Fig 5.3 (a,b). Static water budget model of the watershed of Okefenokee Swamp. The compartments are: x_1 = upland surface storage; x_2 = upland groundwater storage; x_3 = swamp surface storage; x_4 = swamp subsurface storage. Environment is denoted with 0; flow from i to j with f_{ij}; note that in the original paper, as usual for Patten, the flow are indicated differently as f_{ij}. In brackets are listed the destination of the input flow (PPT, Precipitation) and output flows (ET, EvapoTranspiration; SF, Stream Flow; GW, Ground Water). (a) is the static model; (b) is the example of environ when a unit input is applied to x_1.
Figure redrawn from Patten (1985)

swamp and adjacent uplands. The data in Fig. 5.3b illustrate quantitative characteristics of environs. The bold arrow in the diagram identifies the unit input considered. As an example, Fig. 5.3b depicts the environ associated with a unit input to the upland surface water compartment x_1. It is shown that this unit input results in 0.023 units of storage in compartment it comes from the division of storage 0.0546 by the input flow 2.3647, and an internal flow f_{31} of 0.2215 comes from the division of 0.5238 by 2.3647, and so on for the others.

5.4 ECOPATH Software

The software described here ("Ecopath" for short) is designed to help the user to construct trophic network models of an ecosystem. Ecopath is public domain software released by ICLARM (International Center for Living Aquatic Resources Management, Manila, The Philippines) as part of the ICLARM Software Project (Christensen and Pauly, 1992a, 1992b). This software was initially designed for the construction of marine ecosystem models and for estimating the impact performed on marine resources by fishing. Having incorporated the holistic approach of ecosystem evolution theory, however, makes it a useful instrument for considerations of a general nature about the state of the ecosystem. To date, a series of application examples have been published and its use in the management of ecosystems is well acknowledged.

The monograph "Trophic models of Aquatic Ecosystems" (V. Christensen and D. Pauly, 1993) contains a worldwide collection of application examples for—amongst others—culture systems, lakes, rivers, and coastal areas including lagoons.

The software provides useful procedures for the estimation of parameters eventually unknown and for the balancing of the system of equations of conservation of mass or energy (Fig. 5.1), whose dimension is the same as the number of compartments of the web. The procedures included in the software automatically provide results of holistic indices of the model network. Some of these indices are derived from thermodynamics and from information theory (Ulanowicz, 1986).

In contrast to previous versions (Polovina, 1984), version 3.0 (Ecopath for Windows) has introduced the possibility of an accumulation or depletion of biomass by any organism during the time period considered.

Such opportunity allows us to refrain from the restrictive hypothesis of considering the system to be in a steady state. The accumulation does not correspond to a true flow, but it is useful in cases when a compartment has undergone a considerable variation of biomass between the beginning and the end of the period. This is not sufficient, indeed, in cases where it is necessary to study situations in which the dynamics of particular cause–effect relations are important and/or phenomena at a very brief temporal scale. In these cases the use of a dynamic model is more appropriate.

Input data to the model could be of different types, depending on the available information. The software accepts as input biomass values (standing stock or means

of the period), as well as inputs associated with flows (and consequently with the metabolic parameters), determining automatically the unknown parameters by means of energy balance equations. An estimate of the *diet composition* of the various organisms, nevertheless, is always asked for as input. Usually, a biomass estimate is the most readily available input, being also the easiest to obtain by experimental methods.

The necessary input ratios of fundamental metabolic parameters are as follows:

- production/biomass ratio (P/B); and
- consumption/biomass ratio (Q/B) or one of these two; and
- gross efficiency (GE = production/consumption = $(P/B)/(Q/B)$);
- unassimilated part of the food ($\%NA$).

It suffices to know two out of the three ratios of P/B, Q/B and GE since the third is unequivocally determined by the other two.

To these parameter ratios a fifth is added, the ecotrophic efficiency EE, defined as the part of production of a compartment that is consumed by other organisms or exported out of the system. This parameter is actually the most difficult to measure, being bound to the characteristics of the entire web and not just to that of the individual; in most cases this parameter is unknown and can only be determined by the balancing of Eq. (5.1). This equation, rewritten in function of the parameters just defined, then becomes:

$$I_i + B_i \cdot \left(\frac{P}{B}\right)_i = \sum B_j \cdot \left(\frac{Q}{B}\right)_j \cdot DC_{ij} + B_i \cdot \left(\frac{P}{B}\right)_i \cdot (1 - EE_i) + E_i + A_i \tag{5.16}$$

for each compartment i. In this equation the term A_i has been inserted, indicating the false flow associated with the eventual accumulation of biomass; DC_{ij} is the percentage of the i'th element in the diet of organism j; this value corresponds to the element ij of the diet matrix G.

Equation (5.16) could be simplified in the following way:

$$I_i + B_i \cdot \left(\frac{P}{B}\right)_i \cdot EE_i = \sum B_j \cdot \left(\frac{Q}{B}\right)_j \cdot DC_{ij} + E_i + A_i \tag{5.17}$$

where it is evidenced that import I_i, export E_i and accumulated biomass A_i should be provided as additional inputs.

The flow associated with respiration R_i is determined by Eq. (5.1) and can be rewritten in the following way:

$$R_i = B_i \cdot (1 - \%NA_i) \cdot \left(\frac{Q}{B}\right)_i - B_i \cdot \left(\frac{P}{B}\right)_i \tag{5.18}$$

In addition to the features for constructing a trophic network model by means of the balancing of equations, the software also supplies other instruments for the analysis of an ecosystem.

Calculating the equivalent trophic level of an organism is of particular importance. The trophic level is not necessarily indicated by an integer number, as theorized in the past by Lindeman (1942). In nature, a species very frequently finds its food in more than a single trophic level, according to the availability of the resources and to its adaptability. Therefore, it is more appropriate to attribute to an organism a fractional trophic level determined by the mean trophic level of its preys (Odum and Heald, 1975). At the base of the trophic web corresponding to the first trophic level are always the primary producers. At the same level is conventionally placed the compartment of detritus (Baird and Ulanowicz, 1989). Once trophic levels of the elements at the base of the two chains of pasture and of detritus are fixed, it is possible to determine the fractional trophic levels of all the other organisms according to the composition of their diet.

The equivalent trophic level of a species provides a quantitative measure of its position and its role in the web. Significant changes of this level can be indicative of a situation of stress in the ecosystem (Ulanowicz, 1986). The trophic level is also indicative of the quality of the energy used.

In the same way that a fractional trophic level can be attributed to a species, it is also possible to establish the degree of dependency of each species on any of the discrete trophic levels. Therefore, it is possible to analyze the flows aggregated by trophic levels and to establish their energy transfer efficiencies at the level of the whole ecosystem.

Ecopath automatically quantifies the flows aggregated by trophic level, differentiating between the chains of primary producers and those of detritus, and the transfer efficiencies between trophic levels.

Finally, the software provides support for the analysis of the trophic web by means of procedures able to extract all the cycles present in the web, all possible pathways from primary producers to any node, eventually passing also by any other node, and all the pathways from any prey to the top predators.

Even if a model aims to represent all organisms in a system and their connections via the trophic web, a certain degree of aggregation is necessary for a clarifying representation of system characteristics and the management of the model. Of course, there are limitations to the simplification. Christensen and Pauly (1992a) suggest describing an aquatic ecosystem with a model containing not less than 10 compartments. A routine to aggregate system components from 50 compartments down to 1 is included in the software.

From previous modelling approaches of trophic networks it is known that the concept of ecological guilds by far outdates the classical taxonomic approach (Opitz, 1996; Opitz et al., 1996). Therefore, it is strongly recommended that groups of organisms with a similar ecological role be defined instead of aggregating organisms simply by their taxonomic relationships.

Criteria to be applied in the aggregation process are listed below in hierarchical order (for a more elaborate treatment of this subject see e.g. Opitz 1996; Carrer and Opitz, 1999):

- Primary producer/Consumer (exception: symbiotic complexes of organisms with a mixed profile should be included as such and not be separated)
- Habitat (e.g. water column/sediment; this is a facultative criterion which may be included when a spatial separation is required).
- Dimension (micro-, meio-, meso- and macro-).
- Age (juvenile and adult stages, they often differ in their dietary habits).
- Type of diet (plants, meat, detritus, mixed).
- Type of feeding (filtering, grazing, predating, etc.).

Ecopath limitations

- Basically, it assumes the system to be in a steady state although it can accept accumulation and depletion of biomasses.
- Only living and dead (detritus) organic components are included into the model.
- Abiotic effects such as nutrient uptake by primary producers are not considered.
- The software can deal with a maximum of 50 compartments.

Inputs required

- A broad range of currencies can be applied, e.g. wet weight, dry weight, carbon, nitrogen, phosphorus, energy.
- The time period over which average the state variable values is chosen freely by the user.

For each living group, the following parameters are needed as inputs: biomass (B), production/biomass ratio (P/B), consumption/biomass ratio (Q/B). Gross efficiency rates (GE = production/consumption) are needed in cases where no estimate is available for either P/B or Q/B. Additionally, a diet composition estimate (DC, in percentages of volume or weight of food items), an estimate of the percentage of food that is not assimilated (NA), and the amount exported from the system by migration (E), are required as inputs for each ecological group. An additional parameter, usually ecotrophic efficiency (EE = predation mortality expressed as percentage of production), is then calculated using a set of linear equations. If known for a compartment, EE can also be entered and another unknown parameter (e.g. B) can be estimated.

Primary producers are not classified as consumers. Therefore, these groups have no consumption term and do not appear as consumers in the diet matrix.

Model calibration

The first, and perhaps most important, items to consider are the ecotrophic efficiencies *EE*. For each compartment they must be between 0 and 1 (100%), since it is not possible that more of something is eaten and/or caught than is produced. Inputs such as *P/B* ratio, *Q/B* ratio, and diet composition may be modified to adjust *EE*s to the allowable range.

Furthermore, it should be recalled that the gross efficiency *GE*, is defined as the ratio between production and consumption. In most cases *GE* values range from 0.1 to 0.3, but exceptions may occur. In cases of unrealistic *GE* values input parameters should be checked and modified, particularly for groups whose productions have been estimated.

Respiration is, in Ecopath, a factor used for balancing the flows between groups. Thus, it is not possible to enter respiration data. But, of course known values of the respiration of a group can be compared with the output and the inputs can be adjusted to achieve the desired respiration.

Outputs provided

Based on the assumption of mass-balance, the model calculates in absolute numbers the following parameters for each compartment: biomass, accumulated/depleted biomass (*BA*), unassimilated food, flow to detritus, predation mortality (*P·EE*), respiration (*R*), assimilated food (*A*), food intake.

It gives furthermore for each compartment the relationship *R/A*, *P/R*, *R/B*, the fractional trophic level, an omnivory index, a niche overlap index, a selection index, mortality coefficients.

For the entire system the following summary statistics and indices are calculated: total throughput (total *E* + *R* + flow to detritus), net *P*, primary *P/B*, *R/B*, *B/catches*, efficiency of the fishery, connectance index, omnivory index, ascendency/capacity/overheads, cycling index.

Mixed trophic impacts (assessment of the direct and indirect effects that changes of biomass of a group will have on the biomass of the other groups in a system), primary Production required to sustain harvest from the system and ecological footprints are provided.

For more information on the application of the Ecopath model and software see for example Christensen and Pauly (1992b) and the "help" routines of versions 3.0 (Ecopath for Windows) and 4.0 (Ecopath with Ecosim) both available on the internet via: http://www.ecopath.org.

Illustration 5.2

To illustrate an application of a network model and Ecopath Software to an aquatic system, we introduce the case of the Venice Lagoon (Italy) recently studied in detail by S. Carrer and S. Opitz (1999). The example is rather large and detailed to allow us to have an idea of the effort necessary to implement a steady-state model and to appreciate the power of this methodology through the results obtained in this case.

The Ecopath software has been applied to a set of a static model of the trophic interactions within Palude della Rosa—a shallow water area in the northern part of the *Lagoon of Venice*—with the objective of coherently quantifying state variables as well as matter and energy flows between system components. Data available allow us to model trophic interactions including major living system components for such a confined areas of the Lagoon.

Data on hydrobiology, sediments, algae, planktonic and benthic communities, were used to produce a model on a monthly basis of the energy flows among the various biocoenotic components of Palude della Rosa. Rough estimates of biomass density were used for fish communities. Results of experimental campaigns on population size of birds were used for birds' biomass.

The following biocoenotic components are represented by the input data base: macrophytobenthos (macroalgae); phytoplankton; bacterioplankton; zooplankton; zoobenthos: micro- and meiobenthos (protozoa, minor groups, meiobenthic copepods, meiobenthic nematodes), macrobenthos; nekton; and aquatic birds.

The data base was completed with information on detritus, i.e. dead organic material deposited on the ground and suspended in the water column.

The summer situation was considered with the purpose of focusing on the season where main production processes occur. Values used are averages of samples collected at two sampling stations; the homogeneity of the measured values justified the use of an average value. The resulting set of input data represented a wide spectrum of biocoenotic elements and environmental factors surveyed simultaneously in the same period and at the same site.

To render information as homogeneous and comparable as possible, energy has been selected as the unit of measure for biomasses and flows. The currency for biomass is therefore kcal/m^2 (1 kcal = 4.19 kJ); the currency for flows is kcal/(m^2·month).

Conversion factors, assumptions and approximations have been used to transform experimental data into energy content.

Whenever available, values for P/B and/or Q/B were adopted from the literature. In the remaining cases, metabolic models were used to determine daily food intake.

To reduce the number of compartments to an amount that could be handled with some ease and still represent typical features of the trophic network of such a shallow water area, the original number of taxonomic and ecological groups was reduced to 16 compartments by applying a series of ecologically relevant criteria. They are listed below in hierarchical order:

- type of biomass production (producer/consumer);
- habitat (water column/sediment);
- size (micro-, meso- and macro-);
- age group (for fish species: juvenile = fish0 and adult);
- type of food (herbivorous, carnivorous, detritivorous, omnivorous);
- way of feeding (filter feeders, mixed feeders, predators);

For each resulting compartment biomass, metabolic parameters (*P/B*, *Q/B*, *G/E*, *%NA*, *P/R*), diet composition, export and harvest were calculated.

The calibration of the model was accomplished by verifying the mass balance equation. *EE* is determined by solution of Eq. (5.17), thus *EE* is an output of the model used as indicator to check whether the condition is fulfilled. By modifying the diet composition of an organisms regarded groups feeding on zooplankton. Basic inputs and diet composition values resulting from this calibration process are presented in Tables 5.1 and 5.2.

The trophic web of Palude della Rosa—as depicted in Fig. 5.4—spans four trophic levels (*TL*) with fish feeding birds (*TL* = 4.1) and the predatory bass *Morone labrax* (*TL* = 3,9) acting as top predators upon system resources at lower trophic levels.

Benthic feeders feed on all macrobenthic groups (mean *TL* = 2,2) whereas juvenile fish obtain the bulk of their energy by preying on smaller organisms such as zooplankton (*TL* = 2,4) and micro/mesobenthos (*TL* = 2.0). The omnivorous mixed-feeding macrobenthos (*TL* = 2,6) and the predatory macrobenthos (*TL* = 2,4) occupy a slightly higher position in the trophic web than other macrobenthic compartments because 40–50% of their diet consists of other benthic groups with a *TL* of 2,0. Furthermore, up to 30% of the diet of these compartments consist of dead organic matter.

Groups feeding largely (up to 100%) on detritus, such as bacterioplankton, the mullet *Mugil cephalus*, and the micro-, meso-, and macrobenthic detritus feeding compartments are in the same trophic position having *TL*s ranging from 2,0 to 2,1. These results underline the main features of the ecosystem that will be presented in the following: (1) the structure of flows is very poor; (2) the overall system is strongly based on consumption of benthic macrophytes and detritus; and (3) the transfer of energy is mostly confined to first and second trophic level.

The absolute flow matrix reported in Table 5.3 shows that, ranking the compartments by the amount consumed by other compartments, 89% (751 kcal/(m^2 month) of the biomass production consumed within the trophic system originates from the detritus (with 500 kcal/(m^2 month)) and benthic macrophytes compartments (with 252 kcal/(m^2 month)). Phytoplankton herbivorous–detritivorous macrobenthos and detritivorous macrobenthos are of intermediate importance. All other functional groups are of low to negligible importance in terms of the size of energy flow between compartments.

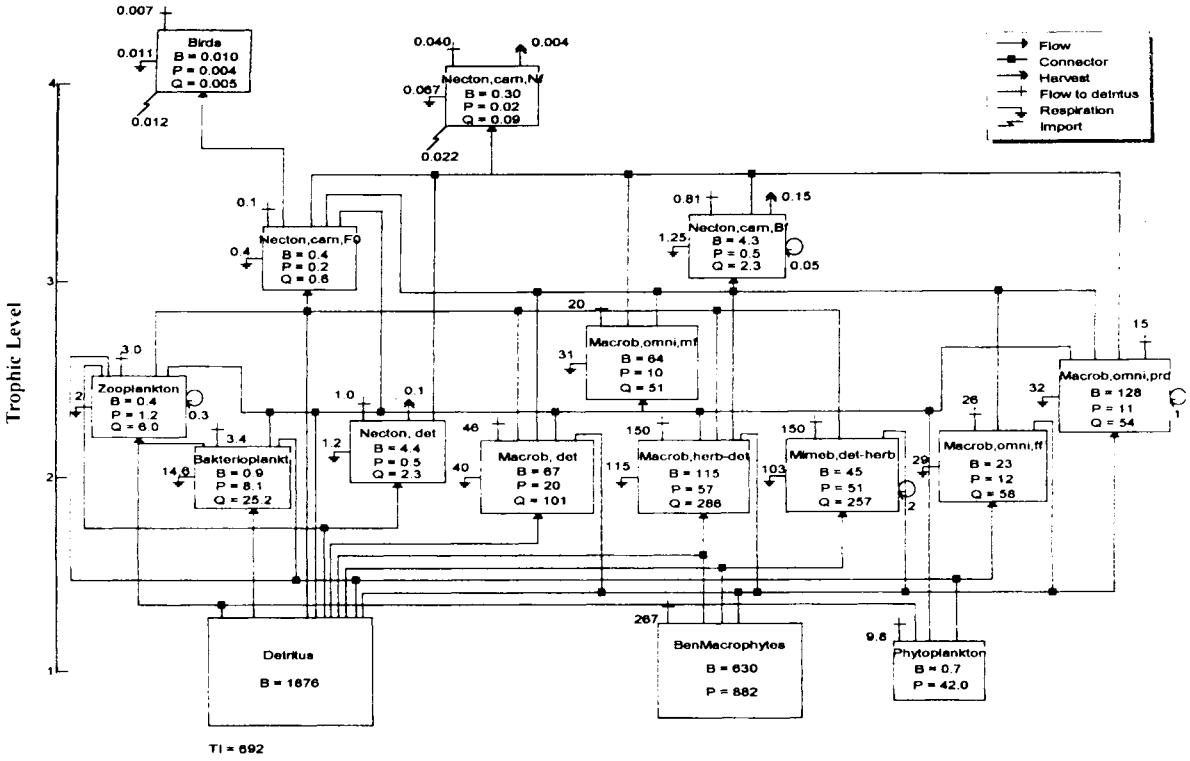

Fig. 5.4. Quantitative representation of trophic interactions within the food web of Palude della Rosa, Lagoon of Venice, during summer 1994. The area of each box is proportional to the logarithm of the biomass (B kcal/m^2) of each group. Flows are in kcal/(m^2 month). Q is the total flow entering a compartment and P is the production of a compartment.

Table 5.1. Basics inputs to the model. Biomass input values were calculated aggregating the species as shown in this table and summing the value of biomass of each species

No.	Functional groups resulting from the aggregation Group name	Abbr.	Basic inputs						
			Biomass (kcal m^{-2})	P/B ($month^{-1}$)	Q/B ($month^{-1}$)	GE	EE	$\%NA$	Harvest
1	Benthic macrophytes	BM	630.0	1.4					
2	Phytoplankton	Phyt	0.7	60.0					
3	Bakterioplankton	Bakt	0.9	9.0	28.0			0.10	
4	Zooplankton	Zoopl	0.4	3.0		0.20		0.50	
5	Micro and mesobenthos detritivorous–herbivorous	mMdh	44.9		5.71	0.20		0.40	
6	Macrobenthos detritivorous	Md	67.3		1.50	0.20		0.40	
7	Macrobenthos herbivorous–detritivorous	Mhd	114.6	0.5		0.20		0.40	
8	Macrobenthos omnivorous–filter feeders	Moff	23.1	0.5		0.20		0.30	
9	Macrobenthos omnivorous–mixed feeders	Momf	63.6		0.80	0.20		0.20	
10	Macrobenthos omnivorous–predators	Mop	128.2		0.42	0.20		0.20	
11	Nekton detritivorous	Ndet	4.4		0.54	0.20		0.30	0.120
12	Nekton carnivorous, fish0	NcF0		0.46		0.30	0.98	0.10	
13	Nekton carnivorous benthic feeders	Ncbf	4.30		0.54	0.20		0.26	0.150
14	Nekton carnivorous nekton feeders	Ncnf	0.30		0.37	0.20		0.20	0.004
15	Birds	Birds	0.01		1.76	0.20		0.20	
16	Detritus (Suspended + Deposited) and DAO	Det	1876						

Detail of the species:
6: Polychaeta: *Streblospio dekhuyzeni*, *Polydora ciliata*, *Spionidae ind.*, *Capitella capitata*, *Nereis diversicolor*
Amphipoda-Isopoda: *Iphinoe* sp., *Microdeutopus grillotalpa*.
Diptera: *Chironomus salinarius*.
7: Gastropoda: *Haminea navicula*, *Hydrobia ventrosa*.
Amphipoda: *Gammarus insensibilis*, *Gammarus aequicauda*, *Corophium insidiosum*, *Corophium orientale*.
8: Bivalvia: *Abra alba*, *Abra ovata*, *Cerastoderma glaucum*, *Tapes* sp.
9: Anthozoa: *Actinia*.
10: Decapoda: *Carcinus mediterraneus*
Gastropoda: *Cyclope neritea*.

The aggregation of flows into discrete trophic levels gives the best quantitative description of the above-mentioned aspects. In Fig. 5.5, fractional trophic levels have been reversed by an approach suggested by Ulanowicz (1995) into six discrete trophic levels *sensu* and flows have been separated according to origin or destination. The figure shows that the combined flows of trophic levels I and II, plus the accumulation of detritus (192 kcal/(m^2 month)) sum up to 2400 kcal/(m^2 month), i.e. 98% of the total system throughput (2458 kcal/(m^2 month)).

Table 5.2. Diet composition matrix. Columns 3 to 15 represent the Diet Matrix. Columns 1 and 2 do not appear because they refer to primary producers. Column 16 is an output of the model and represents flows to detritus normalized by total detritus inflow. This column was added because it is of interest here to compare the resulting matrix (G) with the matrix T_d in Table 5.4.

		Diet matrix (G)													
Abbr.	Group	3	4	5	6	7	8	9	10	11	12	13	14	15	16
BM	1			0.003		0.81			0.35						0.386
Phyt	2		0.30				0.40	0.14							0.014
Bakt	3		0.30				0.05	0.05							0.005
Zoopl	4		0.05				0.003	0.002		0.10	0.60				0.004
mMdh	5			0.005					0.04		0.05				0.217
Md	6							0.10	0.17		0.15	0.1			0.066
Mhd	7							0.29	0.12		0.10	0.29			0.216
Moff	8								0.04			0.33			0.037
Momf	9											0.02	0.03		0.029
Mop	10							0.10	0.02			0.22	0.02		0.021
Nd	11												0.15		0.002
NcF0	12							0.002				0.03	0.05	0.3	
Ncbf	13											0.02	0.55		0.001
Ncnf	14														
Birds	15														
Det	16	1.00	0.35	0.992	1.00	0.19	0.55	0.31	0.25	0.90	0.10				
Import													0.2	0.7	

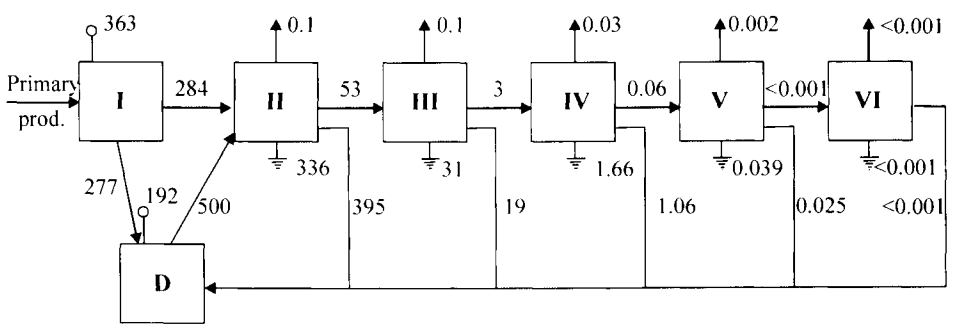

Fig. 5.5. Aggregation of flows by discrete trophic levels.

Table 5.3. Flow matrix. Pred. is the sum of consumption values in the rows, excluding column 16, the flow to detritus. Intake is the sum over the column. %Pred. is the ratio between the predation on the group and total system consumption. %Int. is the ratio between the consumption of the group and total system consumption.

		Flow matrix															
		3	4	5	6	7	8	9	10	11	12	13	14	15	16	Pred.	%Pred.
BM	1	0	0	0.8	0	232	0	0	19	0	0	0	0	0	267.36	251.64	0.299
Phyt	2	0	1.8	0	0	0	23.1	7.3	0	0	0	0	0	0	9.79	32.21	0.038
Bakt	3	0	1.8	0	0	0	2.9	2.5	0	0	0	0	0	0	3.39	7.23	0.009
Zoopl	4	0	0.3	0	0	0	0.2	0.1	0	0.2	0.39	0	0	0	3.00	1.20	0.001
mMdh	5	0	0	1.5	0	0	0	0	2.4	0	0.03	0	0	0	149.96	3.94	0.005
Md	6	0	0	0	0	0	0	5.1	9.1	0	0.10	0.23	0	0	45.92	14.51	0.017
Mhd	7	0	0	0	0	0	0	14.8	6.5	0	0.06	0.67	0	0	149.78	22.05	0.026
Moff	8	0	0	0	0	0	0	0	2.4	0	0	0.76	0	0	25.73	3.13	0.004
Momf	9	0	0	0	0	0	0	0	0	0	0	0.04	0.003	0	20.30	0.04	0.000
Mop	10	0	0	0	0	0	0	5.1	1.2	0	0	0.50	0.002	0	14.77	6.77	0.008
Nd	11	0	0	0	0	0	0	0	0	0	0	0	0.017	0	1.04	0.02	0.000
NcF0	12	0	0	0	0	0	0	0.1	0	0	0	0.08	0.006	0.005	0.07	0.19	0.000
Ncbf	13	0	0	0	0	0	0	0	0	0	0	0.05	0.061	0	0.81	0.11	0.000
Ncnf	14	0	0	0	0	0	0	0	0	0	0	0	0	0	0.04	0.00	0.000
Birds	15	0	0	0	0	0	0	0	0	0	0	0	0	0	0.01	0.00	0.000
Det	16	25.2	2.1	254	101	54	31.6	15.8	13.5	2.1	0.06	0	0	0	0	499.61	0.593
Import		0	0	0	0	0	0	0	0	0	0	0	0.022	0.012			
Tot. Intake		25.2	6.0	256.5	100.7	286.4	57.7	50.8	53.9	2.3	0.6	2.3	0.1	0.02			
%Int.		0.03	0.007	0.304	0.120	0.340	0.069	0.060	0.064	0.003	0.001	0.003	0.000	0.000			

Table 5.4. Total dependency matrix T_{ij}

Abb.	Group	3	4	5	6	7	8	9	10	11	12	13	14	15	16
BM	1	0.943	0.645	0.943	0.943	0.989	0.565	0.820	0.952	0.913	0.768	0.824	0.673	0.225	0.943
Phyt	2	0.057	0.355	0.057	0.057	0.011	0.435	0.180	0.048	0.087	0.232	0.175	0.128	0.068	0.057
Bakt	3	0.016	0.322	0.016	0.016	0.003	0.060	0.059	0.010	0.046	0.198	0.032	0.037	0.058	0.016
Zoopl	4	0.008	0.055	0.008	0.008	0.001	0.008	0.008	0.004	0.107	0.604	0.025	0.063	0.177	0.008
mMdh	5	0.261	0.179	0.265	0.261	0.050	0.157	0.153	0.170	0.253	0.227	0.141	0.136	0.067	0.261
Md	6	0.107	0.073	0.106	0.107	0.020	0.064	0.166	0.210	0.103	0.211	0.185	0.137	0.062	0.107
Mhd	7	0.346	0.237	0.345	0.346	0.066	0.207	0.482	0.296	0.335	0.346	0.484	0.354	0.101	0.346
Moff	8	0.061	0.041	0.060	0.061	0.011	0.036	0.039	0.075	0.059	0.044	0.362	0.212	0.013	0.061
Momf	9	0.046	0.032	0.046	0.046	0.009	0.028	0.026	0.024	0.045	0.034	0.038	0.057	0.010	0.046
Mop	10	0.039	0.027	0.039	0.039	0.007	0.023	0.120	0.042	0.038	0.028	0.236	0.158	0.008	0.039
Nd	11	0.002	0.002	0.002	0.002		0.001	0.001	0.001	0.002	0.002	0.001	0.154	0.001	0.002
NcF0	12							0.002				0.034	0.073	0.294	
Ncbf	13	0.002	0.001	0.002	0.002	0.000	0.001	0.001	0.001	0.002	0.001	0.021	0.550		0.002
Ncnf	14														
Birds	15														
Det	16	1.00	0.684	0.997	1.00	0.190	0.599	0.571	0.524	0.968	0.729	0.506	0.491	0.214	0.384

The system exerts a very high predation pressure on zooplankton (EE = 99.6%) and juvenile fish (EE = 98.0%), A null to low predation pressure is exerted on birds (EE = 0%), omnivorous mixed-feeding macrobenthos (Anthozoa, EE = 0.4%), and the micro/mesobenthos compartment (Protozoa, Nematoda, Copepoda, EE = 7.7%). The main bulk of production of these groups is recycled to the detritus pool.

To survey the dependencies between organisms originating from indirect relationships, the diet matrix G was compared with the matrix T_d, representing the "indirect dependency" of each group of organisms on the others (Table 5.4).

Other interesting relationships are emerging from this kind of analysis. They involve nektonic and benthic compartments which represent species of commercial interest. Looking at columns 13 and 14 of the T_d matrix, it is possible to quantify the dependency of some of the commercially valuable nektonic species on detritus. Approximately 50% of the food of nektonic benthic feeders and nektonic nekton feeders passed through detritus at least once, whereas a null percentage of such food is indicated in the diet matrix related to the direct transfer of matter.

These relations appear like "emerging" links that, when added to the previously mentioned raise of dependencies on detritivorous mesobenthos and herbivorous–detritivorous macrobenthos, show how matter propagates along the trophic network and permit quantification of the impact of eventual disturbances in lower trophic levels on higher ones, based on a holistic criterion.

Such high values of indirect dependency coefficients are illustrated as well by the impressive number of pathways leading from the first trophic level to top predators. 1065 pathways lead from primary producers and detritus to the nektonic apex predator via bivalves and 1558 via macrobenthic omnivorous predators (excluding cycles).

5.5 Response Models

Another class of steady-state models deals with the prediction of the state of a system as a consequence of the value of a forcing function. The state of the system can be expressed as the dependent variable of an equation representing the most sensitive variable of the system taken as an indicator of the system state. This variable is correlated to the independent forcing variable by a simple empirical or semi-empirical statistical model.

Such simple models account neither for the complexity of the ecosystem, nor for the usual complex biological processes, but are often used to discover undesired effects on the system. These empirical or semiempirical models are set up elaborating a set of experimental data and are used to discover and quantify the relation between causes and effects. They depend strictly on the data considered and cannot be used to predict the behaviour of the system when data forcing the system are out of the range of data considered to set up the relation, nor if the considered system is different from that modelled.

As for the network models, this class of steady-state model is also useful in the initial phase of the investigation of a system.

5.5.1 *Response Models in Ecotoxicology*

Some of the statistical models deal with the experimental data of ecotoxicological interest and show the correlation between the concentration of a toxic substance in sediment and that in individuals living in the sediment.

Figure 5.6 shows the relationship between the concentration of heavy metal in animal tissues and in sediment. Such a simple models can be used to find concentrations of heavy metals of benthic animals in new sites. The same relationship can be seen in the data reported in Fig. 5.7: these data are more spread than those of

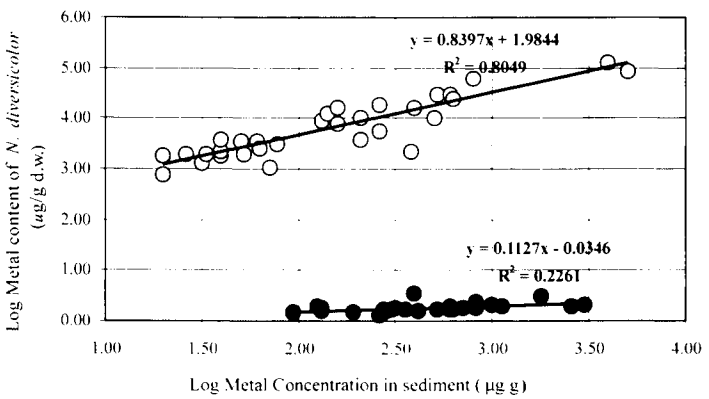

Fig. 5.6. Concentration of zinc (open circles) and copper (filled circles) in the tissues of the polychaete worm *Nereis diversicolor* (expressed as dry weight of tissue) taken from sites in more than 20 estuaries in Devon and Cornwall, and in the sediment at those sites (Bryan, 1976).

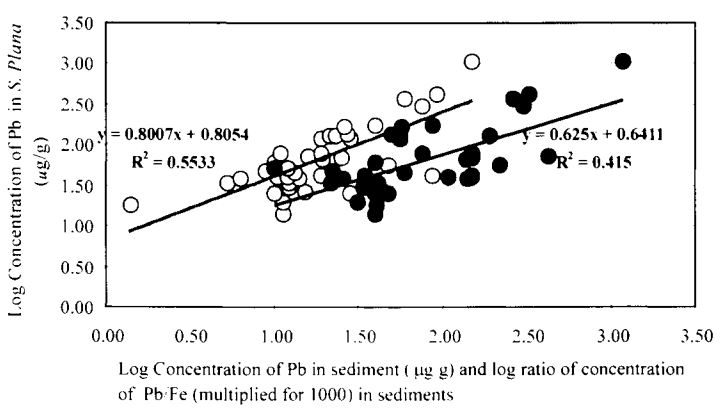

Fig. 5.7. Concentrations of total lead in the soft tissues of 37 samples of the bivalve *Scrobicularia plana* collected from 17 estuaries in south and west England plotted against (filled circles) the lead content of sediment particles and (open circles) the ratio of the concentration of lead to that of iron, multiplied by 10^3 in sediment particles.

zinc in the previous figure and the linear correlation is weaker when only the direct cause–effect process is accounted for.

When the ratio lead/iron in sediment is considered, data are better correlated. Indirectly the iron concentration expresses the binding capacity of the sediment, and when a second process of ecological interest is accounted for, the empirical model predicts the toxicity of lead in the bivalve in a better way. As more processes are accounted for in the model, the better the model predicts the state of the system, but also the more complex the model is.

5.5.2 *Response Models for Trophic State*

Another class of steady-state models deals with the prediction of the trophic states of lakes, usually expressed as concentrations of chlorophyll-a in the water body, or as its primary production.

They are based on a statistical analysis of a dataset reporting the concentrations of some of the most common variables describing the state of a lake such as chlorophyll-a, phosphorus, nitrogen, Secchi disk.

The data base includes lakes, with homogeneous characteristics, in a sufficiently high number to be statistically significant. These models assume that the water body is in steady-state condition and that the trophic states (oligotrophic, mesotrophic, eutrophic) can be calculated by a function of some of the variables describing the state of the lake, as in Table 5.5.

They have been developed to explain the relation between the loads and the trophic state of the lake. Historically, the first attempt of such an analysis was done by Vollenweider (1968), who considered a large number of lakes in temperate climates and correlated in a plot the average concentration of phosphorus and chlorophyll-a, as shown in Fig. 5.8. This figure shows the linear regression:

$$\text{chl-a} = 0.28 \cdot (\text{P})^{0.96}$$

which has a correlation coefficient $r = 0.88$, lakes with a N/P ratio lower then 10 (nitrogen limitation) are not considered in this data base.

A similar strong correlation have been found between P and the maximum chl-a concentration, ($r = 0.90$), between Secchi disc and chl-a concentration ($r = -0.75$). A

Table 5.5. Trophic-state classification based on the values of some variables

Variable	Oligotrophic	Mesotrophic	Eutrophic
Total phosphorus (mg P/m^3)	<10	10–20	>20
Chlorophyll-a (mg chl-a/m^3)	<4	4–10	>10
Secchi-disc (m)	>4	2–4	<2
Hypolimnion oxygen (% sat.)	>80	10–80	<10

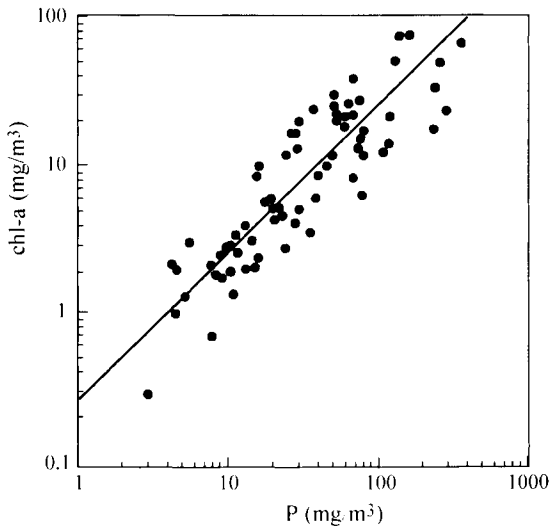

Fig. 5.8. Linear regression between phosphorus and chlorophyll-a in lakes of temperate areas reported by Vollenweider (1968). Note the logarithmic scale in the axes.

weaker one has been found between Secchi disc and P (r = –0.47) because the process of light attenuation involves other factors that are not accounted for in the last correlation.

A hyperbolic model has been tested to predict the planktonic primary production PP (g C/m^2 year^{-1}) as a consequence of average phosphorus concentration P or chl-a concentration.

The models are respectively:

$$PP = 512 \cdot \frac{P}{P + 28.1} \qquad \text{with } r = 0.70$$

$$PP = 631 \cdot \frac{\text{chl-a}}{11.8 + \text{chl-a}} \qquad \text{with } r = 0.74$$

Both the models simulate the saturation process shown by the data in the Fig. 5.9 and set the saturation value around 500 and 600 g C/m^2 year^{-1}, which are not significantly different over a probability $P > 0.95$.

Based on this first rough analysis it was possible to point out the critical role of the phosphorus loads in affecting the trophic state of a lake and to provide a first classification of the temperate lakes.

In a second deeper investigation of the data base, Vollenweider (1975) suggests considering the loading concentration PL and NL (mg/m^2) and adding to the function the residence time t_w of a lake (y).

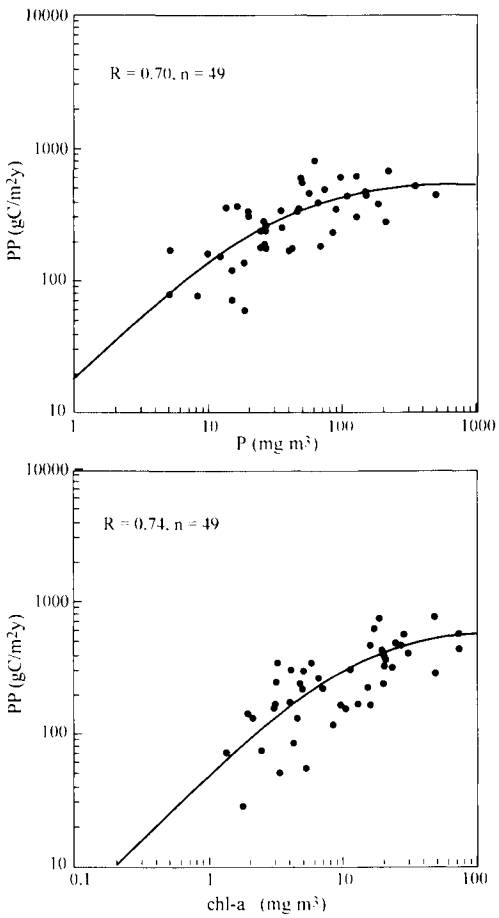

Fig. 5.9. Relation between planktonic production (*PP*) and phosphorus or chlorophyll-a.

Transferring the previous average nutrients concentration *PL* and *NL*, in a corrected nutrient loading function P^* and N^* (mg/m^3) by the formula:

$$P^* = 1.55 \cdot \left[\frac{PL}{(1+\sqrt{t_w})} \right]^{0.82} \quad \text{and} \quad N^* = 5.34 \cdot \left[\frac{NL}{(1+\sqrt{t_w})} \right]^{0.78}$$

This correction does not improve the correlation seen before to a very high level, but allows the model to be used in a predictive way, simulating the effect of a reduction of load on chl-a concentration, Secchi disc and primary production of a lake.

A further elaboration of the data set of temperate lakes done by Vollenweider and presented in details in an OECD report (Vollenweider 1982), shows the uncertainty

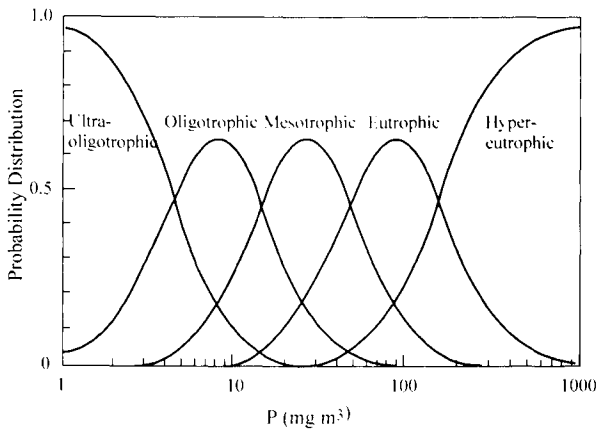

Fig. 5.10. Probability distribution of different trophic states of a temperate lake based on yearly average total phosphorus concentration.

degree, at different levels of confidence, of the results obtained by this response model.

As usual in statistics, it is clear that all the results depend on the data set considered. Also in this case, when we assign a certain category of trophism to a lake, we deal with an uncertainty. For this reason the rigid classification of Table 5.5 has been refined and, according to the Fig. 5.10, it is possible to assign to a lake a certain probability of belonging to a trophic category.

For instance, if we consider an yearly average total phosphorus concentration of 10 mg/m^3, the following probability distribution is associated:

- 10% ultraoligotrophic;
- 63% oligotrophic;
- 26% mesotrophic;
- 1% eutrophic;
- 0% hypereutrophic.

If this diagram were to be used for management purposes to make a prognosis of the rehabilitation of a real lake, it would be necessary to test, by existing data, how much the case study lake fit in the reference data set. The better is the diagnosis of lake trophic category based on the present set of lake, and the narrower is the confidence interval including the lake case, the better the prognosis of the trophic load would be. Also in this case it is clear that the major limit of the response models is the strict dependence of the prognosis on the data set up used to set the statistical relationships.

The temperate lakes data set has been tested to evaluate the trophic state of warm tropical lakes and it appeared totally inadequate.

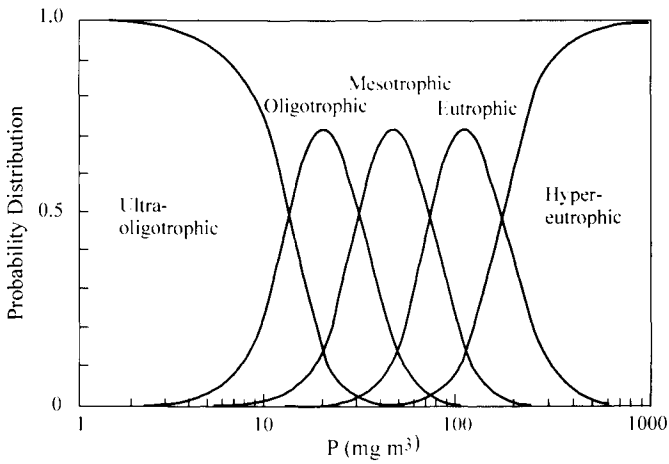

Fig. 5.11. Probability distribution of different trophic states of a tropical and warm lake based on yearly average total phosphorus concentration.

For this reason Salas and Martino (1990) have applied the Vollenweider methodology to a set of 39 tropical and warm lakes and recalculated all the statistics for such a set of data.

A result of such an analysis is plotted in Fig. 5.11 where the probability of a warm tropical lake belonging to a trophic category is shown analogously to the previous one for temperate lakes given in Fig. 5.10.

The comparison of the bell shapes in the two figures clearly and easily shows the difference of the two data bases considered, and highlights how large the error of the prognosis could be if the wrong data base is misused.

In contrast to the previous example, if the same concentration of total phosphorus of 10 mg/m^3 is considered for warm tropical lakes, the following probability distribution results:

- 60% ultraoligotrophic;
- 40% oligotrophic;
- 0% of the other categories.

The simple response model of Vollenweider is surprisingly congruent for such a simplistic relationship but individual lakes can deviate markedly from the "expected" relation. The result is that the lake ecosystem response to reduction in phosphorus inputs can be disappointing. A review of 18 European lakes which had undergone phosphorus input reductions, show that seven did not experience a significant decline in phytoplankton biomass, as expected by model.

Factors, such as light limitations, internal nutrients supply, grazing of zooplankton, and other complex processes usually occurring in lake ecosystems, may

cause failure of the prognosis done by response model and suggest the use of other more reliable models, like dynamic and structurally dynamic ones, to simulate the behaviour of a lake ecosystem.

Illustration 5.3

One of the most important results of the Vollenweider model is the possibility of its use in managing the water quality of a lake. Provided that the conditions for the application of the Vollenweider model are satisfied, it is possible to use Fig. 5.12 to forecast the shift in the lake state forced by a change in the phosphorus load.

Figure 5.12 is a very synthetic way of representing the results of the Vollenweider approach and has been extensively used in limnology. It is a good tool for an early step in modelling a lake.

The x-axis reports the average residence time t_r of the considered lake in a log-scale. This is usually known or it is easy to calculate from the lake limnological parameters.

The y-axis reports the mean value of the concentration of phosphorus loading the lake, this is also usually known or easy to calculate.

Lines in the figure report the average concentration in the lake of phosphorus and chl-a. Trophic categories refer to the classification reported in Vollenweider (1982).

Using Fig. 5.12 it is possible to have a rough estimation of the average phosphorus concentration needed to reach a certain state of the lake. A lake with a $t_r = 10$

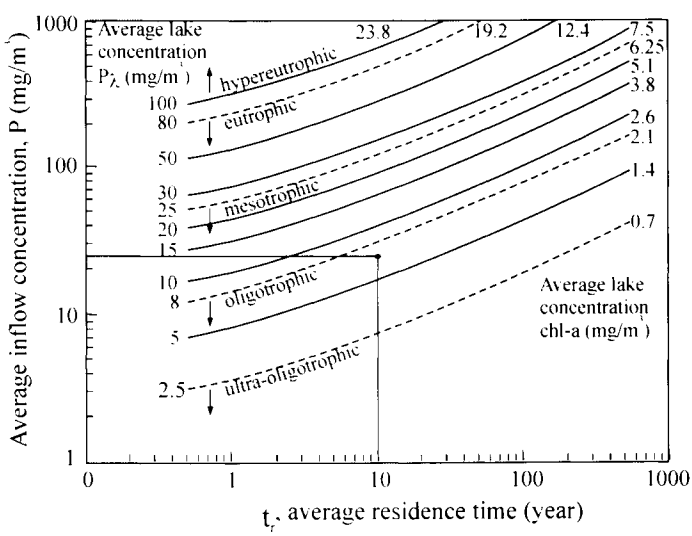

Fig. 5.12. Vollenweider plot for calculation of the trophic state of a temperate lake based on the most important limnological variables. (After OECD report, Vollenweider, 1982).

years, a concentration of 2 mg/m^3 of chl-a, corresponding to an oligotrophic condition, needs an average concentration of about 15 mg/m^3 of phosphorus in the inflow waters. If the volume of the lake is 10^9 m^3, the yearly load supporting such an oligotrophic condition would consequently be 15 ton/year of phosphorus.

CHAPTER 6

Modelling Population Dynamics

6.1 Introduction

This chapter covers population models, where state variables are numbers or biomass of individuals or species. Increasingly complex models are presented, step by step. The growth of one population is mentioned (see Sections 6.2 and 6.3) with a presentation of the basic concepts, while the equations have already been presented in Chapter 3. The interactions between two or more populations are then presented. The famous *Lotka–Volterra model* as well as several more realistic *predator–prey* and *parasitism* models are shown. Age distribution is introduced and computations using matrix models are illustrated, including the relations to growth.

6.2 Basic Concepts

This chapter deals with *biodemographic models*, characterized by numbers or tons of biomass of individuals or species as typical units for state variables.

As early as the 1920s, Lotka and Volterra developed the first population model, which is still widely used today (Lotka, 1956; Volterra, 1926). Most population models have been developed, tested and analyzed since and it will not be possible in this context to give a comprehensive review of these models. The chapter will mainly focus on models of age distribution, growth, and species interactions. Only deterministic models will be mentioned. Those who are interested in stochastic models can refer to Pielou (1966; 1977) who gives a very comprehensive treatment of this type of model.

- A population is defined as a collective group of organisms of the same species. Each population has several characteristic properties, such as *population density* (population size relative to available space), *natality* (birth rate), *mortality* (death rate), *age distribution*, *dispersion*, *growth forms* and others.

A population is a changing entity, and we are therefore interested in its size and growth. If N represents the number of organisms and t the time, then dN/dt = the rate of change in the number of organisms per unit time at a particular instant (t) and $dN/(Ndt)$ = the rate of change in the number of organisms per unit time per individual at a particular instant (t). If the population is plotted against time a straight line tangential to the curve at any point represents the growth rate.

Natality is the number of new individuals appearing per unit of time and per unit of population. We have to distinguish between absolute *natality* and relative natality, denoted by B_a and B_s respectively:

$$B_a = \frac{\Delta N_n}{\Delta t} \tag{6.1}$$

$$B_s = \frac{\Delta N_n}{N\Delta t} \tag{6.2}$$

where ΔN_n = production of new individuals in the population.

Mortality refers to the death of individuals in the population. The absolute mortality rate, M_a, is defined as:

$$M_a = \frac{\Delta N_m}{\Delta t} \tag{6.3}$$

where ΔN_m = number of organisms in the population, that died during the time interval Δt, and the relative mortality rate, M_s, is defined as:

$$M_s = \frac{\Delta N_m}{\Delta t \cdot N} \tag{6.4}$$

6.3 Growth Models in Population Dynamics

The simplest growth models consider only one population. Its interactions with other populations are taken into consideration by the specific growth rate and the mortality, which might be dependent on the magnitude of the population considered but independent of other populations. In other words we consider only one population as state variable.

The simplest growth model assumes *unlimited resources and exponential population growth*. A simple differential equation can be applied:

$$dN/dt = B_s \times N - M_s \times N = r \times N \tag{6.5}$$

where B_s is the instantaneous birth rate per individual, M_s the instantaneous death rate, $r = B_s - M_s$, N the population density and t the time. As seen, the equation represents first-order kinetics (see Section 2.8) and *exponential growth* (see Section 3.6). If r is constant, after integration, we get:

$$N_t = N_0 \times e^{rt} \tag{6.6}$$

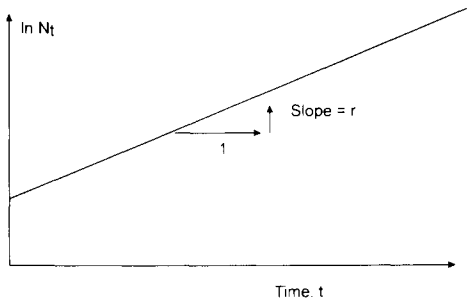

Fig. 6.1. ln N_t is plotted versus time, t.

where N_t is the population density at time t and N_0 the population density at time 0. A logarithmic presentation of Eq. (6.6) is given in Fig. 6.1.

The net reproductive rate, R_0 is defined as the average number of age class zero offspring produced by an average newborn organism during its entire lifetime. Survivorship l_x is the fraction surviving at age x. It is the probability that an average newborn will survive to the age designated x. The number of offspring produced by an average organism of age x during the age period is designated m_x. This is called *fecundity*, while the product of l_x and m_x is called the realized fecundity. According to its definition R_0, can be found as:

$$R_0 = \int_0^\infty l_x m_x \, dx \tag{6.7}$$

A curve that shows l_x as a function of age is called a survivorship curve. Such curves differ significantly for various species, as illustrated in Fig. 6.2.

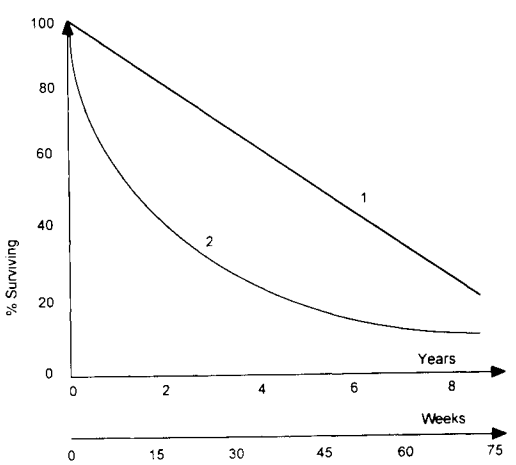

Fig. 6.2. *Survivorship* of (1) the lizard Uta (the lower x-axis) and (2) the lizard Xantusia (the upper x-axis). After Tinkle (1967).

Table 6.1. Estimated maximal *instantaneous rate of increase* (r_{max}, per capita per day) and *mean generation times* (in days) for a variety of organisms

Taxon	Species	r_{max}	Generation time
Bacterium	*Escherichia coli*	ca. 60.0	0.014
Algae	*Scenedesmus*	1.5	0.3
Protozoa	*Paramecium aurelia*	1.24	0.33–0.50
Protozoa	*Paramecium caudatum*	0.94	0.10–0.50
Zooplankton	*Daphnia pulex*	0.25	0.8–2.5
Insect	*Tribolium confusum*	0.120	ca. 80
Insect	*Calandra oryzae*	0.10 (0.09–0.11)	58
Insect	*Rhizopertha Dominica*	0.085 (0.07–0.10)	ca. 100
Insect	*Ptinus tectus*	0.057	102
Insect	*Gibbium psylloides*	0.034	129
Insect	*Trigonogenius globules*	0.032	119
Insect	*Stethomezium squamosum*	0.025	147
Insect	*Mezium affine*	0.022	183
Insect	*Ptinus fur*	0.014	179
Insect	*Eurostus hilleri*	0.010	110
Insect	*Ptinus sexpunctatus*	0.006	215
Insect	*Niptus hololeucus*	0.006	154
Octopus	–	0.01	150
Mammal	*Rattus norwegicus*	0.015	150
Mammal	*Microtus aggrestis*	0.013	171
Mammal	*Canis domesticus*	0.009	ca. 1000
Insect	*Magicicada septendecim*	0.001	6050
Mammal	*Homo sapiens*	0.0003	ca. 7000

The so-called *intrinsic rate of natural increase*, r, is, like l_x and m_x, dependent on the age distribution, and is only constant when the age distribution is stable. When R_0 is as high as possible, i.e., under optimal conditions and with a stable age distribution, the maximal rate of natural increase is realized and designated r_{max}. Among various animals it ranges over several orders of magnitude (see Table 6.1).

Exponential growth is a simplification which is only valid over a certain time interval. Sooner or later every population must encounter the limitations of food, water, air or space, as the world is finite. To account for this we introduce the concept of *density dependence*, i.e., vital rates, like r, depend on population size, N (while we now ignore differences caused by age). Let the *carrying capacity*, K, be defined as the density of organisms at which r is zero. At zero density R_0 is maximal and r becomes r_{max}. The logistic growth equation has already been treated in Chapter 3. The application of the logistic growth equation requires three assumptions:

1. that all individuals are equivalent;
2. that K and r are immutable constants independent of time, age distribution, etc.;
3. that there is no time lag in the response of the actual rate of increase per individual to changes in N.

All three assumptions are unrealistic and can be strongly criticized. Nevertheless, several population phenomena can be nicely illustrated using the logistic growth equation.

Example 6.1

An algal culture shows a *carrying capacity* due to the self-shading effect. In spite of "unlimited" nutrients, the maximum concentration of algae in a chemostat experiment was measured to be 120 g/m^3. At time 0, 0.1 g/m^3 of algae was introduced and 2 days later a concentration of 1 g/m^3 was observed. Set up a *logistic growth* equation for these observations.

Solution

During the first 5 days we are far from the carrying capacity and we have with good approximations:

$$\ln 10 = r_{max} \cdot 2$$

$$r_{max} = 1.2 \text{ day}^{-1}$$

and since the carrying capacity is 120 g/m^3, we have (C = algae concentration):

$$dC/dt = 1.2 \times C \times (120 - C/120)$$

Integration and use of the initial condition $C(0) = 0.1$ yield

$$C = 120/(1 + e^{(a-1.2t)})$$

where

$$a = \ln((120 - 0.1)/0.1) = 7.09.$$

This simple situation, in which there is a linear increase in the environmental resistance with density, i.e., logistic growth is valid, seems to hold good only for organisms that have a very simple life history.

- **In populations of higher plants and animals, that have more complicated life histories, there is likely to be a delayed response.**

Wangersky and Cunningham (1956; 1957) have suggested a modification of the *logistic equation* to include two kinds of time lag: (1) the time needed for an organism to start increasing, when conditions are favourable; and (2) the time required for organisms to react to unfavourable crowding by altering birth and death rates. If these time lags are $t - t_1$ and $t - t_2$ respectively, we get:

$$dN/dt = r \times N_{t-t_1} \times (K - N_{t-t_2})/K \tag{6.8}$$

Population density tends to fluctuate as a result of seasonal changes in environmental factors or due to factors within the populations themselves (so-called intrinsic factors). We shall not go into details here, but just mention that the growth coefficient is often temperature dependent and since temperature shows seasonal fluctuations, it is possible to explain some seasonal population fluctuations in density in that way.

6.4 Interaction between Populations

The growth models presented in Section 6.3 might have a constant influence from other populations reflected in the selection of *parameters*. It is unrealistic, however, to assume that interactions between populations are constant. A more realistic model must therefore contain the interacting populations (species) as *state variables*. For example, in the case of two competing populations we can modify the logistic model and can use the following equations, often called *Lotka–Volterra equations*:

$$dN_1/dt = r_1 N_1 (K_1 - N_1 - \alpha_{12} N_2)/K_1 \tag{6.9}$$

$$dN_2/dt = r_2 N_2 (K_2 - N_2 - \alpha_{21} N_1)/K_2 \tag{6.10}$$

where α_{12} and α_{21} are competition coefficients, K_1 and K_2 are carrying capacities for species 1 and 2, N_1 and N_2 are numbers of species 1 and 2, and r_1 and r_2 are the corresponding maximum intrinsic rate of natural increase.

The steady-state situation is found by setting Eqs. (6.9) and (6.10) equal to zero. We get:

$$N_1 = K_1 - \alpha_{12} \cdot N_2$$

$$N_2 = K_2 - \alpha_{21} \cdot N_1 \tag{6.11}$$

These two linear equations are plotted in Fig. 6.3 giving dN/dt *isoclines* for each species. Below the isoclines populations will increase, above them they decrease. Thus, four cases result, as illustrated in Fig. 6.3 and summarized in Table 6.2. The equation can also be written in a more general form for a community composed of n different species:

$$\frac{dN_i}{dt} = r_i N_i \left(\frac{k_i - N_i - \left(\sum_{i \neq i}^{n} \alpha_{ii} N_i \right)}{k_i} \right) \tag{6.12}$$

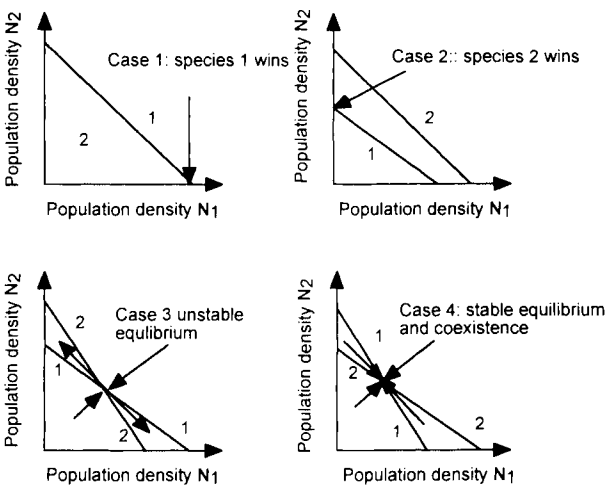

Fig. 6.3. The four cases a, b, c, d: see Eqs. (6.9)–(6.10).

where i and j are species subscripts ranging from 1 to n. At steady state dN_i/dt is equal to zero for all i and

$$N_i \equiv N_{ic} = k_i - \sum_{j \neq i}^{n} \alpha_{ij} N_j \quad (i = 1,2,\ldots, n) \tag{6.13}$$

Lotka–Volterra also wrote a simple pair of *predation* equations:

$$\frac{dN_1}{dt} = r_1 \cdot N_1 - p_1 N_1 \cdot N_2 \tag{6.14}$$

$$\frac{dN_2}{dt} = p_2 \cdot N_1 \cdot N_2 - d_2 \cdot N_2 \tag{6.15}$$

where N_1 is prey population density, N_2 predator population density, r_1 is the intrinsic (maximal) rate of increase of the prey population (per head), d_2 is the mortality of the predator (per head) and p_1 and p_2 are *predation coefficients*. Each population is limited by the other and in the absence of the predator the prey population increases exponentially. By setting the two right-hand sides equal to zero, we find, respectively:

Table 6.2. Summary of the four possible cases of Lotka–Volterra competition equations

	Species 1 can contain Species 2 ($K_2/\alpha_{21} < K_1$)	Species 2 cannot contain Species 2 ($K_2/\alpha_{21} > K_1$)
($K_1/\alpha_{12} < K_2$)	Either species may win (Case 3)	Species 2 always wins (Case 2)
($K_1/\alpha_{12} > K_2$)	Species 1 always wins (Case 1)	Stable coexistence (Case 4)

$$N_2 = \frac{r_1}{p_1} \tag{6.16}$$

$$N_1 = \frac{d_2}{p_2} \tag{6.17}$$

Thus each of the two species *isocline* corresponds to a particular density of the other species. Below the threshold prey density, the predator population will always decrease, whereas above that threshold it will increase. Similarly, the prey population will increase below a particular predator density but decrease above it (see Fig. 6.4). A joint equilibrium exists where the two isoclines cross, but prey and predator densities do not in general converge to this point; instead any given pair of initial densities results in oscillations of a certain magnitude. The amplitude of fluctuations depends on the initial conditions. These equations are unrealistic since most populations encounter either *self-regulation*, *density-dependent feedbacks* or both. The addition of a simple self-damping term to the prey equation results either in a rapid approach to equilibrium or in damped oscillations. Perhaps a more realistic pair of simple equations for modelling the *prey–predator relationship* is:

$$\frac{dN_1}{dt} = r_1 \cdot N_1 - z_1 \cdot N_1^2 - \beta_{12} \cdot N_1 \cdot N_2 \tag{6.18}$$

$$\frac{dN_2}{dt} = \gamma_{21} \cdot N_1 \cdot N_2 - \beta_2 \cdot \frac{N_2^2}{N_1} \tag{6.19}$$

where r_1, z_1, and so on are coefficients.

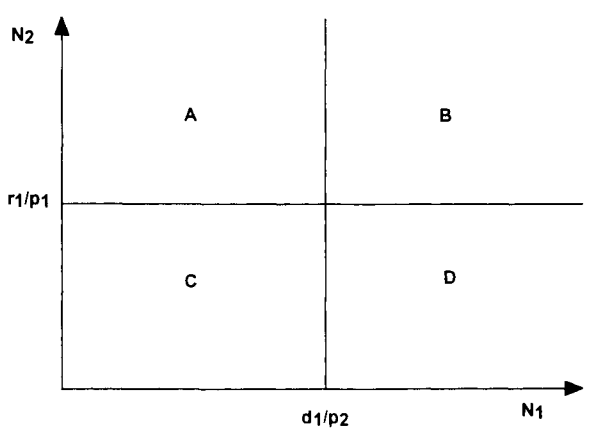

Fig. 6.4. Prey–predator isoclines for the Lotka–Volterra prey–predator equation: (A) both species decrease; (B) predator increase, prey decrease; (C) prey increase, predator decrease; (D) both species increase.

As can be seen, the prey equation is a logistic expression combined with the effect of the predator, while the predator expression considers a *carrying capacity* which is dependent on the prey concentration.

The literature of ecological modelling contains still many papers focusing on modified Lotka–Volterra equations, but the equations can also be criticized for not following the conservation principle. The increase in the biomass of the predator is less than the decrease in the biomass of the prey. Kooijman (2000) has developed many population dynamic models based on the *energy conservation principles* which give new and emerging properties of the energy flow in ecosystems. His approach can be recommended when energy is in focus or if a more complex food web is being considered.

However, Eqs. (6.18) and (6.19) can also easily be criticized. The growth term for the predator is, as can be seen, just a linear function of the prey concentration of density. Other possible relations are shown in Fig. 6.5. The first relationship (A) corresponds to a *Michaelis–Menten expression* (see Chapter 3), while the second relationship (B) only approximates a *Michaelis–Menten expression* by the use of *a first-order expression in one interval and a zero-order expression in another.* The third relationship (C) shown in Fig. 6.5 corresponds to a *logistic expression*: with increasing prey density, the predator density first grows exponentially and afterwards a damping takes place. This relationship is observed in nature and might be explained as follows: the energy and time used by the predator to capture a prey is decreasing with increasing density of the prey. This implies that the predator can not only capture more prey due to increasing density, but also less energy is used to capture the next prey.

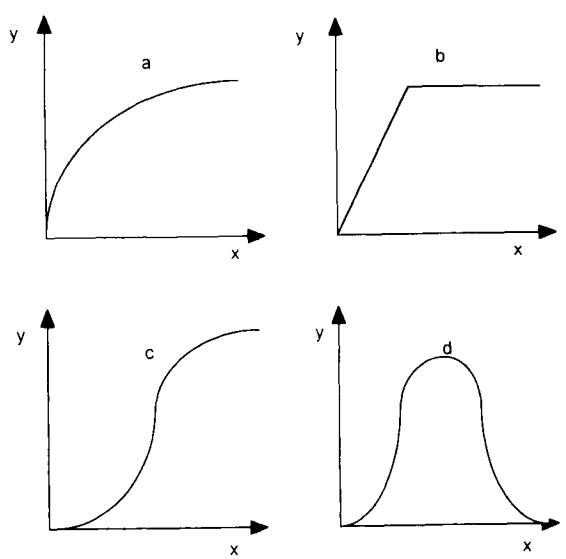

Fig. 6.5. Four functional responses (Holling, 1959) where y is number of prey taken per predator per day and x is the prey density.

Thus, the density of the predator increases more than proportionally to the *prey density* in this phase. Yet, there is a limit to the food (energy) that the predator can consume and at a certain density of the prey, a further decrease in the energy used to capture the prey cannot be obtained. So the increase in predator density slows down as it reaches saturation point at a certain prey density.

The fourth relationship (D) is similar to the often found relation between growth and pH or temperature. It is characteristic here that the *predator density decreases above a certain prey density*. This response might be explained by the effect on the predator of the waste produced by the prey. At a certain prey density the concentration of waste is sufficiently high to have a pronounced negative effect on the predator growth.

Holling (1959; 1966) has developed more elaborate models of prey–predator relationships. He incorporated time lags and hunger levels to attempt to describe the situation in nature. These models are more realistic, but they are also more complex and require a knowledge of more parameters. Besides these complications we have *co-evolution* of predators and prey. The prey will develop better and better techniques to escape the predator and the predator will develop better and better techniques to capture the prey. To account for the co-evolution it is necessary to have a current change of the parameters according to the current selection that takes place.

The effect of *parasitism* is similar to that of *predation*, but differs from the latter in that members of the host species affected are seldom killed, but may live for some time after becoming parasitized. This is accounted for by relating the growth and the mortality of the prey, N_1, to the density of the parasites, N_2. The carrying capacity for the parasites is furthermore dependent on the prey density.

The following equations account for these relations and include a carrying capacity of the prey:

$$\frac{dN_1}{dt} = \frac{r_1}{N_2} \cdot N_1 \left(P \frac{K_1 - N_1}{K_1} \right) \tag{6.20}$$

$$\frac{dN_2}{dt} = r_2 \cdot N_2 \left(\frac{K_2 \cdot N_1 - N_2}{K_2 \cdot N_1} \right) \tag{6.21}$$

Symbiotic relationships are modelled with expressions similar to the Lotka–Volterra competition equations simply by changing the signs for the interaction terms:

$$\frac{dN_1}{dt} = r_1 \cdot N_1 \left(\frac{K_1 - N_1 + \alpha_{12} N_2}{K_1} \right) \tag{6.22}$$

$$\frac{dN_2}{dt} = r_2 \cdot N_2 \left(\frac{K_2 - N_2 + \alpha_{21} N_1}{K_2} \right) \tag{6.23}$$

In nature interactions among populations often become intricate. The expressions presented above might be of great help in understanding population reactions in nature, but when it comes to the problem of modelling entire ecosystems, they are in most cases insufficient.

- **Investigations of stability criteria for Lotka–Volterra equations are an interesting mathematical exercise, but can hardly be used to understand the stability properties of real ecosystems or even of populations in nature.**

Experience from investigations of population stability in nature shows that it is necessary to take into account many interactions with the environment to explain observations in real systems.

The stability concept was widely discussed during the 1970s, but today almost all ecologists agree that the stability of an ecosystem is a very complex problem that cannot be solved by simple methods, at least not by examinations of the stability of two coupled differential equations. It is also acknowledged today that there is no simple relationship between stability and diversity (see May, 1977). Stability must be considered a multidimensional concept, because the stability is dependent on which changes we are concerned with. Some changes the ecosystem might easily adsorb, while others can cause drastic changes in the ecosystem by minor alterations in the forcing function. The buffer capacity introduced in Section 2.6 (see Fig. 2.13), may be a relevant concept to use, as it is multidimensional. There is a buffer capacity for each combination of state variable and forcing function.

Illustration 6.1

This illustration concerns an anaerobic cultivation of two species of yeast, first described by Gause (1934). The two species are *Saccharomyces cerevisiae* (Sc) and *Schizosaccharomyces* (Kephir) (K). Gause cultivated both species in mono-cultures and in mixture and the results suggest that the two species have a mutual effect on each other. His hypothesis was that a production of harmful waste products (alcohols) was the only cause of interactions.

A conceptual diagram of the model to use is shown in Fig. 6.6. The model has three state variables: the two yeast species and the waste products. The amount of

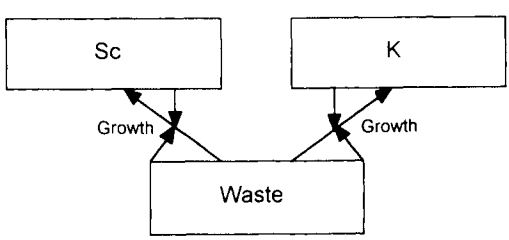

Fig. 6.6. Conceptual diagram of the model presented in Illustration 6.1. Waste is alcohol affecting the growth of two yeast species Sc and K.

Table 6.3. *CSMP Program* for the growth and interference of two yeast species

```
TITLE MIXED CULTURE OF YEAST
    Y1 = INTGRL (IY1, RY1)
    Y2 = INTGRL (IY2, RY2)
IN CON IY1 = 0.45, IY2 = 0.45
    RY1 = RGR1 * Y1 * (1. - RED1)
    RY2 = RGR2 * Y2 * (1. - RED2)
PARAMETER RGR1 = 0.236, RGR2 = 0.049
    RED1 = AFGEN (RED1T, ALC/MALC)
    RED2 = AFGEN (RED2T, ALC/MALC)
FUNCTION RED1T = (0., 0.), (1., 1.)
FUNCTION RED2T = (0., 0.), (1., 1.)
PARAMETER MALC = 1.5
    ALC = INTGRL (ALC, ALCP1 + ALCP2)
    ALCP 1= ALPF1 * 1
    ALCP2 = ALPF2 * RY2
PARAMETER ALPF1 = 0.122, ALPF2 = 0.270
IN CON IALC = 0.

FINISH ALC = LALC
    LALC = 0.99 * MALC
TIMER FINTIM = 150., OUTDEL 2.
PRTPLT Y1, Y2, ALC
END
STOP
```

waste products depends on the growth of yeast. The growth of the yeast species depends on the amount of yeast and the growth rate of the yeast, which is again dependent on the species and a reduction factor, which accounts for the influence of the waste products on the growth. A CSMP-program is presented in Table 6.3. The observed and computed values for the growth of the two yeast species are shown Table 6.4. As can be seen, the fit between observed and calculated values is acceptable for the *monoculture* experiments, but is completely unacceptable for the mixed culture experiments. It can be concluded that the two species do not interfere solely through the production of alcohol. Additional biological knowledge about the interference between the two species must be introduced to the model to explain the observations.

Illustration 6.2

This illustration is a summary of an example presented by Starfield and Bleloch (1986) in their book on population dynamics, "Building Models for Conservation and Wildlife Management". The volume contains many excellent examples on how population dynamics may be used as a management tool. This illustration demonstrates how an analysis of the focal problem can be used to construct a model. The

Table 6.4. Observed and calculated values for the growth of two species of yeasts in mono-cultures and mixtures

	Volume of yeast (arbitrary units)			
	Mono-culture		Mixed	
Hours	Observed	Calculated	Observed	Calculated
		Schizosaccharomyces 'Kephir		
0	0.45	0.45	0.45	0.45
6	–	0.60	0.291	0.59
16	1.00	0.95	0.98	0.81
24	–	1.34	1.47	0.88
29	170	1.64	1.46	0.89
48	2.73	3.04	1.71	0.89
53	–	3.44	1.84	0.89
72	4.87	4.72	–	–
93	5.67	5.51	–	–
117	5.80	5.86	–	–
141	5.83	5.96	–	–
		Saccharomyces cerevisiae		
0	0.45	0.45	0.45	0.45
6	0.37	1.72	0.375	1.70
16	8.87	8.18	3.99	7.56
24	10.66	11.83	4.69	10.86
29	12.50	12.46	6.15	11.47
40	13.27	12.73	–	11.75
48	12.87	12.74	7.27	11.77
53	12.70	12.74	8.30	11.77

equations are all based on semi-quantitative to quantitative known relationships between determining factors on the one side and the influence on the state variables on the other. It is a clear illustration of how "down to earth" considerations might be used to construct models. As many interacting species are involved, the model is made rather complex by including many different relationships between the different state variables of the model. The illustration is concerned with a spectrum of herbivores while no significant predators are present. The principal grazers are warthog, wildebeest, zebra and the white rhinoceros. The principal browsers are giraffe, kudu and the black rhinoceros. Impala and nyala are the two most important mixed feeders.

The problem is illustrated in Fig. 6.7. It implies that the model should consider the interactions between rainfall and vegetation, between vegetation and herbivores and the competition among the herbivores for food.

The first question to consider is: How many classes of species do we need? Clearly giraffe should be a class of its own, as only this animal can browse on tall trees. The black rhinoceros and the kudu browse on shrubs and short trees. Both the white rhinoceros and zebra are grazers that can use relatively tall, coarse grass, while

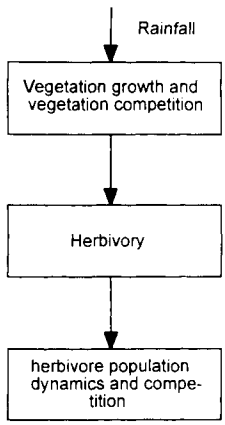

Fig. 6.7. Conceptualization of the problem in Illustration 6.2. The influence of rainfall on the vegetation, the competition among the different forms of vegetation, the food availability for the herbivorous state variables and the competition among the herbivores should all be considered in the model.

wildebeest and warthog are grazers that require short grass. Finally, impala and nyala are mixed feeders, utilizing short grass, shrubs and short trees. By this brief analysis we have suggested how to reduce the number of state variables of herbivores from nine to five. The converting of one variable to another is made using the concept of equivalent animal units (EAU), defined as the daily food intake of a domestic cow. The black rhinoceros is about 2 EAU, a kudu is only about 0.4 EAU. When we lump the two animals together in one group, each black rhinoceros is therefore equivalent to five kudu. The same considerations are made for the other species.

The next problem concerns the food preferences. Here Starfield and Bleloch have suggested setting up the preferences in table form (see Table 6.5). This implies that we have to increase the number of herbivore types from five to six, as shown in the table. For example, impala will first choose palatable grass, then palatable shrubs before resorting to less palatable grass. Kudu on the other hand has only two preferences: first palatable shrubs, then unpalatable shrubs. The effect on switching to a second or third preference is accounted for by a condition index with an arbitrarily chosen scale form 1 to 6: 1 corresponds to the peak of condition, while 6 means extremely poor condition. It is important whether an animal class has an inadequate diet for just one month or for a number of consecutive months. The scale is therefore used to consider the cumulative effect and it is used step-wise. The condition index influences the mortality, particularly the juvenile mortality, which will increase sharply as the condition index approaches 6.

For each of the five classes we consider two sub-classes: adults and juveniles. We estimate for example that an adult kudu requires B kg and a juvenile b kg of food per month, which is selected as the time step of the model. If there are K adult kudu and k juveniles, the kudu population in that park will potentially eat $KB + kb$ kg of leaves

Table 6.5. *Food preferences* of the herbivores

Species	Preference 1	Preference 2	Preference 3
Giraffe	Palatable tall trees	Palatable shrubs	Unpalatable trees
Impala	Grass: palatability > 0.8	Palatable shrubs	Less palatable grass
Kudu	Palatable shrubs	Unpalatable shrubs	
Warthog	Grass: palatability > 0.8	Less palatable grass	
Wildebeest	Grass: palatability > 0.8	Less palatable grass	
Zebra	Grass: palatability > 0.6	Less palatable grass	

in the next month. The model calculates a demand for food, first assuming that every species eats only its first preference. If there is sufficient for all, the food is shared accordingly, but if there is a shortage, the model allocates a share of each animal's second preference, which determines a possible change of the condition index.

Except for zebra, all births take place during the first months of the summer. It is assumed that zebra produce their young throughout the year. The annual birthrate varies from 0.2 for giraffe to 0.95 for warthog.

Six types of vegetation are considered in the model: (A) grass, (B) shrubs + small trees, and (C) tall trees; each with a palatable and unpalatable subclass. The growth in leaf biomass for the two subclasses of B and C are modelled using the following equation:

$$dl/dt = r * f * S * [1 - L/(q * S)] - b \tag{6.24}$$

where L denotes the leaf biomass, r a growth parameter, f is a rainfall correction factor, S the woody component, q the maximum leaf mass that one unit of wood mass normally can support and b is calculated from the herbivore module as the food requirement (see above). The equation is based on the following assumptions:

1. new leaf growth depends on how many bushes/trees, S, there are;
2. rainfall will influence production;
3. herbivores will consume some biomass each month;
4. there is an inhibitory effect of existing leaf biomass, which is considered in the expression: $[1 - L/(q \cdot S)]$;

The application of Eq. (6.24) implies that we have to model the wood mass, S. This is done by using:

$$dS/dt = rs * fs * S * [1 - (\sum S)/T_{max} * C] \tag{6.25}$$

where rs is the growth parameter for woody biomass, fs is the rainfall correction factor for the woody biomass of shrubs and trees, $\sum S$ is the present total wood mass,

T_{max} is the saturation level for woody biomass, and C is the competition from grass. C is found from:

$$C = \exp(-[p * c * A * h + \Sigma l]/U \tag{6.26}$$

where p is a competition factor (must be calibrated), c is converting grass volume to biomass, A is the grass area, h the height of the grass, Σl is the total leaf biomass, and U is the saturation level for green production.

A and h are state variables, too. Equations for the grass area (m^2), A, and for the grass height (m), h, are included in the model:

$$dA/dt = ra * fg * A * C \tag{6.27}$$

$$dh/dt = rh * fg * h[1 - h/h_{max}] - G/(c * A) \tag{6.28}$$

where ra and rh are the growth parameters for A and h, fg is the rainfall correction factors for grass area and grass height, h_{max} is the saturation height for grass, and G is the grass biomass consumed by herbivores (kg/month), obtained from the herbivore module. Empirical tables are available for f. For instance, fg is dependent on the rainfall, whether it is low medium and high, and it is dependent on the season.

Figures 6.8 and 6.9 show some of the simulations carried out by the model. The number of kudu versus the number of years is plotted in Fig. 6.8, while Fig. 6.9 gives the palatable browse on shrubs in the same period. The condition index will be roughly opposite to this curve. When the palatable browse is high the condition index is low and *vice versa*.

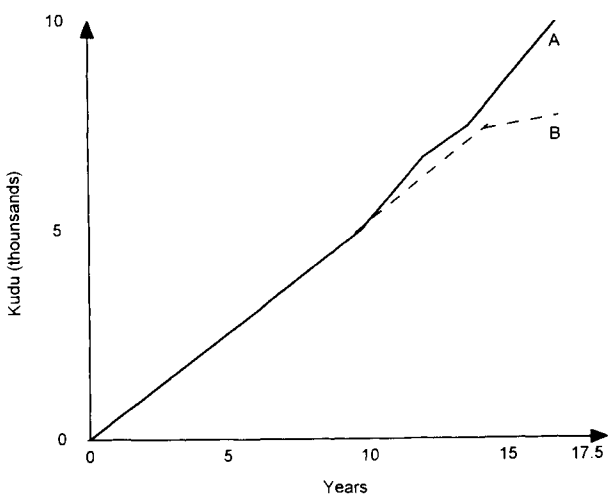

Fig. 6.8. The kudu population is plotted versus the number of years: (A) corresponds to cropping of the impala, whenever their population exceeds 6000; (B) corresponds to no cropping of impala under otherwise similar conditions.

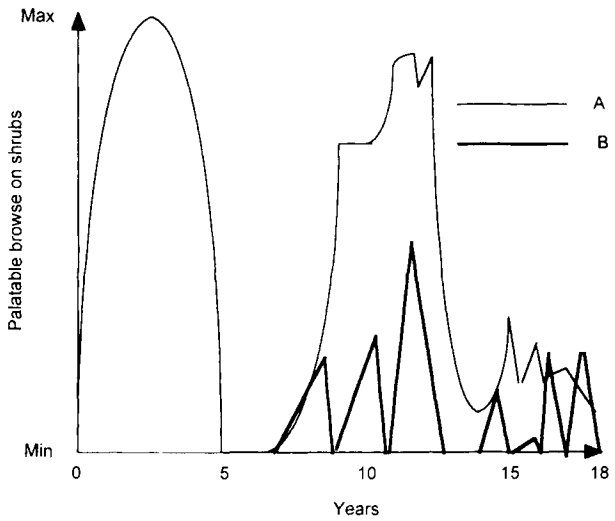

Fig. 6.9. The amount of palatable browse on shrubs and short trees is plotted versus the time: (A) corresponds to cropping of the impala, whenever their population exceeds 6000; (B) corresponds to no cropping of impala under otherwise similar conditions.

Rain is—unsurprisingly—of very great importance for the herbivorous populations, as is also expected from the diagram in Fig. 7.7, where the indirect effect of rain on herbivores is obvious. It can be seen by the violent fluctuations in palatable browse on shrubs, that they can almost entirely be explained by fluctuations in rainfall.

6.5 Matrix Models

Another important aspect of modelling population dynamics is the influence of the *age distribution*, which shows the proportion of the population belonging to each age class. If a population has unchanged l_x and m_x schedules, it will eventually reach a stable age distribution, meaning that the percentage of organisms in each age class remains the same. Recruitment into every age class is exactly balanced by its loss due to mortality and aging.

The *growth equations* presented in Chapter 3 and Eqs. (6.6) and (6.8) all assume that the population has a stable age distribution. The *intrinsic rate of increase*, r, *the generation time*, T, and the reproductive value, v_x is conceptually independent of the age distribution, but might of course be different for populations of the same species with different age distributions. Therefore the models presented in the two previous sections did not need to consider age distribution, although in actual cases the parameters do, of course, reflect the actual age distribution.

A model predicting the future age distribution was developed by Lewis (1942) and Leslie (1945). The population is divided into $n + 1$ equal age groups: group 0, 1, 2, 3,..., n. The model is then presented by the following *matrix equation*:

$$\begin{matrix} f_0 & f_1 & f_2 & \dots & f_{n-1} & f_n \\ p_0 & 0 & 0 & \dots & 0 & 0 \\ 0 & p_1 & \dots & \dots & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & \dots & p_{n-1} & 0 \end{matrix} \times \begin{matrix} n_{t,0} \\ n_{t,1} \\ n_{t,2} \\ \cdot \\ \cdot \\ n_{t,n} \end{matrix} = \begin{matrix} n_{t+1,0} \\ n_{t+1,1} \\ n_{t+1,2} \\ \cdot \\ \cdot \\ n_{t+1,n} \end{matrix} \tag{6.29}$$

The number of organisms in the various age classes at time $t + 1$ are obtained by multiplying the numbers of animals in these age classes at time t by a matrix, which expresses the *fecundity* and *survival rates* for each age class. $f_0, f_1, f_2 \dots f_n$ give the reproduction in the i'th age group and $P_0, P_1, P_2, P_3, P_4 \dots P_n$ represent the probability that an organism in the i'th age group still will be alive after promotion to the $(i+1)$th group.

The model can be written in the following form:

$$\boldsymbol{A} * \boldsymbol{a}_t = \boldsymbol{a}_{t+1} \tag{6.30}$$

where $\boldsymbol{A}$ is the matrix, $\boldsymbol{a}_t$ is the column vector representing the population age structure at time t and $\boldsymbol{a}_{t+1}$ is a column vector representing the age structure at time $t + 1$. This equation can be extended to predict the age distribution after k periods of time:

$$\boldsymbol{a}_{t+k} = \boldsymbol{A}^k * \boldsymbol{a}_t \tag{6.31}$$

The matrix $\boldsymbol{A}$ has $n + 1$ possible *eigenvalues* and *eigenvectors*. Both the largest eigenvalues, λ, and the corresponding eigenvectors are ecologically meaningful. λ gives the rate at which the population size is increased:

$$\boldsymbol{A} * v = \lambda * v \tag{6.32}$$

where v is the stable age structure. ln λ is the intrinsic rate of natural increase. The corresponding *eigenvector* indicates the stable structure of the population.

Example 6.2

Usher (1972) has given a very illustrative example on the use of matrix models. The model is based on data provided by Laws (1962) and Ehrenfeld (1973) for the blue whale before its extinction and sharp changes in survival rates.

The eigenvalue can be used to find the number of individuals that can be removed from a population to maintain the same number in each age class. It can be shown that the following equation is valid:

$$H = 100(\lambda - 1)/\lambda$$

where H is the percentage of the population that can be removed.

Blue whales reach maturity at between four and seven years of age. They have a gestation period of about one year. A single calf is born and is nursed for about seven months. On average, not more than one calf is born to a female every two years. The numbers of the two sexes are approximately equal. Survival rates are about 0.7 each two years for the first ten years and 0.78 for whales above 12 years. We divide the population into 7 groups with a two-year period for the first six groups and the age of 12 years and above as the seventh group. The fecundity for the first two groups is, according to the information, about zero. The third group has a fecundity of 0.19 and the fourth group of 0.44. The maximum fecundity of 0.50 is reached at the age of 8–11 years. The fecundity of the last group is 0.45.

Find the intrinsic rate of natural increase, the stable structure of the whale population and the harvest, which can be taken to maintain a stable population size.

Solution

The *eigenvalue* can be found either by an iterative method or by plotting the number of whales (totally or for each age class separately) versus the period of time. The slope of this plot will, after a stabilization period, correspond to r, the intrinsic rate of increase, or ins. We find by these methods that $r = 0.0036\ \text{year}^{-1}$ or l = antilog 0.0036 = 1.0036 (for one year) or 1.00362 = 1.0072 for two years. Using Eq. (7.36), the corresponding *eigenvector* is found to be:

a = [1000, 764, 584, 447, 341, 261, 885] as the Leslie matrix is:

$$\begin{matrix} 0 & 0 & 0.19 & 0.44 & 0.50 & 0.50 & 0.45 \\ 0.77 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0.77 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.77 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.77 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0.77 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0.77 & 0.78 \end{matrix}$$

The harvest that can be taken from the population is estimated to be:

$$H = 100(\lambda - 1)/\lambda = 0.71\%$$

every two years, or about 0.355% every year.

If the harvest exceeds this value the population will decline. Population models of *r*-strategies might generally cause more difficulties to develop than models of *K*-strategies, due to the high sensitivity of the fecundity. The number of offspring might be known quite well, but the number of survivors to be included in the first age class, the number of recruits, is difficult to predict. This is the central problem of fish population dynamics, since it represents nature's regulation of population size (Beyer, 1981).

PROBLEMS

1. Set up a STELLA model representing Lotka–Volterra equations. How is it possible to consider the conservation principles, which are a prerequisite for the application of STELLA?
2. Express the model in Illustration 6.1 by STELLA.
3. Make a conceptual diagram of a four-species model based on Eqs. (6.12).
4. Mention at least three reasons for the unrealistic nature of the Lotka–Volterra model.
5. A fish culture has a carrying capacity of 50 g/l. Set up a logistic growth equation for the fish culture, when the initial concentration at day 0 is 1 g/l and the concentration 2 g/l is obtained after 10 days. How long does it take to increase the concentration 24 g/l to 48 g/l? Find an equation that expresses the doubling time as function of the time.
6. Explain under which conditions the four functional responses may occur.
7. Set up a matrix model for a bird population that has the following characteristics:

   (a) life span 7 years;

   (b) 4 eggs from the second year per pair, increasing to 5 eggs the third year and 6 eggs the following years;

   (c) the mortality is 30% the first year, 20% the following years, except the last year where it is 100%

   What is the steady state age distribution?

CHAPTER 7

Dynamic Biogeochemical Models

7.1 Introduction

This chapter gives detailed examples of typical dynamic *biogeochemical models*. A wide application and pronounced development of this type of model has taken place during the last 25 years. The models are often formulated as a set of differential equations combined with some algebraic equations and a parameter list. Obviously, the differential equations require the definition of an initial state.

The following biogeochemical models are included in the chapter: three *eutrophication* models with very different complexities and a wetland model. The classical Streeter–Phelps BOD/DO model which belongs to this type of model has already been discussed in Section 2.12 and Chapter 3. As an introduction to the three eutrophication models, an overview of the available eutrophication models will be given. Eutrophication models are used to show the complexity spectrum of models available today. In this context the selection of model complexity will be discussed with reference to Chapter 2. Furthermore, the generality of models and the possibilities of setting up prognoses will be discussed using eutrophication models as examples. All four models presented are discussed in detail. It is hoped that the reader will thereby gain a good impression of how to develop and use a biogeochemical model and how to assess the advantages and disadvantages of this type of model. Furthermore, it is hoped that the reader will learn to be critical and will understand the considerations involved in modelling, including the selection of a balanced *model complexity*.

Wetlands models have been very much in focus during the last five to eight years due to an increasing interest in these ecosystems as habitats for birds and amphibians. The restoration of existing wetlands or the construction of new wetlands seems to be the most effective abatement method of nutrient pollution from non-point sources (mainly agricultural pollution). This has obviously increased the demand for good management models in the area. One relatively simple wetland model will be presented: a model of the nitrogen removal by *denitrification* processes in wetlands, using *STELLA*.

Biogeochemical models have been widely used to solve very concrete problems, examples of which are given below.

- Optimization of biological treatment plants: treated comprehensively in Snape et al. (1995); the *submodels* applied are presented with all information about process equations, parameters and forcing functions.
- Ground water contamination: covered in National Research Council (1990).
- The acidification problem: the Rains Model is presented in a very detailed way in Alcamo et al. (1990).
- *Forest growth* and yield: Vanclay (1994).
- *Air pollution problems*: a number of applicable models are published in Gryning and Batchvarova (2000) and Baldasano et al. (1994).
- *Optimization of agriculture*: a very detailed treatment is given in France and Thornley (1984).

7.2 Application of Dynamic Models

Ecosystems are dynamic systems and it might therefore be the ultimate goal for a modeller to construct *dynamic models of ecosystems*. Models of population dynamics focusing on changes in the size of population caused by the production of offspring and various forms of mortality were given in Chapter 6. The growth of individuals or age classes was considered using growth dependence of various factors. Ecosystem management at the population level seems feasible using of this type of model, including the important management of renewable resources.

This chapter is devoted to another type of model, one which has gained wide application both in science and in a management context. *Biogeochemical models* attempt to capture the dynamics and cycling of biochemical and geochemical compounds in ecosystems. When models are used as an instrument in pollution control, they must account for the fate and distribution of both pollutants and of nature's own compounds. This will require the application of biogeochemical models, since they focus on the processes and transformation of various compounds in the ecosystem.

Total ecosystem models which couple population models with biogeochemical models have also been developed. These have been touched on in Chapter 4 where the application of hierarchical models are discussed. The food available for growth is dependent on the biogeochemical cycling in ecosystems and the growth rate is dependent on the general life condition in the ecosystem, which again is dependent on the biogeochemical cycling. The coupling between the two types of model takes place through such relationships, and will often require application of at least a two-hierarchical model.

As pointed out in Sections 2.7 and 2.8, the construction of dynamic models requires data, which can elucidate the dynamics of the processes included in the

model. Generally, a more comprehensive database is required to build a dynamic model than a static model. Therefore, in a data-poor situation it might be better to draw up an average situation under different circumstances using a static model than to construct an unreliable dynamic model which contains uncertainty in the most crucial parameters.

The first biogeochemical model to be constructed was the *Streeter–Phelps BOD-DO model* in 1925 (Streeter and Phelps, 1925); it is described in detail in Chapter 3 which illustrates quite clearly the concept of biogeochemical models. As opposed to most dynamic models, the *Streeter–Phelps model* consists of only one differential equation, which can be solved analytically (see Chapter 3).

Hydrodynamic models can be considered as *biogeochemical models*, since they describe the fate and distribution of the important compound water in ecosystems. The output from hydrodynamic models might often be used as forcing functions in ecological models. Although they are not ecological models as they do not account for any biological processes, they are often used in conjunction with ecological models as the distribution of chemical compounds and living organisms is dependent on the hydrodynamics. During the 1990s, three-dimensional hydrodynamic models were applied more and more frequently, but it is only in recent years that well developed ecological models, e.g., *eutrophication models*, were coupled with three-dimensional hydrodynamic models. It is important to emphasize that it there is no sense in coupling simple, insufficiently developed ecological models with three-dimensional models, because the standard deviations of validation and the reliability of the prognosis will be determined by the weakest component in the chain of calculations. Hydrodynamics models are, however, beyond the scope of this book and will therefore not be described in detail.

Experience throughout the 1970s has shown that even very complex models cannot account for all the processes which need to be included in generally applicable models of a given ecosystem type, for example, lakes, rivers, grasslands, etc. Simple models can be applied more generally as they may eventually include the few processes that are almost always the most important.

Experience gained after ten years of intensive application of ecological modelling during the 1970s can be summarized in the following points: (see also the discussion in Chapter 2, particularly Sections 2.5 and 2.12)

1. **A good knowledge of the ecosystem is required to capture the essential features, which should be reflected in the model.**
2. **The scope of the model determines the *complexity*, which in turn determines the quality and quantity of the data needed for calibration and validation.**
3. **If good data are not available it is better to go for a somewhat over-simplified model than one which is too complex.**
4. **Simple models are more general than *complex models*. However, if the data base allows one to develop a more complex model, it will probably be more specific as it will almost inevitably contain some processes and components specific to the ecosystem under consideration.**

During the 1970s and the early 1980s, much experience was gained in modelling many different types of ecosystem and many different aspects including a number of pollution problems. The modellers also learned which *modifications* it was necessary to make, when a model was applied to the *same* problem but for a different ecosystem from that for which it was originally developed. It was seen that the same model could not be applied to another ecosystem *without* some changes unless, as mentioned above, the model was very simple. More and more models became well calibrated and validated. They could often be used as a practical management tool, but in most cases it was necessary to combine the use of the model with a good knowledge of general environmental issues. Also, in cases when the model could not be applied to set up accurate predictions, the model was useful to enable the manager to see the qualitative reaction of the ecosystem to various management strategies. The scientists who applied models found that they were very useful in indicating research priorities and also in capturing the system features of ecosystems (see also the discussion in Sections 1.4 and 1.5).

7.3 Eutrophication Models I: Overview and Two Simple Eutrophication Models

Eutrophication

From a thermodynamic view, a lake can be considered as an open system, which exchanges material (waste water, evaporation, precipitation) and energy (evaporation, radiation) with the environment. However, in some great lakes the input of material per year is not able to change the concentration measurably. In such cases the system can be considered as almost closed, which means that it exchanges energy, but not material, with the environment.

The flow of energy through the lake system leads to at least one cycle of material in the system (provided that the system is in a steady state; see Morowitz, 1968). As illustrated in Figs. 2.1, 2.9, 2.10 and 7.1, the important elements all participate in the cycles that control eutrophication.

The word eutrophy is generally taken to mean "nutrient rich". In 1919, Nauman introduced the concepts of oligotrophy and eutrophy, distinguishing between oligotrophic lakes containing little planktonic algae and eutrophic lakes containing much phytoplankton.

The eutrophication of lakes all over the world has increased rapidly during the last decade due to increased urbanization and, consequently, increased discharge of nutrient per capita. The production of fertilizers has grown exponentially in this century and the concentration of phosphorus in many lakes reflects this.

The word eutrophication is used increasingly in the sense of the artificial addition of nutrients, mainly nitrogen and phosphorus, to waters. Eutrophication is generally considered to be undesirable, but this is not always true. The green colour of

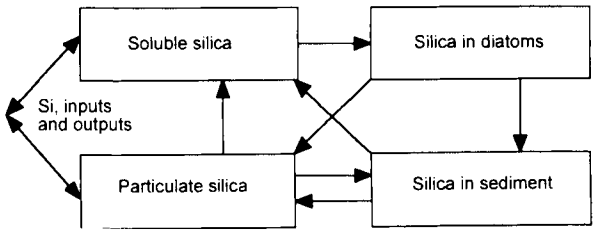

Fig. 7.1. The silica cycle.

eutrophied lakes makes swimming and boating less safe due to the increased turbidity, and from an aesthetic point of view the chlorophyll concentration should not exceed 100 mg m^{-3}. However, the most critical effect from an ecological point of view is the reduced oxygen content of the *hypolimnion*, caused by the decomposition of dead algae. During summer, eutrophic lakes sometimes show a high oxygen concentration at the surface, but a low concentration of oxygen in the hypolimnion which is lethal to fish.

About 16–20 elements are necessary for the growth of freshwater plants; Table 7.1 lists the relative quantities of essential elements in plant tissue. The present concern about *eutrophication* relates to the rapidly increasing amount of phosphorus and nitrogen, which are normally present at relatively low concentrations. Of the two, phosphorus is considered to be the major cause of eutrophication in lakes, as it was formerly the growth-limiting factor for algae in the majority of lakes, but as mentioned previously, its use has increased tremendously during the last decade. The concept of the *limiting factor* is treated in Chapter 3.

Nitrogen is limiting in a number of East African lakes as a result of the nitrogen depletion of soils by intensive erosion in the past. Today, however, nitrogen may become limiting in lakes as a result of the tremendous increase in the phosphorus concentration caused by discharge of waste water, which contains relatively more

Table 7.1. *Average freshwater plant composition* on a wet weight basis

Element	Plant content (%)	Element	Plant content (%)
Oxygen	80.5	Chlorine	0.06
Hydrogen	9.7	Sodium	0.04
Carbon	6.5	Iron	0.02
Silicon	1.3	Boron	0.001
Nitrogen	0.7	Manganese	0.0007
Calcium	0.4	Zinc	0.0003
Potassium	0.3	Copper	0.0001
Phosphorus	0.08	Molybdenum	0.00005
Magnesium	0.07	Cobalt	0.000002
Sulphur	0.06		

phosphorus than nitrogen. While algae use four to ten times more nitrogen than phosphorus, waste water generally contains only three times as much nitrogen as phosphorus in lakes and a considerable amount of nitrogen is lost by *denitrification* (nitrate $\rightarrow N_2$).

The growth of phytoplankton is the key process of *eutrophication* and it is therefore important to understand the interacting processes that regulate growth. Primary production has been measured in great detail in a number of lakes. This process represents the synthesis of organic matter and the overall process can be summarized as follows (for further details see Chapter 3):

$$\text{Light} + 6CO_2 + 6H_2O \rightarrow C_6H_{12}O_6 + 6O_2$$

The composition of phytoplankton is not constant (note that Table 7.1 gives only an average concentration), but reflects to a certain extent the concentration of the water. If, e.g., the phosphorus concentration is high, the phytoplankton will take up relatively more phosphorus—this is called luxury uptake.

As can be seen from Table 7.1, phytoplankton consists mainly of carbon, oxygen, hydrogen, nitrogen and phosphorus: without these elements no algal growth will take place. This leads to the concept of limiting nutrient mentioned above and in Chapter 3, and which has been developed by Liebig as the *law of the minimum*. This states that the yield of any organism is determined by the abundance of the substance that in relation to the needs of the organism is least abundant in the environment (Hutchinson, 1970). However, the concept has been considerably misused due to oversimplification. First of all, growth might be limited by more than one nutrient. The composition is not constant but varies with the composition of the environment. Furthermore, growth is not at its maximum rate until the nutrients are used, and is then stopped, but the growth rate slows down when the nutrients become depleted.

Chapter 3 discusses how this may be considered in terms of a relationship between phytoplankton growth and nutrient concentrations. Consideration is also given to how the interaction of several limiting nutrients can simultaneously be taken into account. Another side of the problem is the consideration of the nutrient sources. It is of importance to set up mass balances for the most essential nutrients.

The sequence of events leading to *eutrophication* has often been described as follows: *oligotrophic* waters will have a ratio of N:P greater than or equal to 10, which means that phosphorus is less abundant than nitrogen for the needs of phytoplankton. If sewage is discharged into the lake the ratio will decrease, since the N:P ratio for municipal waste water is 3:1, and consequently nitrogen will be less abundant than phosphorus relative to the needs of phytoplankton. In this situation, however, the best remedy for the excessive growth of algae is not the removal of nitrogen from the sewage, because the mass balance might then show that nitrogen-fixing algae will give an uncontrollable input of nitrogen into the lake. It is necessary to set up mass balances for each of the nutrients and these will often reveal that the input of nitrogen from nitrogen-fixing blue green algae, precipitation and tributaries is contributing too much to the mass balance for the removal of nitrogen from the

sewage to have any effect. On the other hand, the mass balance may reveal that the phosphorus input (often more than 95%) comes mainly from sewage, which means that it is better management to remove phosphorus from the sewage than nitrogen. Thus, it is not important which nutrient is most limiting, but which nutrient can most easily be made to limit the algal growth.

Eutrophication Models: An Overview

Several eutrophication models with a wide spectrum of complexity have been developed. As for other models the right complexity of the model is dependent on the available data and the ecosystem. Table 7.2 reviews various eutrophication models, indicating the characteristic features of the models, the number of case studies to which each has been applied (with some modification from case study to case study, because a general model is non-existent and site-specific properties should be reflected in the selected modification, unless the model is very simple) and whether the model has been calibrated and validated.

Table 7.2. Various eutrophication models

Model name	No. of st. var.	Nutrients	Segments	Dimension (D) or layer (L)	CS or NC*	C and/or V**	No. of case studies
Vollenweider	1	P (N)	1	1L	CS	C+V	many
Imboden	2	P	1	2L.1D	CS	C+V	3
O'Melia	2	P	1	1D	CS	C	1
Larsen	3	P	1	1L	CS	C	1
Lorenzen	2	P	1	1L	CS	C+V	1
Thomann 1	8	P,N,C	1	2L	CS	C+V	1
Thomann 2	10	P,N,C	1	2L	CS	C	1
Thomann 3	15	P,N,C	67	2L	CS	-	1
Chen & Orlob	15	P,N,C	sev.	2L	CS	C	min. 2
Patten	33	P,N,C	1	1L	CS	C	1
Di Toro	7	P,N	7	1L	CS	C+V	1
Biermann	14	P,N,Si	1	1L	NC	C	1
Canale	25	P,N,Si	1	2L	CS	C	1
Jørgensen	17–20	P,N,C	1	1–2L	NC	C+V	22
Cleaner	40	P,N,C,Si	sev.	sev. L	CS	C	many
Nyholm, Lavsoe	7	P,N	1–3	1–2L	NC	C+V	25
Aster/Melodia	10	P,N,Si	1	2L	CS	C+V	1
Baikal	>16	P,N	10	3L	CS	C+V	1
Chemsee	>14	P,N,C,S	1	profile	CS	C+V	many
Minlake	9	P,N	1	1	CS	C+V	>10
Salmo	17	P,N	1	2L	CS	C+V	16

*CS: constant stoichiometric; NC: independent nutrient cycle.
**C: calibrated; V validated.

It is not, of course, possible to treat all the more complex models in detail. One of the more complex models has therefore been selected and is presented in more detail in Section 7.3. *Eutrophication models* demonstrate quite clearly the ideas behind *biogeochemical models* and it is therefore fruitful to go into some illustrative details about the validation of this type of model and particularly its prognosis. The results presented were obtained using a complex eutrophication model and demonstrate what can be achieved today using ecological models, provided that sufficient effort is made to obtain good data and good ecological background knowledge about the ecosystem being modelled.

Simple Eutrophication Models

Some of the most simple models that can be used in a data-poor situation are presented below. These models will give the reader a good impression of the problems involved in modelling the eutrophication process.

Simple eutrophication models are based on three steps:

1. Determination or calculation of nutrient loading.
2. Prediction of the nutrient concentration (usually only one nutrient is considered). Two or more steady-state situations may be compared.
3. A relationship between the nutrient concentration and the level of eutrophication is applied to "translate" the nutrient level to a chlorophyll level, which is "translated" into a transparency. Determination of nutrient balances is the basis of all eutrophication models. It is possible by measuring the concentrations and flow rates of inputs and outputs. Alternatively, it is possible to calculate the nutrient loading as demonstrated below, although it is only recommended that the calculation method be used when data are not available.

Calculation of the *nutrient loading* of lakes

The first step is to set up a nutrient balance for the lake system. Even with a lack of data it is possible to give some general lines.

(a) Natural P and N loads from land

Table 7.3 shows a phosphorus-export (E_p) and a nitrogen-export (E_n) scheme based on a geological classification.

The figures are based on an interpretation of the following references: Dillon and Kirchner (1975), Lønholdt (1973; 1976), Vollenweider (1968; 1969) and Loehr (1974).

To calculate the natural nutrient loading to a lake, one must know (1) the area A_i of the watershed of each tributary to the lake, and (2) classify each as to geology and land use.

Table 7.3. Export scheme of phosphorus, E_p, and nitrogen E_n (mg m^{-2} year^{-1})

Land use	E_p		E_n	
	Geological classification		Geological classification	
	Igneous	Sedimentary	Igneous	Sedimentary
Forest runoff				
Range	0.7–9	7–18	130–300	150–500
Mean	4.7	11–7	200	340
Forest + pasture				
Range	6–12	11–37	200–600	300–800
Mean	10.2	23.3	400	600
Agricultural areas				
Citrus	18			2240
Pasture	15–75			100–850
Cropland	22–100			500–1200

The total amount of phosphorus, I_{Pl}, and nitrogen, I_{Nl}, supplied to the lake from the land is therefore calculated using the following equations:

$$I_{Pl} = \sum A_i E_{Pi} \tag{7.1}$$

$$I_{Nl} = \sum A_i E_{Ni} \tag{7.2}$$

where the index i refers to the area number i in the *catchment area*. The area is indicated by A and the export per unit of area by E (see Table 7.3).

(b) Natural P and N loads from precipitation

Table 7.4 is a compilation of the references of Schindler and Nighswander (1970) and Dillon and Rigler (1974) and those supplied by some recent measurements by the authors and Lake Biwa Research Institute, LBRI. Based upon the annual precipitation of Pr (mm year^{-1}) it is possible to find the supply of phosphorus I_{PP} and nitrogen I_{NP} from precipitation:

$$\begin{aligned} I_{PP}(\text{mg y}^{-1}) &= Pr\, C_{PP}\, A_S \\ I_{NP}(\text{mg y}^{-1}) &= Pr\, C_{NP}\, A_S \end{aligned} \tag{7.3}$$

where A_S is the surface area (m^2) of the lake, and C_{PP} and C_{NP} are the phosphorus and nitrogen concentrations in rainwater (see Table 7.4).

Table 7.4. Nutrient concentration in *rainwater* (mg l^{-1})

	C_{PP}	C_{NP}
Range	0.025–0.1	0.3–1.6
Mean	0.07	1.0

Table 7.5. *Retention coefficients* (Brandes et al., 1974). D = grain size.

Filter bed	R
4% sed. mud 96% sand (70 cm)	0.76
75 cm sand D = 0.3 mm	0.34
75 cm sand D = 0.6 mm	0.22
75 cm sand D = 0.24 mm	0.48
75 cm sand D = 1.0 mm	0.01
10% sed. mud 90% sand (37 cm)	0.88
50% limestone 50% sand (37 cm)	0.73
Silty sand (70 cm)	0.63
50% clay silt 50% sand (37 cm)	0.74

(c) Artificial P and N loads

The calculation of the artificial nutrient supply to a lake must necessarily be based on per capita and yearly figures, and great care must be taken when selecting the appropriate value. The following points must be taken into consideration:

1. The discharge per capita and per year is approx. 800–1800 g P and 3000–3800 g N.
2. Mechanical treatment removes 10–15% of the nutrients.
3. Biological treatment removes 10–15% of the nutrients.
4. Chemical precipitation removes 80–90% of the phosphorus.
5. The retention coefficients, R, of total phosphorus for septic tile filter beds of different characteristics are shown in Table 7.5 (after Brandes et al., 1974). The retention coefficients of total nitrogen for septic tile filter beds are of the order 0.01–0.1.

Based on the considerations indicated above, the P load (I_{Pw}) and N load (I_{Pw}) can be found.

Predictions of Eutrophication

The equations for a description of the recycling of nutrients in a lake have been given in Chapter 3. Here, we will try to answer the question: how can we translate the phosphorus and/or nitrogen concentration to a measure of the *eutrophication*?

Dillon and Rigler (1974) developed a relationship for estimating the average summer *chlorophyll a* concentration (chl.a) with the N:P ratio of the water > 12:

$$\log_{10}(\text{chl.a}) = 1.45 \log_{10}[(\text{P}) \cdot 1000] - 1.14 \tag{7.4}$$

For the case where the N:P ratio is < 4, the following equation was evolved, based on eight case studies:

$$\log_{10}(\text{chl.a}) = 1.4 \log_{10}[(\text{N}) \cdot 1000] - 1.9 \tag{7.5}$$

(N) and (P) are expressed as mg l^{-1} and (chl.a) is found in mg l^{-1}. If the N:P ratio is between 4 and 12, the use of the smallest value of (chl.a) found on the basis of the two equations is recommended.

Many correlations between phosphorus concentrations and chlorophyll concentrations have been developed. Dillon et al. (1975) set up a relationship between the *Secchi disc transparency*, SE and (chl.a) which is shown in Fig. 7.2. Kristensen et al. (1990) have developed eight different equations, which relate the phosphorus concentration (P_{lake}) with the average *transparency depth* (z_{eu}). The influence of the mean depth, z, is included in three of the equations (see Table 7.6).

The simple model presented above will never be as good a predictive tool as a model based on more accurate data and which takes more processes into consideration. However, the semi-quantitative estimations that can be obtained using the simple model are better than none at all and in a data-poor situation it may be the only model the data can support. Furthermore, it is often an advantage to use simple models to find first estimations before a more advanced model is developed.

From the equations given in Chapter 3, it is possible to estimate the P concentrations in the lake water as a function of time. The N concentration can be estimated by a parallel set of equations. These considerations can be translated into chlorophyll a by means of equations (7.4) and (7.5). The *transparency* can be found when (chl.a) is known from Fig. 7.2 and Fig. 7.3—or by means of the relations in

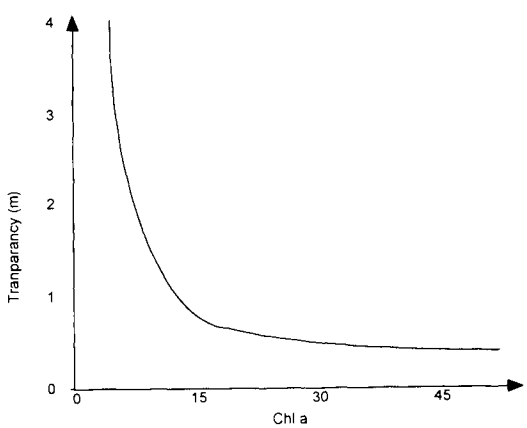

Fig. 7.2. *Transparency* (m) versus (chl.a).

Table 7.6. Relations between average transparency depth, z_{eu}, phosphorus concentration, P_{lake} and mean depth, z (after Kristensen et al., 1990)

Number	Equation
1	$z_{eu} = 0.44\ (\pm\ 0.038)\ P^{-0.54(\pm 0.031)}$
2	$z_{eu} = 0.36(\pm\ 0.029)\ P^{-0.29(\pm 0.028)} z 0.51(\pm 0.042)$
3	$z_{eu} = 0.39(\pm\ 0.038)\ P^{-0.58(\pm 0.034)}$
4	$z_{eu} = 0.34(\pm\ 0.028)\ P^{-0.29(\pm 0.028)} z 0.55(\pm 0.040)$
5	$z_{eu} = 0.52\ (\pm\ 0.042)\ P^{-0.48(\pm 0.031)}$
6	$z_{eu} = 0.43\ (\pm\ 0.026)\ P^{-0.20(\pm 0.022)} z 0.55(\pm 0.030)$
7	$z_{eu} = 0.40\ (\pm\ 0.055)\ P^{-0.69(\pm 0.064)}$
8	$z_{eu} = 0.34\ (\pm\ 0.0424)\ P^{-0.60(\pm 0.041)}$

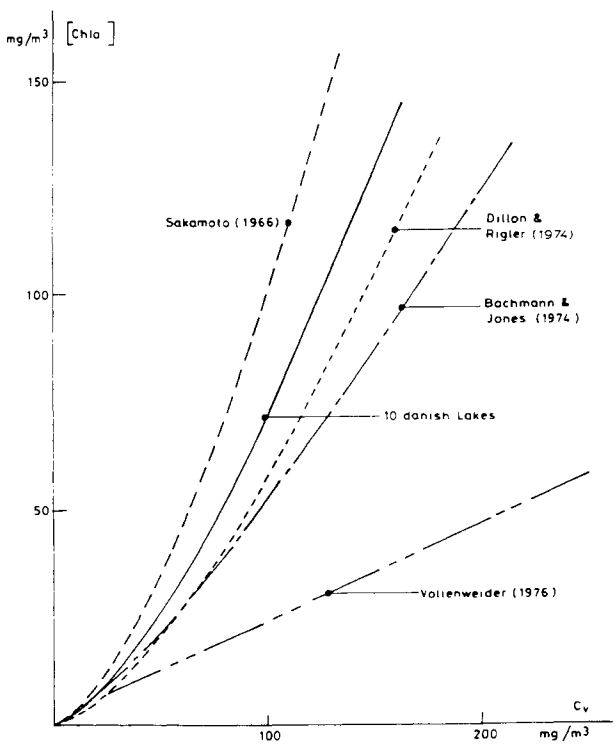

Fig. 7.3. Empirical relationships between summer chlorophyll (chl.a) and annual average phosphorus concentration, C_v (reproduced from Kamp Nielsen, 1986).

Table 7.6—directly from phosphorus concentrations. In this way, it is possible to test *different waste water treatment* programs and answer such questions as: should N or P be removed? What would be the increase in efficiency required, if the transparency were to be improved by a factor two or more?

7.4 Eutrophication Models II: A Complex Eutrophication Model

The model shown in Figs. 2.1, 2.9, and with modifications in Fig. 2.10, has been selected as an illustrative example of a *eutrophication* model of medium to high complexity. The results given in Table 2.12 also relate to this model. The model was developed for *Lake Glumsø*—a case study having the following advantages:

1. The lake is shallow (mean depth 1.8 m) and no formation of a *thermocline* takes place. The case study is thus relatively simple.
2. The lake is small (volume 420,000 m^3) and well mixed, which implies that a model needs not to consider hydrodynamics but can focus on ecological processes.
3. Retention time is short (< 6 months), which means that any change due to a management action can be observed fairly rapidly.
4. A radical change in nutrient input occurred in April 1981, and the water quality changes have been observed (Jørgensen et al., 1986).
5. It is unique in that a *prognosis* of change was published *before* any changes actually took place (Jørgensen et al., 1978). It has since been possible to validate this prognosis.
6. The lake has been intensely studied during 1973–1984. The model is therefore based on comprehensive data.

The model has also been applied in 21 other case studies, of course with the necessary modifications, which will be presented below. It is probably one of the most well examined *eutrophication* models published to date, due to:

- the comprehensive investigation of the applicability of the model to Lake Glumsø on the basis of a very good data base;
- the unique feature that the model predictions by radically changed loading were validated;
- the wide application of the same model with modifications.

This implies that the results represent what is obtainable in relation to validation under almost unchanged loading, accuracy in predictions (see below), and general applicability. Emphasis is therefore placed on these results.

The ecology of *Lake Glumsø* was investigated before the model was developed (Jørgensen et al., 1973). The phases in modelling given in Section 2.3 were followed very carefully so as to be able to obtain a model with the predictive power necessary for it to be used as a management instrument.

Figures 2.1 and 2.9 are the conceptual diagrams of the N- and P-flows of the model. Many of the equations can be found in other eutrophication models and in

Chapter 3 on unit processes. It seems of little value in this context, therefore, to present all the equations of the model, and the following pages are devoted to the most characteristic features of the model to illustrate typical modelling considerations. They are:

1. *independent cycling* of N,P and C which is a result of the two-step process description of phytoplankton growth;
2. a more detailed description of the water–sediment interactions that are extremely important for shallow lakes where a significant amount of the nutrient is stored in the sediment.

The two steps describing the growth of phytoplankton are:

1. *uptake of nutrients* in accordance with *Monod's kinetics*, and
2. growth determined by the internal substrate concentration.

In other words, independent nutrient cycles of phosphorus, nitrogen and carbon are considered. Phytoplankton biomass as well as carbon, phosphorus and nitrogen in algal cells must be included as state variables, all expressed in the units g/m^3. This is more complex than the *constant stoichiometric approach*, but as Jørgensen (1976a) has shown, it was impossible to obtain an accurate time at which the maximum phytoplankton concentration and production occurred using the simpler non-causal *Monod's kinetic* for growth of phytoplankton. The proportions of nitrogen and phosphorus in both zooplankton and fish are included in the model to ensure element conservation.

The growth of phytoplankton is described using a growth rate coefficient μ_{max}, which is limited by four factors:

A temperature factor:

$$FT1 = \exp\left(A(T - T_{opt})\right)(T_{max}T)/(T_{max} - T_{opt})A(T_{max} - T_{opt}) \tag{7.6}$$

where A, T_{opt} and T_{max} are species dependent constants. T is temperature.

A factor for intracellular nitrogen, NC:

$$FN3 = 1 - NC_{min}/NC \tag{7.7}$$

A parallel factor for intracellular phosphorus:

$$FP3 = 1 - PC_{min}/PC \tag{7.8}$$

and similarly

A factor for intracellular carbon:

$$FC3 = 1 - CC_{min}/CC \tag{7.9}$$

This means that we have:

$$dPHYT/dt = \mu_{max} FT1 \cdot FP3 \cdot FN3 \cdot FC3 \tag{7.10}$$

Notice that the usually applied μ_{max} is $\mu_{max} FP3 \cdot FN3 \cdot FC3$, which can be found in Jørgensen et al. (1991; 2000). If it is presumed that the nitrogen content of algae varies between 5 and 12% and the phosphorus content between 0.5 and 2.5%, we get, omitting $FC3$, that the here applied $\mu_{max} = \mu_{max}$-usually-applied$\times$ 2.14.

NC, PC and CC are determined by nutrient uptake rates:

$$UC = UC_{max} FC1 \cdot FC2 \cdot FRAD \tag{7.11}$$

$$UN = UN_{max} \cdot FN1 \cdot FN2 \tag{7.12}$$

$$UP = UP_{max} \cdot FP1 \cdot FP2 \tag{7.13}$$

where UC_{max}, UN_{max} and UP_{max} are species dependent constants (maximum uptake rates); generally, UC_{max} will be greater, the smaller the size of the phytoplankton considered. $FC1$, $FN1$ and $FP1$ are expressions that give the limitations in uptake:

$$FC1 = (FC_{max} - FCA) / (FCA_{max} - FCA_{min}) \tag{7.14}$$

$$FN1 = (FN_{max} - FNA) / (FNA_{max} - FNA_{min}) \tag{7.15}$$

$$FP1 = (FP_{max} - FPA) / (FPA_{max} - FPA_{min}) \tag{7.16}$$

where FCA_{max}, FCA_{min}, FNA_{max}, FNA_{min}, FPA_{max} and FPA_{min} are constants indicating the maximum and minimum contents respectively of nutrients in phytoplankton. FCA, FNA and FPA are determined as $CC/PHYT$, $NC/PHYT$ and $PC/PHYT$. $FC2$, $FN2$ and $FP2$ give the limitations in uptake caused by the nutrient level in the lake water:

$$FC2 = C / (KC + C) \tag{7.17}$$

$$FN2 = NS / (NS + KN) \tag{7.18}$$

$$FP2 = PS / (PS + KP) \tag{7.19}$$

As will be seen, these last expressions are in accordance with the *Michaelis–Menten* formulation. KC, KN and KP are half saturation constants. FRAD is a complex expression, covering the influence of solar radiation. This influence is integrated over depth and the *self-shading effect* is included. The intracellular nitrogen, phosphorus and carbon can now be determined by differential equations:

$$dNC/dt = UN \cdot PHYT - (SA + GZ / F + Q / V)NC \tag{7.20}$$

$$dPC/dt = UP \cdot PHYT - (SA + GZ / F + Q / V)PC \tag{7.21}$$

$$dCC/dt = UC \cdot PHYT - (SA + RESP + GZ / F + Q / V)CC \tag{7.22}$$

where *PHYT* is the phytoplankton concentration, *GZ* is the grazing rate corresponding to gross growth of zooplankton, *F* a yield factor (approximately 2/3, i.e., zooplankton utilizes 66.7% of the food), *Q* is the outflow rate, *SA* is the settling rate (day^{-1}) and *V* the volume. *RC* is the respiration rate, found as

$$RC = RC_{max}(CC / CC_{max})^{2/3} \tag{7.23}$$

A more detailed *sediment submodel* is another characteristic feature of the model presented. As the sediment accumulates nutrients it is important to describe quantitatively the processes determining the mass flows from *sediment* to water, particularly in shallow lakes, where the sediment may contain the major part of the nutrients. To what extent will accumulated compounds in the sediment be redissolved in the lake water? The exchange processes between mud and water of phosphorus and nitrogen have been extensively studied, as these processes are important for the *eutrophication* of lakes. Several of the earlier developed models did not consider the importance of these sediment–water interactions. Chen and Orlob (1975) ignored the exchange of nutrients between mud and water and, as pointed out by Jørgensen et al. (1975), this will inevitably give a false prognosis. Ahlgren (1973) applied a constant flow of nutrients between sediment and water, and Dahl-Madsen and Strange-Nielsen (1974) used a simple first-order kinetic to describe the exchange rate.

A more comprehensive submodel (Fig. 7.4) for the exchange of phosphorus has been developed by Jørgensen et al. (1975). The settled material, *S*, is divided into

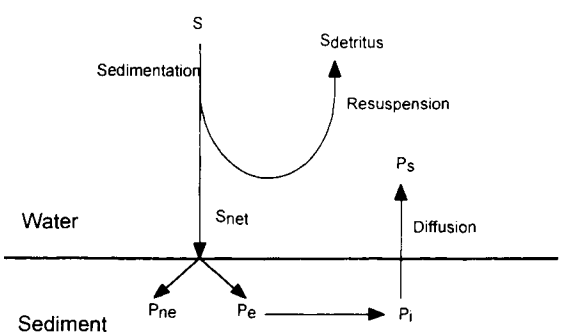

Fig 7.4. Sedimentation, *S*, divided into $S_{detritus}$ and S_{net}; P_{ne} *non-exchangeable phosphorus* in unstabilized sediment: P_e *exchangeable phosphorus* in unstabilized sediment: P_i phosphorus in *interstitial water*: P_s dissolved phosphorus in water.

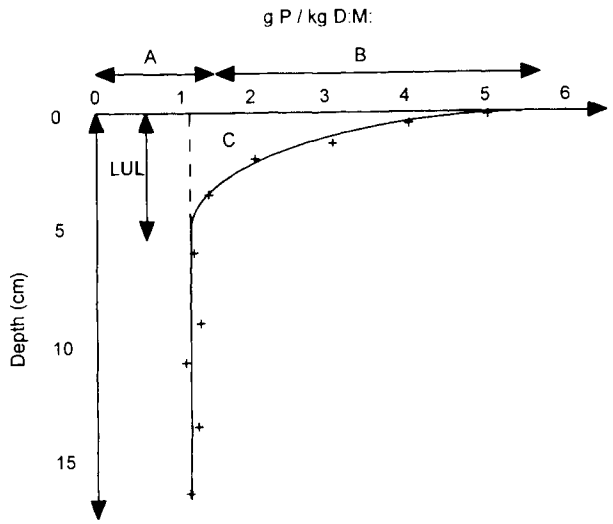

Fig. 7.5. Analysis of core from *Lake Esrom*. mg P per g dry matter is plotted against the depth. The area C represents *exchangeable phosphorus*. $f = (B \cdot A^{-1})$. *LUL* is the unstabilized layer.

S_{detritus} and S_{net}, the former being mineralized by microbiological activity in the water body, and the latter being the material actually transported to the sediment. S_{net} can also be divided into two flows:

$$S_{\text{net}} = S_{\text{net,s}} + S_{\text{net,e}} \tag{7.24}$$

where $S_{\text{net,s}}$ = flow to the stable non-exchangeable sediment, and $S_{\text{net,e}}$ = mass flow to the exchangeable unstable sediment.

Correspondingly, P_{ne} and P_{e}, *non-exchangeable* and *exchangeable phosphorus* concentrations, both based on the total dry matter in the sediment, can also be distinguished. An analysis of the phosphorus profile in the sediment (Fig. 7.5) will give the ratio (f) of the exchangeable to the total settled phosphorus:

$$f = (S_{\text{net}} - S_{\text{net,s}}) / S_{\text{net}} = S_{\text{net,e}} / S_{\text{net}} \tag{7.25}$$

and

$$dP_{\text{e}}/dt = a \times f \times S_{\text{net,e}} - K5 \times P_{\text{e}} K6^{(T-20)} \tag{7.26}$$

where a = factor converting water concentration units to concentration units in the sediment (mg P kg^{-1} DM). $S_{\text{net,e}}$ can be found from sediment profile studies. The increases of the stabilized sediment can be found by numerous methods. The application of lead isotopes is, for example, a fast and reliable method. Exchangeable phosphorus is mineralized similarly to detritus in a water body, and a first-order

reaction as indicated gives a reasonably good description of the conversion of P_c into *interstitial phosphorus*, P_i: $K5 \times P_c K6^{(T-20)}$, where $K5$ = a rate coefficient, $K6$ = a temperature coefficient, and T = temperature.

Finally, the interstitial phosphorus, P_i, will be transported by diffusion from the pore water to the lake water. This process, which has been studied by Kamp-Nielsen (1974), can be described by means of the following empirical equation (valid at 7°C):

$$\text{Release of P} = 1.21\,(P_i - P_s) - 1.7\ (\text{mg P m}^{-2}\ 24\ \text{h}^{-1}) \tag{7.27}$$

where P_s is the dissolved phosphorus in the lake water.

It thus turns out that:

$$dP_i/dt = K5 \times P_c K6^{(T-20)} - \beta(1.21(P_i - P_s) - 1.7) \times T/280 \tag{7.28}$$

where β converts concentration units in the *sediment* to those for lake water, and T is the absolute temperature as the release rate was found to be proportional to T.

This *submodel* was validated in three case studies (Jørgensen et al., 1975) examining sediment cores in the laboratory. Kamp-Nielsen (1975) has added an adsorption term to these equations.

A similar submodel for nitrogen release has been set up by Jacobsen and Jørgensen (1975). The nitrogen release from sediment is expressed as a function of the nitrogen concentration in the sediment and the temperature, taking into account both aerobic and anaerobic conditions.

The grazing on phytoplankton by zooplankton Z, and the *predation* on zooplankton by fish F are both expressed by a modified *Monod expression*:

$$\mu Z = \mu Z_{max}(PHYT - GL) / (PHYT - KA) \tag{7.29}$$

$$\mu F = \mu F_{max}(ZOO - KS) / (ZOO - KZ) \tag{7.30}$$

where GL, KA, KS and KZ are constants. These expressions are according to Steele (1974). GL and KS express the very low concentration at which grazing and *predation*, respectively, do not take place. The time to find the food and the energy spent on searching for food is simply too high at this low concentration.

The following points in the model were changed during 1979–83 and thus gave a better validation:

1. $FC3$, $FN3$ and $FP3$ were changed to:

$$FC3 = \frac{FCA - FCA_{min}}{FCA_{max} - FCA_{min}} \tag{7.31}$$

and similarly for $FN3$ and $FP3$. Notice that, compared with expressions (7.7)–(7.9), this expression has the advantage that μ_{max} becomes the usually applied maximum growth rate in the differential equation.

2. The T_{opt} in the temperature factor was changed to the actual temperature in the lake water during the summer months to allow for temperature adaptation.

3. The temperature dependence of phytoplankton respiration was changed to an exponential expression.

4. *RC* was changed to:

$$RC = RC_{max}\, CC / CC_{max} \tag{7.32}$$

The exponent 2/3 in Eq. (7.23) is valid for individual cells as the surface is approximately proportional to the weight or volume of the cells, but since phytoplankton concentration is used here, application of the exponent 2/3 is irrelevant.

5. As mentioned above, only part of the settled phosphorus is exchangeable. In the case study referred to, it was found that 15% of the settled phosphorus was non-exchangeable to be able to account for the observed phosphorus profile in the sediment. In the new version exchangeable and non-exchangeable nitrogen were also distinguished. It is possible (based upon the nitrogen profile in the sediment) to estimate that non-exchangeable nitrogen is 4–5 times higher than non-exchangeable phosphorus. As algae contain on average seven times as much nitrogen as phosphorus, the exchangeable part of the settled nitrogen, called *KNEX*, can be estimated by the following equation:

$$KNEX = \left(\frac{5}{7} KEX + \frac{2}{7}\right) \tag{7.33}$$

where *KEX* is the exchangeable fraction on the settled phosphorus; in this particular study $KEX = 0.85$, which means that

$$KNEX = \left(\frac{5}{7} \cdot 0.85 + \frac{2}{7}\right) = 0.89 \tag{7.34}$$

These changes gave a better correspondence between the modelled and the observed nitrogen balance; and finally:

6. A *carrying capacity* of zooplankton was introduced to give a better simulation of zooplankton and phytoplankton. Carrying capacities are often observed in ecosystems (see Chapter 6), but their necessity in this case may be due to a too-simple simulation of the grazing process. Phytoplankton might not be grazed by all zooplankton species present, and some species might use detritus as a food source. The zooplankton *growth rate*, μZ, is computed in accordance with these modifications as:

$$\mu Z = \mu Z_{max} \cdot FPH \cdot FT2 \cdot F2CK \tag{7.35}$$

where $FPH = (PHYT - GL) / (PHYT - KA)$, see the expression in Eq. (7.29), $FT2$ is a temperature regulation expression, and $F2CK$ accounts for carrying capacity:

$$F2CK = 1 - ZOO/CK \tag{7.36}$$

where

$$CK = 26 \text{ mg/l} \tag{7.37}$$

was chosen in this case.

An *intensive measuring period* was applied to improve parameter estimation as described in Section 2.9. The results of this effort can be summarized as follows:

A. Different optional expressions of simultaneous limiting factors (see Chapter 3) were tested and only two expressions gave an acceptable maximum growth rate for phytoplankton and an acceptable low standard deviation. These are: multiplication of the *limiting factors*, and averaging the limiting factors (see the discussion in Chapter 3).

B. The previously applied expression for the influence of temperature on phytoplankton growth gave unacceptable parameters with too high standard deviations. A better expression, Eq. (7.6), was introduced as a result of the intensive measuring period.

C. It was possible to improve the parameter estimation, giving more realistic values for some of the parameters. Whether this would give an improved validation when observations from a period with drastic changes in the nutrients loading are available could not be stated.

D. Two zooplankton state variables based on phytoplankton grazing and detritus feeding was tested but did not give any advantages.

E. The other expressions applied for process descriptions were confirmed.

It is urgently needed to validate models against independent set of measurements. No general method of validation is available, but almost the same method suggested by WMO (1975) for validation of hydrological models was applied to this model. Table 7.7 gives results of the validation improved as described above. The following numerical validation criteria were applied:

1. *Y, coefficient of variation* of the residuals of errors for the state variables for the validation period, defined as

$$Y = [\Sigma(y_c - y_m)^2]^{1/2} / (n\, Y_{a.m}) \tag{7.38}$$

where y_c = calculated values of the state variables, y_m = measured values of the state variables, n = number of comparisons, $Y_{a.m}$ = average of measured values over the validation period.

2. R, the relative error of *mean values*:

$$R = (Y_{a,c} - Y_{a,m}) / Y_{a,m} \tag{7.39}$$

where $Y_{a,c}$ = is the average of measured values over the validation period.

3. A, the relative error of *maximum values*:

$$A = (Y_{max,c} - Y_{max,m}) / Y_{max,m} \tag{7.40}$$

where $Y_{max,c}$ = maximum value of the calculated state variable in the validation period, and $Y_{max,m}$ = maximum value of the measured state variable in the validation period. A for the phytoplankton concentration or the *production* (d*Phyt*/d*t*) are often considered the most important validation criteria, as they describe the *"worst case" situation*. This is also often reflected in validations of prognoses.

4. *TE*, *timing error*:

$$TE = \text{date of } Y_{max,c} - \text{date of } Y_{max,m} \tag{7.41}$$

Y, R and A give the errors in relative terms. Multiplication by 100 will give the errors as percentages. The standard deviation, Y, for all measured state variables, is as seen

Table 7.7. Numerical *validation of the model* described

Validation criteria	State variable	Value
Y	all	0.31
R	P_{total} (*P4*)	0.26
R	$P_{soluble}$ (*PS*)	0.16
R	N_{total} (*N4*)	0.02
R	$N_{soluble}$ (*NS*)	0.14
R	Phytoplankton (*CA*)	0.10
R	Zooplankton (*Z*)	0.27
R	Production	0.03
A	P_{total} (*P4*)	0.12
A	$P_{soluble}$ (*PS*)	0.18
A	N_{total} (*N4*)	0.07
A	$N_{soluble}$ (*NS*)	0.03
A	Phytoplankton (*CA*)	0.15
A	Zooplankton (*Z*)	0.00
A	Production	0.08
TE	P_{total} (*P4*)	105 days
TE	$P_{soluble}$ (*PS*)	60 days
TE	N_{total} (*N4*)	15 days
TE	$N_{soluble}$ (*NS*)	15 days
TE	Phytoplankton (*CA*)	0 days*; 120 days**
TE	Zooplankton (*Z*)	60 days
TE	Production	0 days

*Based on measuring suspended matter 1–60 μm.
**Based on chlorophyll.

31%. It is the standard deviation for one comparison of model value and measured value. As the standard deviation for a comparison of n sets of model values and measured values is $\sqrt{n}$ times smaller and n is in the order of 225 in the Lake Glumsø case, the overall average picture of the lake is given with a standard deviation of about 2%, which is very acceptable. Y is, for instance, generally five times larger for hydrodynamics models (WMO, 1975).

The relative errors of mean values, R, are 3% for production, 10% for phytoplankton and 2% for nitrogen; are all acceptable values. However, the relative error for total phosphorus is 26% and for zooplankton 27%, which must be considered a little too high. The relative errors of the maximum values, A, are from 0% to 18%, which is acceptable. The ability of the model to predict maximum production and maximum phytoplankton concentration has special interest for a *eutrophication model*; the relative errors are 8% and 15%, respectively—fully acceptable.

The ability to predict the time when maximum values occur is expressed by using *TE*. Production and phytoplankton (use for suspended matter 1–60 m) give full accordance between model values and measured values. *TE* for nitrogen total and soluble are also acceptable, while the zooplankton and phosphorus values are on the high side. All in all, the validation has demonstrated that the model should have value as a predictive tool, although the dynamics of phosphorus and zooplankton could be improved.

The changes made to the model during the period 1979–1983 by very frequent measurements, i.e, the six points mentioned above, improved the validation further, as Y was reduced from 31% to 16%.

As mentioned previously, this model has been applied with modifications to 21 other case studies. The changes to the model were all based on ecological observations. Table 7.8 reviews the modifications needed for 20 out of the 22 case studies in order to get a workable model. By calibration carried out according to Section 2.8, it was found that the most crucial parameters were all approximately in the range of values found in the literature (see also Table 2.13). Note that the parameters shown here were all found by:

1. using literature values as initial guesses (see Jørgensen et al., 1991; 2000);
2. using frequent measuring periods to get good first estimations of parameters;
3. a first rough calibration of the model to improve parameter estimations;
4. using an automatic calibration procedure to allow a finer calibration of 6–8 of the most important parameters (most sensitive to the phytoplankton concentration) with ranges partly based on the frequent measurements. This procedure was repeated at least twice and only when the same parameter values were found, was the calibration considered to be satisfactory.

The model presented and other models of similar complexity are widely applied as environmental management tools (see below). They represent what can be achieved with the use of ecological models, *provided* that all steps of the procedure shown in

Table 7.8. Survey of *eutrophication* studies based upon the application of a modified *Glumsø model*

Ecosystem	Modification	Level*
Glumsø (version A)	basis version	6
Glumsø (version B)	non-exchangeable nitrogen	6
Ringkøbing Firth	boxes, nitrogen fixation	5
Lake Victoria	boxes, thermocline, other food chain	4
Lake Kyoga	other food chain	4
Lake Mobuto Sese Seko	boxes, thermocline, other food chain	4
Lake Fure	boxes, nitrogen fixation, thermocline	3
Lake Esrom	boxes, Si-cycle, thermocline	4
Lake Gyrstinge	level fluctuations, sediment exposed to air	4–5
Lake Lyngby	basis version	6
Lake Bergunda	nitrogen fixation	2
Broia Reservoir	macrophytes, 2 boxes	
Lake Great Kattinge	resuspension	5
Lake Svogerslev	resuspension	5
Lake Bue	resuspension	5
Lake Kornerup	resuspension	5
Lake Balaton	adsorption to suspended matter	2
Roskilde Fjord	complex hydrodynamics	4
Stadsgraven, Copenhagen	4–6 interconnected basins	5 (level 6: 93)
Internal lakes of Copenhagen	5–6 interconnected basins	5

*Levels: 1. *Conceptual diagram* selected. 2. *Verification* carried out. 3. *Calibration* using intensive measurements. 4. Calibration of entire model. 5. *Validation*. Object function and regression coefficient are found. 6. *Validation of a prognosis* for significant changed loading.

Section 2.3 are carefully included in the model development. Eutrophication models are probably also the types of ecological model to have received most attention and effort during the last 25 years. The results therefore reflect what could be obtained for all ecosystem models, if sufficient effort is used in the examination and development of models.

The *eutrophication models* of medium to high complexity also illustrate to what extent the ecosystem properties can be revealed using models. For instance, it is possible using eutrophication models to illustrate the importance of the indirect effect of the network representation and of the element cycles. These models also show, however, the "soft points" of modelling, particularly the discrepancy between the rigidity of the model and the enormous flexibility of the ecosystem. This point is discussed in more detail in Chapter 9. All in all, it may be concluded that eutrophication models represent the state of the art of modelling.

Prognoses for the development of eutrophication by different removal efficiencies for phosphorus, nitrogen or phosphorus and nitrogen simultaneously have been made in almost all the case studies listed in Table 7.8. It has been stated for *Lake Glumsø* that removal of nitrogen has little or no effect, while removal of phosphorus would give substantial reduction in the phytoplankton concentration.

The results of two cases are summarized in Table 7.9.

- Case A: The treated waste water has a concentration of 0.4 mg P l^{-1}, corresponding to about 92% removal efficiency, which is achievable by proper chemical precipitation.
- Case B: The treated waste water has a concentration of 0.1 mg P l^{-1}, corresponding to about 98% removal efficiency, which will require chemical precipitation in combination with, e.g., ion exchange.

As seen in Table 7.9, the water quality will improve significantly in accordance with the prognosis. Case B, 98% removal of phosphorus, must be preferred. In the third year Case B will give a reduction in production from 1100 g C/m^2 y^{-1} to 500 g C/m^2 y^{-1} and the *transparency* is increased from a minimum value of 20 cm to 60 cm. The ninth year would even result in a reduction of the production to 320 g C/m^2 y^{-1}, which corresponds (almost) to a mesotrophic lake, which is an acceptable improvement for a shallow lake situated in an agricultural area. The prognosis predicts a pronounced effect of 98% phosphorus removal, which could therefore be recommended to the environmental authorities. Further improvements after nine years should not be expected (the *retention time* of the water is only about six months).

Conveyance of the waste water was also considered but has the following disadvantages:

1. it is slightly more expensive than the Case B solution, taking interests, depreciation and running costs into consideration;
2. the phosphorus is not removed but only transported to Susaa River, where its effects have not been considered;
3. the sludge produced at the biological treatment plant will be less valuable as a soil conditioner, since the phosphorus concentration will be lower than when phosphorus removal is included; and
4. the freshwater is not retained in the lake, from where, after storage for some time, it could have been reclaimed if needed. Freshwater is not at present a problem in this area, but it is foreseen that it might be in 20 to 40 years.

In spite of these arguments the community, having a preference for traditional methods, has chosen to convey waste water to the Susaa River. The pipeline was

Table 7.9. *Predictions* by means of the model in two cases for concentration of treated waste water. Case A: 0.4 mg P/l; Case B: 0.1 mg P/l

	Third year		Ninth year	
	Case A	Case B	Case A	Case B
g C/m^2 year	650	500*	500	320*
Minimum *transparency* (cm)	50	60	60	75

*An error of 3% on this value could be expected if the validation results hold, see *R* in Table 7.7 for production.

constructed in 1980, and it began operation in April 1981, which has enabled a validation of the prognosis presented.

Lake Glumsø was ideal for these studies, not only because of its limited depth and size, but also because a reduced nutrient input to the lake was relatively easy to realize. The limited retention time (about six months) makes it realistic to obtain a validation of a prognosis within a relatively short time interval (a few years). On 1 April 1981 the input of waste water directly to the lake was stopped. As the capacity of the sewerage system is still too small, a minor input of mixed rain water and waste water is, from time to time, discharged through an upstream tributary of the lake. The phosphorus loading is therefore reduced not by 98% but only by 88% (determined by a *phosphorus balance* 1981–1984). The prognosis of Case A should thus be used for comparison.

During the third year after the reduction in loading took place, a pronounced effect was observed. Table 7.10 compares some of the most important data of the *prognosis*. This table also includes data obtained during the first two months of the third year. In the table errors are indicated as ± for g C/24 h m^2 and chlorophyll maximum mg/m^3.

For the prognosis values the results from Table 7.7 (production 8% and phytoplankton concentration 15%) are used to determine standard deviations. For the

Table 7.10. Comparison of prognosis and observations

	Prognosis (Case A: 92% P reduction)	Measurement approximately (88% reduction)
Minimum *transparency*		
First year	20 cm	20 cm
Second year	30 cm	25 cm
Third year	45 cm	50 cm
g C/24 h m^2 maximum		
First year	9.5 ± 0.8	5.5 ± 0.5
Second year (spring)	6.0 ± 0.5	11 ± 1.1
Second year (summer)	4.5 ± 0.4	3.5 ± 0.4
Second year (autumn)	2.0 ± 0.2	1.5 ± 0.2
Third year (spring)	5.0 ± 0.4	6.2 ± 0.6
Chlorophyll in spring maximum mg/m^3		
First year	750 ± 112	800 ± 80
Second year	520 ± 78	550 ± 55
Third year	320 ±48	380 ± 38

Table 7.11. *Validation of the prognosis* (3rd year)

Y (see Eq. (7.38))	0.72*
SDPC (st. dev. of predicted and measured max. phyt. conc.	0.08

*Phytoplankton, soluble and total nutrient concentrations were considered.

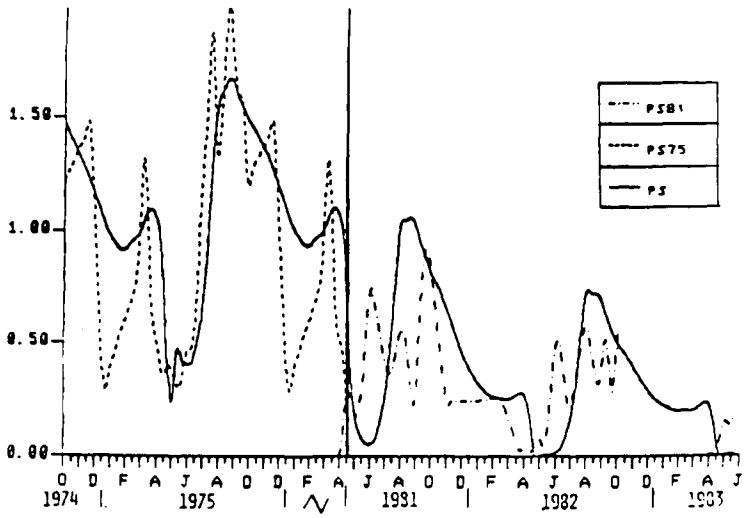

Fig. 7.6. Prognosis validation, soluble phosphorus.

measured values an error of 10% is estimated. A comparison between the prognosis and measured values is illustrated in Figs 7.6 and 7.7. As seen from Table 7.10, the prognosis has given an almost correct production in the third year for maximum spring production and phytoplankton concentration, but the maximum concentration of phytoplankton occurs about 1st April, while the prognosis predicts the beginning of May (Fig. 7.7). Previously, the lake was dominated by *Scenedesmus*, but now by diatoms which have a lower optimum temperature and therefore bloom earlier in the spring than *Scenedesmus*. This seems to explain the discrepancy between prognosis and measurements on this point, and thereby the relatively high Y value (see Table 7.11).

If it was possible to account for shifts in species composition, the model might improve its predictions. Results published by Jørgensen (1981; 1986; 1992a,b) and Jørgensen and Mejer (1979) indicate that this would be possible by introducing a maximum growth rate of phytoplankton which is variable and currently determined as the value that gives the highest *exergy* (for further explanations see Chapter 9). Such models are called *structurally dynamic models*. However, since diatoms take up silica, it was also necessary to introduce a silica cycle into the model.

The other production and chlorophyll values are well predicted except the spring production in the second year (Table 7.10). The predictions on minimum transparency are acceptable as they are given with a difference of 5 cm or less (Table 7.10).

The general trends in the phosphorus concentrations (Fig. 7.6) give good accordance between predicted and measured values, although the fluctuations in phosphorus concentration were not well predicted. However, it cannot be excluded that the fluctuations are an artifact.

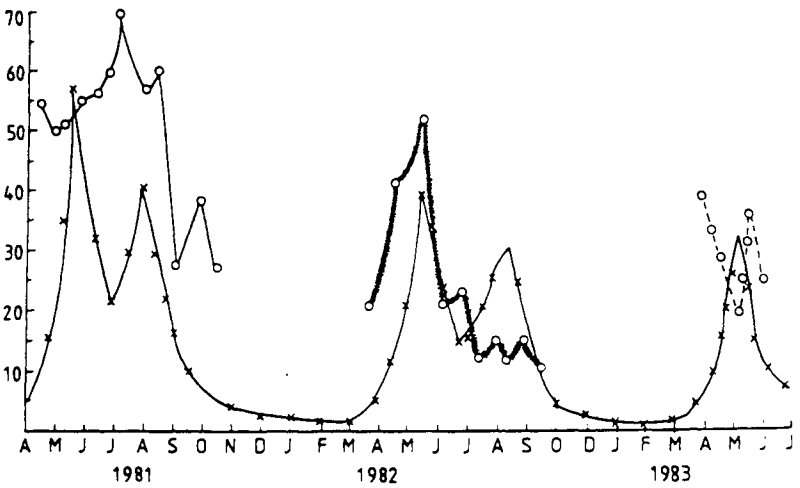

Fig. 7.7. Phytoplankton concentration versus time. Prognosis validation: O corresponds to measured values. × corresponds to model output.

The prognosis was validated by use of Y (see Table 7.11) and the average standard deviation of the predicted and measured maximum phytoplankton concentration, designated SDPC. The results are shown in Table 7.11. The Y value is 72% compared with 16 (or 31%) for the validation under unchanged loading. The increased standard deviation, Y, between model values and measured values is due to the above-mentioned shift in species composition. The maximum phytoplankton concentration is, however, predicted with an error of only 8% (Table 7.11), which is fully acceptable. A better accordance between observed and predicted values in time for the maximum phytoplankton concentration will therefore improve the Y value considerably. It should most probably be attainable by a structurally dynamic model.

7.5 A Wetland Model

Introduction

Wetland is defined by Cowardin et al. (1979) as an ecosystem transitional between aquatic and terrestrial ecosystems, where the water table is usually at or near the surface or the land is covered by shallow water. Recently, several models of wetlands have been developed in response to an increasing interest in the use of wetlands as buffer zones in the landscape and to denitrify the drainage water from agriculture. Models of forested swamps, bogs, marshes and tundra have appeared in the literature during the last 10 years (see Jørgensen et al., 1995).

Mitsch (1976; 1983) has given a more comprehensive review of wetland models than it is possible to give here. He distinguishes between energy/nutrient models, hydrological models, models of spatial ecosystems, models of tree growth, process models, causal models and regional energy models. Mitsch et al. (1988) have reviewed several types of wetland models in their book "Wetland Modelling". Other literature sources are Mitsch and Gosselink (1993; 2000), and Mitsch and Jørgensen (1989, second edition expected 2001).

A Model of Nitrogen Removal by Wetlands

Non-point sources have been in focus since the late 1970s. Nitrogen and phosphorus balances have shown that agriculture and other non-point sources contribute significantly to overall pollution and, in particular, to the *eutrophication* problem. It has been implied that environmental technology is not sufficient, but must be supplemented by other methods to cope with the problems of non-point sources. These methods are covered by the term *ecological engineering* or *ecotechnology*. Mitsch and Jørgensen (1989) give an overview of the methods of ecological engineering used to abate eutrophication of lakes and have compared the efficiency of the methods for a particular lake by a eutrophication model. The result of this case study (other case studies have given similar results) is that the application of wetlands is often a very effective method, at least where nitrogen plays a role for the eutrophication.

A nitrogen balance for agricultural regions has revealed that nitrogen from non-point sources plays a major role and that a solution to the eutrophication problem of freshwater and marine ecosystems cannot be found without solving the problems associated with non-point pollution. The entire spectrum of available ecological engineering methods touched on above have been implemented so far to solve the problem. In this context, there is a need for a wetland model, able to make predictions of the nitrogen removal capacity of a wetland on the basis of certain information about an existing or a planned wetland. This chapter presents such a model. Its aim is to make as general a model as possible, but as ecological models have only a certain generality, it has been necessary to distinguish between the general relationships and the more site-specific parameters and forcing functions. Thus, it is necessary to accept that it is not possible to achieve a complete generality for wetland models. According to Mitsch's classification (see above), the model is a causal process model.

The model is based upon previous approaches by Jørgensen et al. (1988) and Dørge (1991). The model differs from previous models by being simpler, which was necessary to make it more general. Furthermore, the model is dynamic in the hydrological as well as in the biological part where Dørge's model is a steady-state model for the biological components. A dynamic model is more difficult to calibrate, but the calibration of a dynamic model will often reveal bias relations more clearly. This feature of dynamic models has been used to make a site-specific calibration, as

will be demonstrated below. The results of model application on two case studies are presented. The procedure for a more general application of the model in an environmental management context is proposed.

A conceptual diagram of the model and the equations are presented in Figs. 7.8 and 7.9. The software *STELLA* is applied. The climatic forcing functions are: precipitation, evaporation, temperature and solar radiance. The last is given as a cosine function (see Dørge, 1991) and the first three functions as tables (see Fig. 7.9). The same functions are applied to both case studies. The site-specific forcing functions are: the nitrate and ammonium concentrations in the in-flowing water and the flow rate.

The model construction considers one square metre of wetland and looks at the conversion of nitrogen in this area. The result of the model will therefore be how much nitrogen can be removed, accumulated and/or released per unit of area. Two hydrological state variables are applied, one representing the surface layer, where nitrification can take place, and the other the reactive zone, where a pronounced *denitrification* and accumulation take place. The depth of this layer is not very important, because in the great majority of cases the *limiting factor* is the *hydraulic conductivity*. The amount of organic matter and the room for denitrifying micro-organisms in this zone are under no circumstances limiting.

The nitrogen state variables are nitrate and ammonium in the surface layer and nitrate, ammonium, detritus-N, plant-N and adsorbed N in the so-called active layer. Cycling of nitrogen takes place in the active layer: ammonium and nitrate are taken up by plants. Plant-N forms detritus-N by decay and after *mineralization* ammonium is formed. Nitrification and denitrification are described by the *Michaelis–Menten equations*, while the uptake of nitrate and ammonium by the plants is formulated by first-order kinetics and proportional to the light. There are no differences between the uptake rates for ammonium and nitrate. The uptake is therefore proportional to the concentration of inorganic nitrogen = ammonium + nitrate. The mineralization follows a first-order kinetics, too.

The decay is dependent on the uptake and a mortality function, which can be formulated as a table according to the seasonal variations generally observed in a given area and a given type of wetland. All biological rates are dependent on the temperature with a more pronounced dependence for the nitrification and *denitrification*. The following site-specific measured parameters are used: hydrological conductivity, nitrification capacity, denitrification capacity, the detritus-N pool (the initial value of this state variable) and the initial and maximum value of plant N. The following parameters are calibrated: uptake rates for nitrate and ammonium and the mineralization rate. These parameters are adjusted to give the observed trends in detritus-N and the maximum value of plant-N.

The model has been applied in several case studies, of which two are shown. The site specific parameters, the basis for the model application, are shown in Table 7.12. Uptake rates for nitrate and ammonium and the mineralization rate are found by calibration. These two parameters are given in Table 7.13. The calibration of the two case studies was easy to perform and gave reasonable values, as seen in Table 7.14.

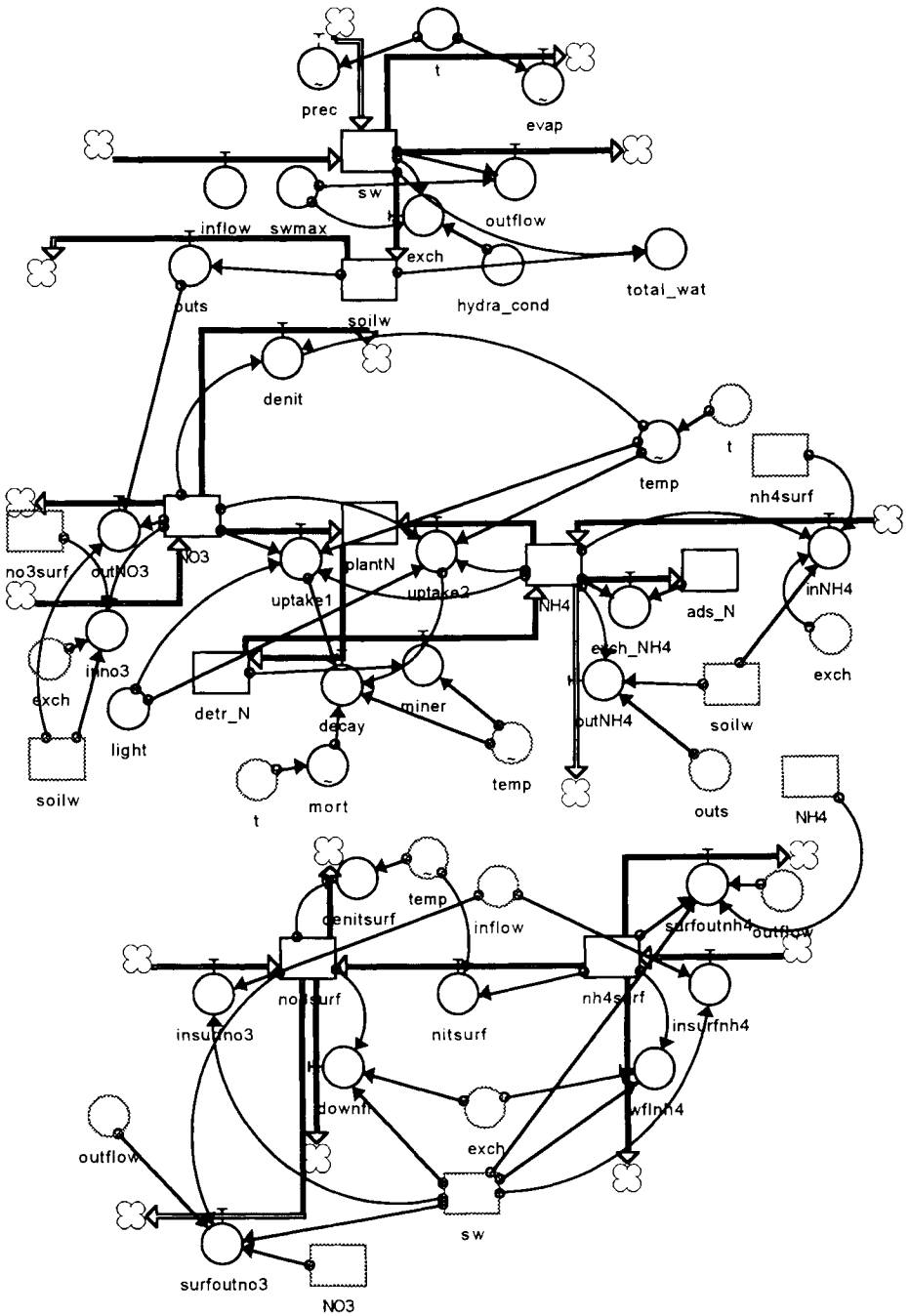

Fig. 7.8. A *STELLA* diagram of the model of *nitrogen removal* by *wetlands*.

Model Equations (*STELLA*)

```
ads_N = ads_N + dt * (exch_NH4)
INIT(ads_N) = 200/9
detr_N = detr_N + dt * (decay - miner)
INIT(detr_N) = 1200
NH4 = NH4 + dt * (-uptake2 + miner - exch_NH4 - outNH4 + inNH4)
INIT(NH4) = 1.0
nh4surf = nh4surf + dt * (-nitsurf + insurfnh4 - wflnh4 - surfoutnh4)
INIT(nh4surf) = 0.1
NO3 = NO3 + dt * (-uptake1 - outNO3 - denit + inno3)
INIT(NO3) = 10
no3surf = no3surf + dt * (insurfno3 + nitsurf - downfl - denitsurf - surfoutno3)
INIT(no3surf) = 5
plantN = plantN + dt * (uptake1 + uptake2 - decay)
INIT(plantN) =20
soilw = soilw + dt * (exch - outs)
INIT(soilw) = 2.0
sw = sw + dt * (inflow - outflow + prec - evap - exch)
INIT(sw) = 0.015
decay =(1.04 ^ (temp-20))*mort*(uptake1+uptake2)
denit = (1.12 ^ (temp-20))*8*NO3/(12+NO3)
denitsurf = (1.12 ^ (temp-20))*8*no3surf/(12+no3surf)
downfl = exch*no3surf/sw
exch = IF sw > swmax THEN hydra_cond ELSE sw*hydra_cond/swmax
exch_NH4 = IF ads_N < 200*NH4/(8+NH4) THEN NH4 (8+NH4) ELSE 0
hydra_cond = 0.09
inflow = 0.035
inNH4 = (exch*nh4surf+0.01*(nh4surf-NH4)) soilw
inno3 = (exch*no3surf+0.01*(no3surf-NO3)) soilw
insurfnh4 = inflow*0.2/sw
insurfno3 = inflow*5/sw
light = 1.91 - 1.68*COS(6.1*(TIME-355)/365)
miner = 0.0001*detr_N*1.07 ^ (temp-20)
nitsurf = 8*(1.12 ^ (temp-20))*nh4surf/(8+nh4surf)
outflow = IF sw > swmax THEN 1.0*(sw-swmax) ELSE 0
outNH4 = outs*NH4/soilw
outNO3 = outs*NO3/soilw
outs = IF soilw > 2.45 THEN 0.1 ELSE 0
surfoutnh4 = (nh4surf*outflow+0.01*(nh4surf-NH4)) sw
surfoutno3 = (outflow*no3surf+0.01*(no3surf-NO3)) sw
swmax = 0.05
t =TIME
total_wat = soilw+sw
uptake1 =IF NO3 > 0.05 THEN light*0.15*(1.05 ^ (temp-20))*NO3/(NO3+NH4) ELSE 0
uptake2 = IF NH4 > 0.05 THEN light*0.15*(1.05 ^ (temp-20))*NH4/(NO3+NH4) ELSE 0
wflnh4 = exch*nh4surf/sw
evap = graph(t)
mort = graph(t)
prec = graph(t)
temp = graph(t)
```

Fig. 7.9. The equations used in the *STELLA* program. "Statement goes here" implies that table functions are required.

Table 7.12. *Wetland properties* (based on 1 m^2)

Parameter	Rabis *wet meadow*	*Glumsø reed-swamp*
Hydrological conductivity (m/24 h)	0.009	0.009
Production (N/year)	7.0	40.0
Detritus-N (g)	800	1200
Max. nitrification (g N/24 h)	11	7
Max. denitrification (g N/24 h)	22	72

Table 7.13. Calibrated parameters

Parameter	Rabis wet meadow	Glumsø reed-swamp
Uptake rate (1/24 h)	0.025	0.125
Mineralization rate (1/24 h)	0.00005	0.00025

Table 7.14. *Nitrogen balance* (based on 1 m^2). The numbers are found by the simulations; numbers in brackets are previously measured values.

Nitrogen flow (g N/year)	Rabis wet meadow	Glumsø reed-swamp
Loading (L)	55	64
Removed by denitrification (1)	24 (20)	89(92)
Released (2)	0(0)	37(40)
Accumulate (3)	3(5)	7(5)
% (1) + (3) – (2) / L	49(45)	92(89)

The most interesting results of the model applications are the nitrate concentration in the out-flowing water (shown in Figs 7.10 and 7.11) and the nitrogen balances, given in Table 7.14. The accordance with measured results is acceptable, particularly in the light of the uncertainty, which should be accepted in environmental planning.

It is the aim of model development to construct a model with a general applicability. The idea may be expressed as follows: give some pertinent information about the wetland and the model will give you the capability of the wetland to remove nitrogen. The environmental planner will thus be able to say how much wetland is needed to achieve certain goals for the removal of nitrogen from non-point sources on a regional basis.

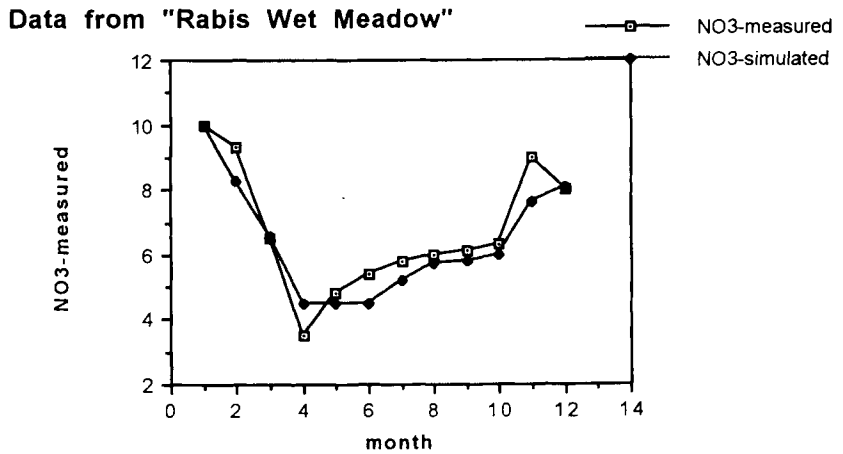

Fig. 7.10. Comparison of measured and simulated values of nitrate in mg/l for a *wet meadow.*

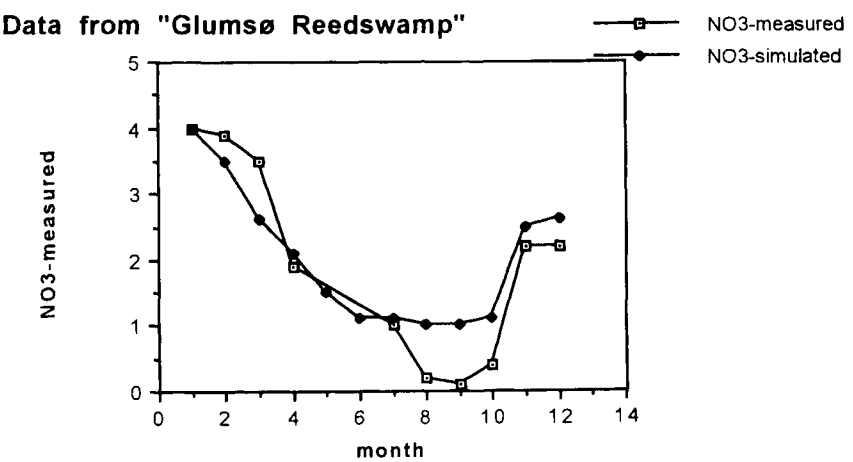

Fig. 7.11. Comparison of nitrate measured and simulated for *Glumsø Reed-swamp.*

The model has been applied in several case studies with acceptable results, which is promising for the model application. However, it is recommended that more experience from even more case studies be gained before attempting a wider application on a regional basis. The procedure for a wider application seems ready from the experience obtained in the case studies. A tentative procedure is summarized in a flow chart (see Fig. 7.12). The methods to be applied, if the wetland does not exist, but is planned for construction, are similar. The climatic forcing

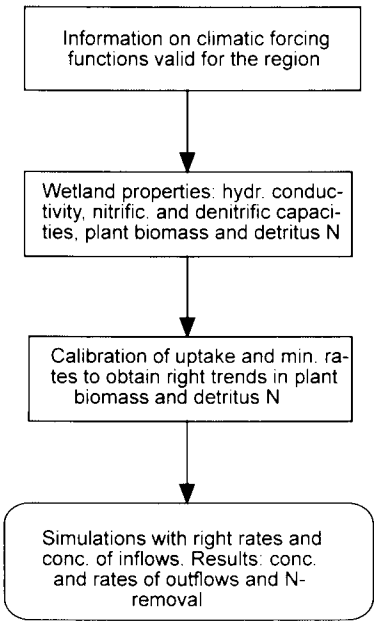

Fig. 7.12. A procedure applicable for development of a wetland model for a specific site, from the general model presented in the text.

Table 7.15. Spectrum of *hydraulic conductivity* (m/24 h)

Type of soil	Hydraulic conductivity (m/24 h)
Clay	0.0005
Sand	50
Sandy soil	10
Medium humic soil	1–5
Compact peat	0.01–0.05

functions used are regionally based, but the wetland properties for a non-existing *wetland* can not be found but only estimated.

Hydrological conductivity can still be estimated from the soil characteristics and by comparison with wetlands with similar vegetation and soil types. Table 7.15 gives the spectrum of *hydrological conductivity*.

The initial and maximum values of plant-N and the trends in detritus-N are estimated from a wetland with similar vegetation as the one chosen for the planned wetland. The height of the surface layer is estimated from wetlands with similar vegetation and from the slope of the landscape, where the wetland is planned.

PROBLEMS

1. Two alternatives exist for improving the visual quality of Lake X: (1) increase the dilution (flushing) rate, and (2) decrease the concentration of nutrients in the inflow by waste water treatment. The present detention time is 8 months and the average inflow of phosphorus, which is considered the most limiting nutrient is 120 mg l^{-1}. The lake can be considered a completely mixed reactor. Which alternative would you choose and why?

2. The average flow velocity of a stream is 0.7 m/s and the average depth is 1.5 m. Estimate the rate of oxygen transfer from the atmosphere to the water at 12°C, 15°C and 20°C.

3. A stream has the following characteristics during a low flow period: flow rate 70 $m^3 s^{-1}$ and 0.4 m s^{-1}, temperature 24°C, depth 2 m, dissolved oxygen 85% and BOD_5 2 mg/l at point X. How many kg of BOD_5 can be discharged into the stream at point X, if a minimum of 5 mg/l is to be maintained in the stream? Average rate constants can be assumed. Nitrification is negligible.

4. A steam receives waste water at a rate 7 $m^3 s^{-1}$. The waste water has BOD_5 12 mg/l and the ammonium concentration is 23 mg/l. The stream has a flow rate of 60 $m^3 s^{-1}$ and 0.5 m s^{-1}, temperature 18°C, depth 2 m, dissolved oxygen 95%. Which minimum oxygen concentration will be recorded in the stream at which distance from the discharge point. Use the constant given in the text.

5. Estimate the difference in the estimation of the reaeration coefficient using all the expressions presented in the text.

6. BOD_5 at room temperature 20°C is found to be 14 mg/l in a sample. What is BOD_7 at 18°C?

7. Determine the BOD_5 and the oxygen concentration in a completely mixed lake with an inflow of 40 l/s, a depth of 3 m and an area of 15 ha. The average wind speed is approximately 4.5 m/s, the oxygen concentration in the inflow is 8 mg/l and contains no BOD. 120 kg of BOD is discharged to the lake by waste water per day. The lake has a sandy bottom. The photosynthesis corresponds to 3 mg oxygen/l/day).

8. Set up a STELLA program for Lorenzen's model (see Chapter 3).

9. Explain why the relationship between summer chlorophyll and annual average phosphorus concentration is so different for the various investigations of the relationship.

10. Find the transparency for a lake with an annual average phosphorus concentration of 1 mg/l and a depth of 2 m using Table 7.6. Use also Eq. (7.4) and Fig. 7.2. Explain the discrepancy.

11. Explain why any new lake model development inevitably requires an examination of possible model modifications.

12. Why is validation of a model compulsory?
13. How will you describe the generality of eutrophication models?
14. Explain why it is expected that a structurally dynamic model will be able to offer a better validation.

CHAPTER 8

Ecotoxicological Models

8.1 Classification and Application of Ecotoxicological Models

Ecotoxicological models are increasingly applied to assess the environmental risk of the emission of chemicals to the environment. We can distinguish between fate models, the results of which are concentrations of a chemical in one or more environmental compartments (e.g., the concentration of a chemical compound in a fish or in lake), and effect models, which translate a concentration or body burden in a biological compartment to an effect either on an organism, a population, a community, an ecosystem, a landscape (consisting of two or more ecosystems) or the entire ecosphere.

The results of a *fate model* can be used to find the ratio, RQ, between the computed concentration, the *predicted environmental concentration* (PEC), and the non-observed-effect concentration (NOEC), which is determined by the application of literature values or laboratory experiments. Further details about the applied procedure for environmental risk assessment (ERA) and how to account for the uncertainty of the assessment will be presented in the next section.

The effect models presume that we know the concentration of a chemical in a focal compartment, either by a model or by analytical determinations. The effect models translate the concentrations found into an effect on either the growth of an organism, the development of a population or the community, the changes of an ecosystem or a landscape, or on the entire ecosphere.

Obviously, it is also possible to merge fate models with effect models and thereby combine the two results. We could call them *FTE models*, meaning fate–transport–effect models.

Many fate models, fewer effect models and only a few FTE models have been applied to solve ecotoxicological problems and perform *ERA*s. The development is, however, towards a wider application of effect and FTE models.

*A. **Fate models** may be divided into three classes:*

I. Models that map the fate and transport of a chemical in a region or a country. These models are sometimes called *McKay-type models* after Don McKay who first developed them. A detailed discussion of the application of these models can be found in Mackay (1991) and SETAC (1997). This type of fate model is rarely calibrated and validated, although a attempt has been made to indicate the standard deviation of the results (see *SETAC*, 1997).

II. Models that consider a specific case of toxic substance pollution, e.g., discharge of a chemical to a coastal zone from a chemical plant or a sewage treatment plant. This type of fate model must always be calibrated and validated.

III. Models that focus on a chemical that is used locally. This implies that an evaluation of the risk will require us to determine a typical concentration (which is much higher than the regional concentration that would be obtained from model Type I) in a typical locality. A typical example is the application of pesticides, where the model will have to look into a typical application on an agriculture field close to a stream and with a ground water mirror close to the surface. This model type can be considered to be a hybrid of I and II. The conceptual diagram and the equations of the Type III model are similar to model Type II, but the interpretation of the model results are similar to model Type I. This model type should always be calibrated and validated by data obtained for a typical case study, but the prognosis is most commonly applied for the development of "a worst case situation" or "an average situation", which in general may be different from the case study applied for the calibration and validation.

Examples of all three types of models will be presented in this chapter. Chapter 5 on steady-state models has already presented an ecotoxicological model Type II. Only examples of dynamic models are included in this chapter.

*B. **Effect models** may be classified according to the hierarchical level of concern:*

I. Organisms models, where the core of the model is the influence of a toxic substance on an organism, for instance the influence on the growth, represented in the model by a relationship between the growth parameters and the concentration of a toxic substance.

II. Population models, where the population models presented in Chapter 6, including individual based models, may be applied with the addition of relationships between toxic substance concentrations and the model parameters.

III. An ecosystem model where the influences of a toxic substance on several parameters are included. The result of these impacts of a chemical is an ecosystem with a different structure and composition.

IV. As ecosystems are open systems, the effects of chemicals may change several interrelated ecosystems. Landscape models can be used in these cases.

V. Global models where the impacts of chemicals are the core of the model. A typical global model is a model of the ozone layer and its decomposition due to the discharge of chemicals (e.g., freon).

FTE models can be any combination of the fate and effect models, although the combinations of Types AII and AIII fate models with Types BII and BIII effect models will be most used in practical ecotoxicological management.

The effect models applied up to now are mainly of Types I and II, although the effects on ecosystem levels may be of particular importance due to their frequent irreversibility. In some cases, ecosystems may change their composition and structure significantly due to discharge of toxic substances. In such cases it is recommended that consideration be given to applying structurally dynamic models, also called variable parameter models (see Chapter 9).

The ecotoxicological models are applied either for registration of chemicals to solve site specific pollution problems or to follow the recovery of an ecosystem after pollution abatement or remediation has taken place.

Types AI and AIII models are widely used for registration of chemicals. About 100,000 chemicals are registered, but only about 20,000 chemicals are in use on a scale which is likely to threaten the environment. It is the long-term goal to perform an ERA for all these 20,000 chemicals, which were in use prior to 1984 when an ecotoxicological evaluation of all new chemicals became compulsory throughout the European Union (EU). Among the 20,000 chemicals, 2500 have been selected as high volume chemicals which are obviously of most concern. Among the 2500 chemicals, 140 have been selected by the EU to be examined in detail, included performance of *ERA* which will require the application of models. These are called HERO-chemicals (highly expected regulatory output chemicals). A proper ecotoxicological evaluation of the chemicals in use prior to 1984 is important: if we continue with the same low rate of evaluation as we have done in the last decade, it will take 100 years before we have a proper ecotoxicological evaluation of the 2500 high volume chemicals and 800 years before we have evaluated all the chemicals in use!

About 300–400 new chemicals are registered per year. These chemicals *must* be evaluated properly, although it may be possible in some cases for chemical manufacturers to postpone the evaluation and the final decision for a few years.

Types AII fate models, BII, BIII and, in a few cases, BIV effect models are applied, sometimes in combination as an FTE model, to solve site specific pollution problems caused by toxic substances or to make predictions on the recovery of ecosystems after the impacts have been removed. These applications are mainly carried out by environmental protection agencies and rarely by chemical manufacturers.

It can be concluded from this short overview of model types and classes and their application in practical environmental management that there is an urgent need for good ecotoxicological models and for extensive experience in the applicability of

these models. The application of ecotoxicological models up to now has been relatively minor compared with the environmental management possibilities that these models offer.

Section 8.2 reviews the performance of an ERA. Section 8.3 presents the characteristics and structure of ecotoxicological models. Section 8.4 gives an overview of some of the ecotoxicological models published during the last 10–15 years. The description of the chemical, physical and biological processes will, in general, be according to the equations presented in Chapter 3. Section 8.5 is devoted to parameter estimations methods, which are of particular importance in ecotoxicological models.

The following sections are used to present ecotoxicological models of case studies. Section 8.6 presents a very simple ecotoxicological model of chromium pollution in *Fåborg Fjord*, Denmark. This case study illustrates clearly that a simple model can give an acceptable and sufficiently accurate answer to an environmental management question, provided that the modeller knows his ecosystem and can select the processes of importance for the management question in focus. The case study in Section 8.7 covers an ecotoxicological model for relating contamination of agricultural products by cadmium and lead with the heavy metal pollution of soil due to the content of cadmium and lead in fertilizers, dry deposition and sludge. The model presented in Section 8.9 is a more complex but still a relatively simple model compared with the more complex eutrophication models. This case study is devoted to mercury contamination of *Mex Bay* in Egypt. Section 8.9 gives examples of fate models, *fugacity models*, in general including the basic equations. A case study, where the fugacity modelling approach is used, is presented. The case study illustrates the application of a fugacity model to the PCB pollution of the Great Lakes.

8.2 Environmental Risk Assessment

A brief introduction to the concepts of *environmental risk assessment* (*ERA*), is given below to familiarize the reader with the concepts and ideas that are behind the application of ecotoxicological models to assess an environmental risk.

Treatment of industrial waste water, solid waste and smoke is very expensive. Consequently, industries attempt to change their products and production methods in a more environmentally friendly direction to reduce the treatment costs. Industries need to know, therefore, how much the different chemicals, components and processes are polluting our environment. Or expressed differently: what is the environmental risk of using a specific material or chemical compared with other alternatives? If industries can reduce their pollution just by switching to another chemical or process, they will of course consider doing so to reduce their *environmental costs* or improve their green image. An assessment of the environmental risk associated with the use of a specific chemical and a specific process gives the industries the possibility of making the right selection of materials, chemicals and

processes to the benefit of the economy of the enterprise and the quality of the environment.

Similarly, society needs to know the environmental risks of all chemicals applied so as to phase out the most environmentally threatening chemicals and set standards for the use of all other chemicals. The standards should ensure that there is no serious risk involved in using the chemicals, provided that the standards are followed carefully. Modern abatement of pollution includes, therefore, environmental risk assessment (*ERA*), which may be defined as the process of assigning magnitudes and probabilities to the adverse effects of human activities. The process involves identifying hazards such as the release of toxic chemicals to the environment by quantifying the relationship between an activity associated with an emission to the environment and its effects. The entire ecological hierarchy is considered in this context, implying that the effects at the cellular (biochemical) level, the organism level, the population level, and the ecosystem level as well as for the entire ecosphere should be considered.

The application of environmental risk assessment is rooted in the recognition that:

1. the cost of elimination of all environmental effects is impossibly high;
2. decisions in practical environmental management must always be made on the basis of incomplete information;

We use about 100,000 chemicals in such amounts that they may threaten the environment, but we know only about 1% of what we need to know to be able to make a proper and complete environmental risk assessment of these chemicals. Later in this chapter a short introduction will be given to available estimation methods which it is recommended be applied if we cannot find information about properties of chemical compounds in the literature. A list of the relevant properties is also given in this context and their implication for environmental impact is discussed.

ERA is in the same family as environmental impact assessment (EIA), which attempts to assess the impact of a human activity. EIA is predictive, comparative and concerned with all possible effects on the environment, including secondary and tertiary (indirect) effects, while ERA attempts to assess the probability of a given (defined) adverse effect as result of a considered human activity.

Both ERA and EIA use models to find the expected environmental concentration (EU) which is translated into impacts for EIA and to *risks of specific effects* for ERA. The development of the ecotoxicological models that are applicable to the assessment of environmental risks is treated in detail below. An overview of ecotoxicological models is given in Jørgensen et al. (1995a).

Legislation and regulation of domestic and industrial chemicals with respect to the protection of the environment have been implemented in Europe and North America for decades. Both regions distinguish between existing chemicals and introduction of new substances. For existing chemicals the European Union requires

(e.g. according to Council Regulation No. 793/93) an assessment of risk to man and environment of priority substances by principles given in the Commission Regulation No. 1488/94. An informal priority setting (IPS) is used for selecting chemicals among the 100,000 listed in The European Inventory of Existing Commercial Chemical Substances. The purpose of IPS is to select chemicals for detailed risk assessment from among the EU high production volume compounds, i.e., >1000 t/year (about 2500 chemicals). Data necessary for the IPS and an initial hazard assessment are called Hedset and cover such issues as environmental exposure, environmental effects, exposure to man and human health effects.

In the EU, the risk assessment of new notified substances is based on data submitted according to Directive 67/548/EEC. The directive provides a scheme of step-wise procedure which, in both North America and Europe, is approximately as presented below. Tests are often required to provide the data needed for the ERA.

At the UNCED meeting on the Environment and Sustainable Development, in Rio de Janeiro in 1992, it was decided to create an Intergovernmental Forum on Chemical Safety (IGFCS, Chapter 19 of Agenda 21). The primary task is to stimulate and coordinate global harmonization in the field of chemical safety, covering the following principal themes: assessment of chemical risks, global harmonization of classification and labelling, information exchange, risk reduction programmes and capacity building in chemicals management.

The uncertainty plays an important role in risk assessment (Suter, 1993). Risk is the probability that a specified harmful effect will occur, or in the case of a graded effect, the relationship between the magnitude of the effect and its probability of occurrence.

Risk assessment has emphasized risks to human health and has to a certain extent ignored ecological effects. However, it has been acknowledged that some chemicals that have little or no risk to human health can cause severe effects on aquatic organisms, for instance. Examples are chlorine, ammonia and certain pesticides. **A up-to-date *risk assessment* therefore comprises considerations of the entire *ecological hierarchy*** which is the ecologist's view of the world in terms of levels of organization. Organisms interact directly with the environment and it is organisms that are exposed to toxic chemicals. The species-sensitivity distribution is therefore more ecologically credible (Calow, 1998). The reproducing population is the smallest meaningful level in ecological sense. However, populations do not exist in vacuum, but require a community of other organisms of which the population is a part. The community occupies a physical environment with which it forms an ecosystem.

Moreover, both the various adverse effects and the ecological hierarchy have different scales in time and space which must be included in a proper environmental risk assessment (see Fig. 8.1). For example, oil spills occur at a spatial scale similar to those of populations, but they are briefer than population processes. Therefore a *risk assessment* of an *oil spill* requires consideration of reproduction and recolonization that occur on a longer time scale and that determine the magnitude of the population response and its significance to natural population variance.

Uncertainties in risk assessment are most commonly taken into account by the application of safety factors. Uncertainties have three basic causes:

1. the inherent randomness of the world (*stochasticity*),
2. errors in execution of assessment,
3. imperfect or incomplete knowledge.

The inherent *randomness* refers to uncertainty that can be described and estimated but cannot be reduced because it is characteristic of the system. Meteorological factors such as rainfall, temperature and wind are effectively stochastic at levels of interest for risk assessment. Many biological processes such as colonization, reproduction and mortality also need to be described stochastically.

Human errors are inevitably attributes of all human activities. This type of uncertainty includes incorrect measurements, data recording errors, computational errors and so on.

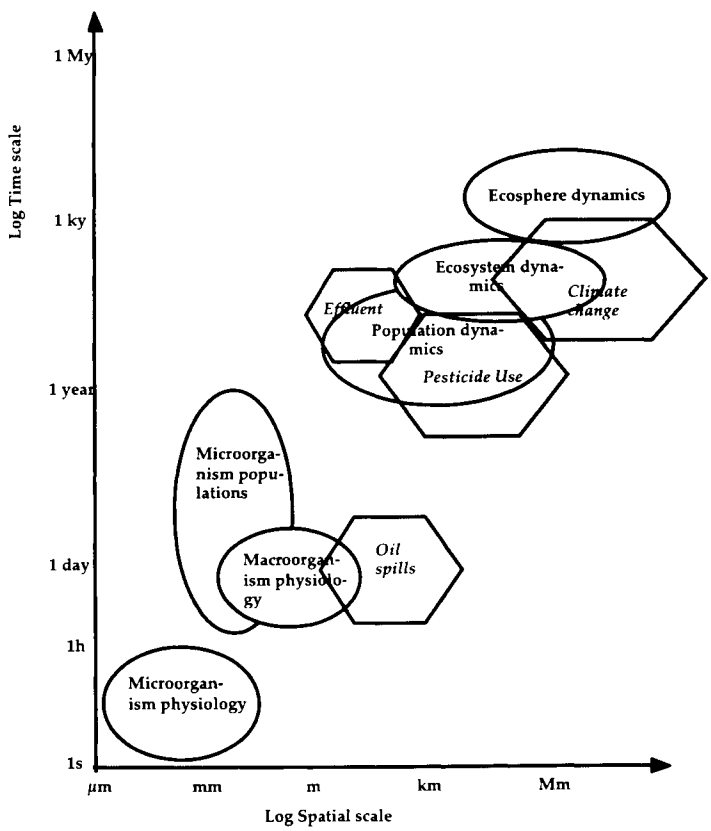

Fig. 8.1. The spatial and time scale for various *hazards* (hexagons, italic) and for the various levels of the *ecological hierarchy* (circles, non-italic).

Table 8.1. Selection of *assessment factors* to derive *PNEC* (see also step 3 of the procedure presented below)

Data quantity and quality	Assessment factor
At least one short-term LC_{50} from each of the three trophic levels of the base set (fish, zooplankton and algae)	1000
One long-term NOEC (non-observed effect concentration, either for fish or Daphnia)	100
Two long-term NOECs from species representing two trophic levels	50
Long-term NOECs from at least three species (normally fish, Daphnia and algae) representing three trophic levels	10
Field data or model ecosystems	case by case

Uncertainty is considered by use of an *assessment (safety) factor* from 10 to 1000. The choice of assessment factor depends on the quantity and quality of toxicity data (see Table 8.1). The assessment or safety factor is used in step 3 of the environmental risk assessment procedure presented below. Relationships other than the uncertainties originating from randomness, errors and lack of knowledge may be considered when the assessment factors are selected, e.g., cost-benefit. This implies that the assessment factors for *drugs* and *pesticides* for instance may be given a lower value due to their possible benefits.

Lack of knowledge results in undefined uncertainty that cannot be described or quantified. It is a result of practical constraints on our ability to accurately describe, count, measure or quantify everything that pertains to a risk estimate. Clear examples are the inability to test all toxicological responses of all species exposed to a pollutant and the simplifications needed in the model used to predict the expected environmental concentration.

The most important feature distinguishing risk assessment from impact assessment is the emphasis in risk assessment on characterizing and quantifying uncertainty. It is therefore of particular interest in risk assessment to be able to analyze and estimate the analyzable uncertainties. They are natural *stochasticity*, parameter errors and model errors. Statistical methods may provide direct estimates of uncertainties. They are widely used in model development.

The use of statistics to quantify uncertainty is complicated in practice by the need to consider errors in both the dependent and independent variables and to combine errors when multiple extrapolations should be made. *Monte Carlo analysis* is often used to overcome these difficulties (see, e.g., Bartell et al., 1992).

Model errors include inappropriate selection or aggregation of variables, incorrect functional forms and incorrect boundaries. The uncertainty associated with model errors is usually assessed by field measurements utilized for calibration ad validation of the model (see Chapter 2). The modelling uncertainty for ecotoxicological models is not, in principle, different from that already discussed in Chapter 2.

Risk assessment of chemicals can be divided into nine steps, as shown in Fig. 8.2. The nine steps correspond to the questions that the *risk assessment* attempts to

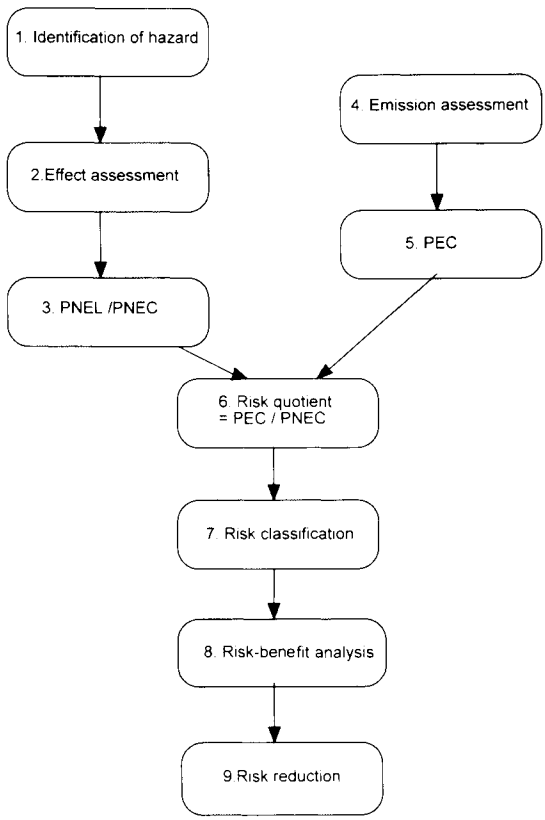

Fig. 8.2. The procedure presented in nine steps to assess the risk of chemical compounds. Steps 1–3 require extensive use of ecotoxicological handbooks and ecotoxicological estimation methods to assess the toxicological properties of the chemical compounds considered, while Step 5 requires the selection of a proper ecotoxicological model.

answer in order to be able to quantify the risk associated with the use of a chemical. These nine steps are presented in detail below with reference to Fig. 8.2.

Step 1: Which hazards are associated with the application of the chemical? This involves gathering data on the types of hazards—possible environmental damage and human health effects. The health effects include *congenital*, *neurological*, *mutagenic*, *endocrine disruption* (so-called oestrogen) and *carcinogenic effects*. It may also include characterization of the behaviour of the chemical within the body (interactions with organs, cells or genetic material). The possible environmental damage includes lethal effects and *sublethal effects* on growth and reproduction of various populations.

As an attempt to quantify the potential danger posed by chemicals, a variety of toxicity tests have been devized. Some of the recommended tests involve experiments with subsets of natural systems, e.g., microcosms, or with entire ecosystems.

The majority of testing of new chemicals for possible effects has, however, been confined to studies in the laboratory on a limited number of test species. Results from these laboratory assays provide useful information for the quantification of the relative toxicity of different chemicals. They are used to forecast effects in natural systems, although their justification has been seriously questioned (Cairns et al., 1987).

Step 2: What is the relation between dose and responses of the type defined in Step 1? It implies knowledge of *NEC* (*non-effect concentration*), LD_x values (the dose which is lethal to $x\%$ of the organisms considered), LC_y values (the concentration which is lethal to $y\%$ of the organisms considered) and EC_z values (the concentration giving the indicated effect to $z\%$ of the considered organisms) where x, y and z express a probability of harm. The answer can be found by laboratory examination or we may use estimation methods. Based upon these answers, a most probable level of no effect (NEL) is assessed. Data needed for Steps 1 and 2 can be obtained directly from scientific libraries, but are increasingly found via on-line data searches in bibliographic and factual databases. Data gaps should be filled with estimated data. It is very difficult to obtain complete knowledge about the effect of a chemical on all levels from cells to ecosystem. Some effects are associated with very small concentrations, e.g., the *oestrogen effect*. It is therefore far from sufficient to know NEC, LD_x, LC_y and EC_z values.

Step 3: Which uncertainty (safety) factors reflect the amount of uncertainty that must be taken into account when experimental laboratory data or empirical estimations methods are extrapolated to real situations? Usually, safety factors of 10–1000 are used. The choice is discussed above and will usually be in accordance with Table 8.1. If good knowledge about the chemical is available, a safety factor of 10 may be applied. On the other hand, if it is estimated that the available information has a very high uncertainty, a safety factor of 10,000 may be recommended in a few cases. Most frequently, safety factors of 50–100 are applied. *NEL* (non-effect level) times the safety factor is named the predicted non-effect level (*PNEL*). The complexity of environmental risk assessment is often simplified by deriving the predicted no effect concentration (PNEC) for different environmental components (water, soil, air, biotas and *sediment*).

Step 4: What are the sources and quantities of emissions? The answer to this question requires a thorough knowledge of the production and use of the chemical compounds considered, including an assessment of how much of the chemical is wasted in the environment by production and use. The chemical may also be a waste product which makes it very difficult to determine the amounts involved. For instance, the very toxic dioxins are waste products from incineration of organic waste.

Step 5: What is (are) the actual exposure concentration(s)? The answer to this question is called the predicted environmental concentration (*PEC*). Exposure can be assessed by measuring environmental concentrations. It may also be predicted by

a model, when the emissions are known. The use of models is necessary in most cases either because we are considering a new chemical, or because the assessment of environmental concentrations requires a very large number of measurements to determine the variations in concentrations in time and space. Furthermore, it provides an additional certainty to compare model results with measurements, which implies that it is always recommended both to develop a model and make at least a few measurements of concentrations in the ecosystem components, when and where it is expected that the highest concentration will occur. Most models will demand an input of parameters, describing the properties of the chemicals and the organisms, which also will require extensive application of handbooks and a wide range of estimation methods. The development of an environmental, ecotoxicological model therefore requires extensive knowledge of the physical–chemical–biological properties of the chemical compound(s) considered. The selection of a proper model is discussed in this chapter and in Chapter 2.

Step 6: What is the ratio *PEC/PNEC*? This ratio is often called the *risk quotient*. It should not be considered an absolute assessment of risk but rather a relative ranking of risks. The ratio is usually found for a wide range of ecosystems, e.g., aquatic ecosystems, terrestrial ecosystems and ground water.

Steps 1–6 are shown in Fig. 8.3 which is completely in accordance with Fig. 8.2 and the information given above.

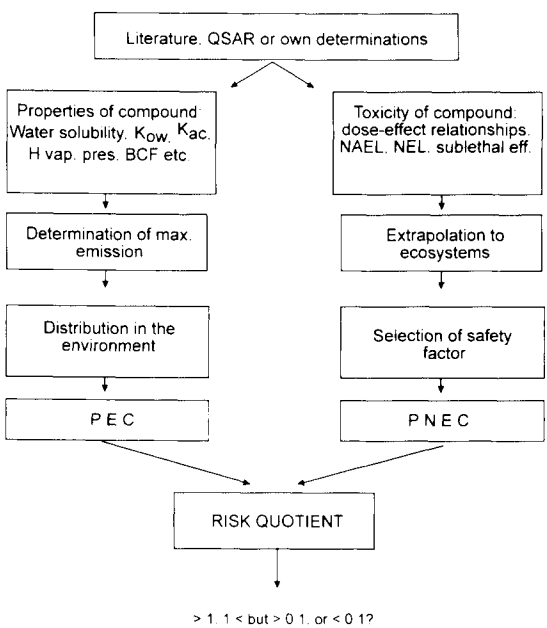

Fig. 8.3. Steps 1–6 are shown in more detail for practical applications. The result of these steps also leads naturally to assessment of the *risk quotient*.

Step 7: How will you classify the risk? The valuation of risks is made in order to decide on risk reductions (Step 9). Two risk levels are defined: (1) the upper limit, i.e., the maximum permissible level (MPL); and (2) the lower limit, i.e., the negligible level (NL). It may also be defined as a percentage of MPL, for instance 1% or 10% of MPL.

The two risk limits create three zones: a black, unacceptable, high risk zone > MPL, a grey, medium risk level and a white, low risk level < NL. The risk of chemicals in the grey and black zones must be reduced. If the risk of the chemicals in the black zone cannot be reduced sufficiently, consideration should be given to phasing out the use of these chemicals.

Step 8: What is the relation between risk and benefit? This analysis involves examination of socioeconomic, political and technical factors, which are beyond the scope of this volume. The cost–benefit analysis is difficult, because the costs and benefits are often of a different order.

Step 9: How can the risk be reduced to an acceptable level? The answer to this question requires deep technical, economic and legislative investigation. Assessment of alternatives is often an important aspect in risk reduction.

Steps 1, 2, 3 and 5 require knowledge of the properties of the focal chemical compounds, which again implies an extensive literature search and/or selection of the best feasible estimation procedure. In case literature values are not available, it is recommended to have at hand (in addition to "Beilstein") the following very useful handbooks of environmental properties of chemicals and methods for estimation of these properties.

- S.E. Jørgensen, S. Nors Nielsen and L.A. Jørgensen, 1991. Handbook of Ecological Parameters and Ecotoxicology, Elsevier, 1991. Published in 2000 as a CD called Ecotox, it contains three times the number of parameters of the 1991 book edition.
- P.H. Howard et al., 1991. Handbook of Environmental Degradation Rates. Lewis Publishers.
- K. Verschueren, 1983. Handbook of Environmental Data on Organic Chemicals. Van Nostrand Reinhold.
- P.H. Howard. Handbook of Environmental Fate and Exposure Data. Lewis Publishers. Volume I: Large Production and Priority Pollutants, 1989. Volume II: Solvents, 1990. Volume III: Pesticides, 1991. Volume IV: Solvents 2, 1993. Volume V: Solvents 3, 1998.
- G.W.A. Milne, 1994. CRC Handbook of Pesticides. CRC.
- W. J. Lyman, W.F. Reehl and D.H. Rosenblatt, 1990. Handbook of Chemical Property Estimation Methods. Environmental Behaviour of Organic Compounds. American Chemical Society.

- D. Mackay, W.Y. Shiu and K.C.Ma. Illustrated Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals. Lewis Publishers. Volume I: Mono-aromatic Hydrocarbons, Chloro-benzenes and PCBs, 1991. Volume II: Polynuclear Aromatic Hydrocarbons, Polychlorinated Dioxins, and Dibenzofurans, 1992. Volume III: Volatile Organic Chemicals, 1992.
- Jørgensen, S.E., Mahler, H. and Halling Sørensen, B., 1997. Handbook of Estimation Methods in Environmental Chemistry and Ecotoxicology. Lewis Publishers.

Steps 1–3 are sometimes denoted as effect assessment or effect analysis and Steps 4–5 exposure assessment or effect analysis. Steps 1–6 may be called risk identification, while environmental risk assessment (*ERA*) encompasses all the nine steps presented in Fig. 8.2. Step 9 in particular is very demanding, as several possible steps in reduction of the risk should be considered, including treatment methods, cleaner technology and substitutes for the chemical under examination.

In North America, Japan and the EU during the last 5–6 years, it consideration has been given to treating medicinal products similarly to other chemical products, as there is in principle no difference between a medicinal product and other chemical products. However, this only resulted in the introduction from 1st January 1998 of the application of *environmental risk assessment* for new veterinary medicinal products. At present, technical directives for human medicinal products in the EU do not include any reference to ecotoxicology and the assessment of their potential risk (Jensen et al., 1998). However, a detailed technical draft guideline issued in 1994 indicates that the approach applicable to veterinary medicine would also apply to human medicinal products. Presumably, ERA will be applied to all medicinal products in the near future when sufficient experience with veterinary medicinal products has been achieved. Veterinary medicinal products, on the other hand, are released into the environment in larger amounts: for instance, in spite of its possible content of veterinary medicine, manure is used as fertilizer on agricultural fields.

It is also possible to perform an environmental risk assessment where the human population is in focus. The ten steps applied in this case are shown in Fig. 8.4, which is not significantly different from Fig. 8.3. The principles for the two types of environmental risk assessment are the same. Figure 8.4 uses the *non-adverse effect level* (*NAEL*) and *non-observed adverse effect level* (*NOAEL*) to replace the predicted non-effect concentration and the predicted environmental concentration is replaced by the *tolerable daily intake* (TDI).

This type of environmental risk assessment has particular interest for *veterinary medicine* which may contaminate food products for human consumption. For instance, the use of antibiotics in pig feed has attracted a lot of attention, as they may be found as residues in pig meat or may contaminate the environment though the application of manure as natural fertilizer.

The selection of a proper ecotoxicological model is the first step in the development of an environmental *exposure model*, as required in Step 5. This will be discussed in more detail in the next section.

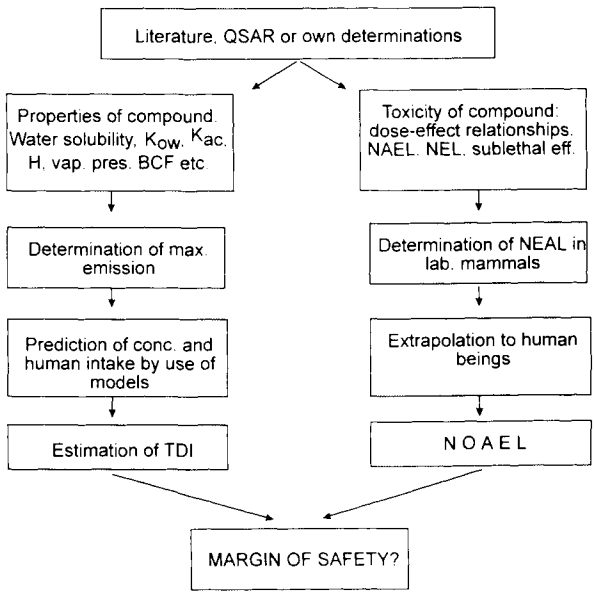

Fig. 8.4. *Environmental risk assessment* for human exposure. This leads to a margin of safety which corresponds to the risk quotient in Figs. 8.2 and 8.3.

8.3 Characteristics and Structure of Ecotoxicological Models

Toxic substance models are most often biogeochemical models, because they attempt to describe the mass flows of the toxic substances considered, although there are effect models of the population dynamics which include the influence of toxic substances on the birth rate and/or mortality and should therefore be considered toxic substance models.

Toxic substance models differ from other ecological models in that:

1. The need for *parameters* to cover all possible toxic substance models is great, and general estimation methods are therefore used widely. Section 8.5 is devoted to this question, which has to a certain extent also been discussed in Section 2.8.

2. The *safety margin*, *assessment factors* should be high, for instance, expressed as the ratio between the predicted concentration and the concentration that gives undesired effects. This is discussed in Section 8.2, where RQ = PEC/NOEC is applied *after* an *assessment factor* (a safety margin) has been used. The selection of the assessment factor is, as presented in Section 8.2, a question of our knowledge about the effect of the chemical.

3. They require possible inclusion of an effect component, which relates the output concentration to its effect. It is easy to include an effect component in the model; it is, however, often a problem to find a well examined relationship to base it on.

4. Because of points (1) and (2), we need simple models. Our knowledge of process details, parameters, *sublethal effects*, *antagonistic* and *synergistic effects* is limited.

It may be an advantage to outline the approach before developing a toxic substance model according to the procedure presented in Section 2.3:

1. Obtain the best possible knowledge about the processes of the toxic substances in the ecosystem. As far as possible, knowledge about the quantitative role of the processes should be obtained.

2. Attempt to get parameters from the literature and/or from experiment (*in situ* or in the laboratory).

3. Estimate all parameters by the methods presented in Sections 2.9 and 8.5.

4. Compare the results from (2) and (3) and attempt to explain discrepancies.

5. Estimate which processes and state variables it would be feasible and relevant to include in the model. At this stage, if there is the slightest doubt, then include too many processes and state variables rather than too few.

6. Use a sensitivity analysis to evaluate the significance of the individual processes and state variables. This may often lead to further simplification.

To summarize, ecotoxicological models differ in general from ecological models by:

1. being most often more simple,

2. requiring more *parameters*,

3. a wider use of parameter estimation methods,

4. a possible inclusion of an effect component.

Ecotoxicological models may be divided into five classes according to their structure. These five classes also illustrate the possibilities of simplification which is urgently needed as previously discussed.

1. *Food Chain or Food Web Dynamic Models*

This class of model considers the flow of toxic substances through the food chain or food web. Such models will be relatively complex and contain many state variables. They will furthermore contain many parameters, which often have to be estimated by one of the methods presented in Section 8.5. This type of model will typically be

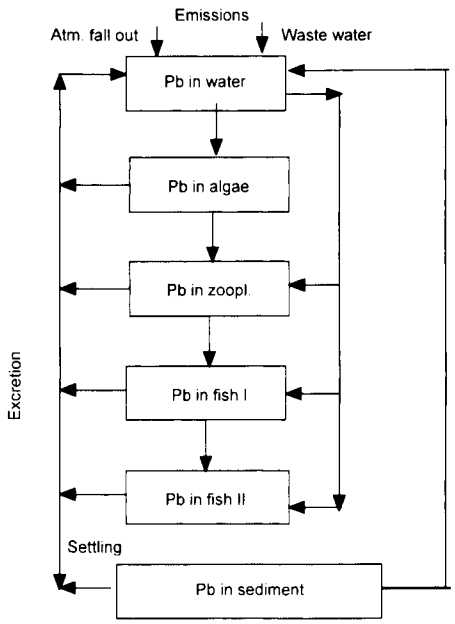

Fig. 8.5. Conceptual diagram of the *bioaccumulation* of lead through a food chain in an aquatic ecosystem.

used when many organisms are affected by the toxic substance, or the entire structure of the ecosystem is threatened by the presence of a toxic substance. Because of the complexity of these models, they have not been used widely. They are similar to the more complex *eutrophication models* that consider the flow of nutrients through the food chain or even through the food web. Sometimes they are even constructed as *submodels* of a *eutrophication model* (see, e.g., Thomann et al., 1974). Figure 8.5 shows a conceptual diagram of an ecotoxicological food chain model for lead. There is a flow of lead from atmospheric fallout and waste water to an aquatic ecosystem, where it is concentrated through the food chain—the so-called 'bioaccumulation'. A simplification is hardly possible for this model type, because it is the aim of the model to describe and quantify the *bioaccumulation through the food chain*.

2. *Static Models* of the Mass Flows of Toxic Substances

If the seasonal changes are minor, or of minor importance, a static model of the mass flows will often be sufficient to describe the situation and even to show the expected changes if the input of toxic substances is reduced or increased. This type of model is based on a mass balance, as can clearly be seen from the example in Fig. 8.6. It will often, but not necessarily, contain more trophic levels, but the modeller is frequently concerned with the flow of the toxic substance through the food chain. The example

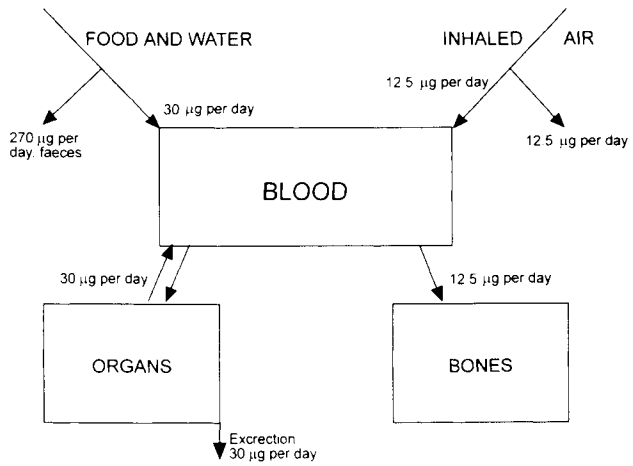

Fig. 8.6. A *static model* of the lead uptake by an average Dane.

in Fig. 8.6 considers only one trophic level, while the example in Section 8.5 shows a much more complex steady-state model of *dioxine* in the Lagoon of Venice. If there are some seasonal changes, this type (which is usually simpler than type one), can still be an advantage to use if, for instance, the modeller is concerned with the worst case or the average case and not with the changes.

3. A Dynamic Model of a Toxic Substance in One Trophic Level

It is often only the toxic substance concentration in one trophic level that is of concern. This includes the zero trophic level, which is understood as the medium—either soil, water or air. Figure 8.7 gives an example: a model of copper contamination in an aquatic ecosystem. The copper concentration in the water is the main concern as it may reach a toxic level for the phytoplankton. Zooplankton and fish are much less sensitive to copper contamination, so an alarm first rings at a

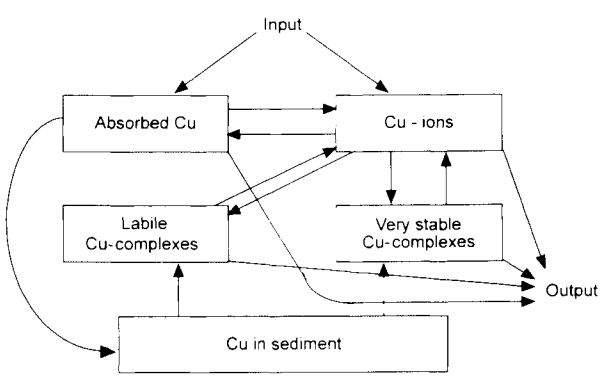

Fig. 8.7. Conceptual diagram of a simple copper-model.

concentration level harmful to phytoplankton. However, only the ionic form is toxic and it is therefore necessary to model the partition of copper in ionic form, complex bound form and adsorbed form. The exchange between copper in the water phase and in the sediment is also included, because the sediment can accumulate relatively large amounts of heavy metals. The amount released from the sediment may be significant under certain circumstances, e.g., under low pH.

Figure 8.8 gives another example. Here the main concern is the *DDT* concentration in fish, where there may be such high concentration of DDT that, according to the *WHO standards*, they are not recommended for human consumption. The model can therefore be simplified by including only the fish and not the entire food chain. Some physical–chemical reactions in the water phase are still of importance and they are included as shown on the conceptual diagram in Fig. 8.8. As can be seen from these examples, simplifications are often feasible when the problem is well defined, including which component is most sensitive to toxic matter and which processes are most important for concentration changes.

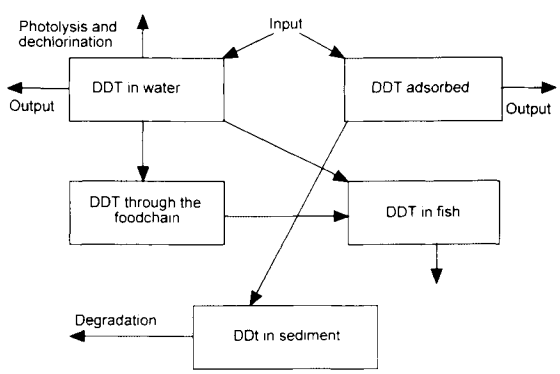

Fig. 8.8. Conceptual diagram of a simple *DDT-model*.

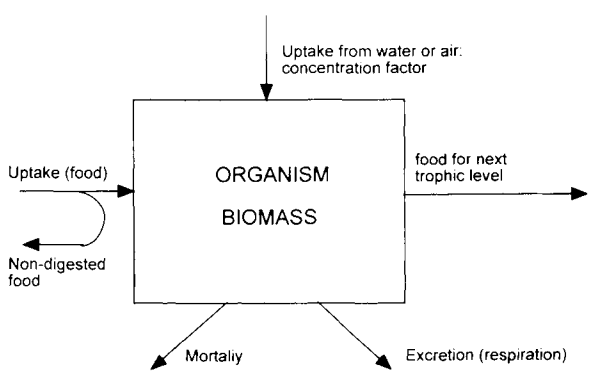

Fig. 8.9. Processes of interest for modelling the concentration of a toxic substance at one *trophic level*.

Figure 8.9 shows the processes of interest for modelling the concentration of a toxic component at one trophic level. The inputs are uptake from the medium (water or air) and from digested food = total food – non-digested food. The outputs are mortality (transfer to detritus), excretion and *predation* from the next level in the food chain.

4. Ecotoxicological Models in *Population Dynamics*

Population models are *biodemographic models* and therefore have numbers of individuals or species as state variables. The simple population models consider only one population. The growth of the population is a result of the difference between natality and mortality:

$$dN/dt = B * N - M * N = r * N \tag{8.1}$$

where N is the number of individuals, B is the *natality* (i.e., the number of new individuals per unit of time and per unit of population), M is the *mortality* (i.e., the number of organisms that die per unit of time and per unit of population), and r is the increase in the number of organisms per unit of time and per unit of population, and is equal to $B - M$. B, N and r are not necessarily constants as in the exponential growth equation, but are dependent on N, the *carrying capacity* and other factors. The concentration of a toxic substance in the environment or in the organisms may influence natality and mortality, and if the relationship between a toxic substance concentration and these population dynamic parameters is included in the model, it becomes an ecotoxicological model of population dynamics.

Population dynamic models may include two or more trophic levels and ecotoxicological models will include the influence of the toxic substance concentration on *natality*, *mortality* and interactions between these populations. In other words, an ecotoxicological model of population dynamics is a general model of population dynamics with the inclusion of relations between toxic substance concentrations and some important model parameters.

5. Ecotoxicological Models with *Effect Components*

Although Class 4 models may already include relations between concentrations of toxic substances and their effects, these are limited to, for instance, population dynamic parameters, not to a final assessment of the overall effect. In comparison, Class 5 models include more comprehensive relations between toxic substance concentrations and effects. These models may include not only lethal and/or *sublethal effects* but also effects on biochemical reactions or on the enzyme system. The effects may be considered at various levels of the biological hierarchy from the cells to the ecosystems.

In many problems it may be necessary to go into more detail about the effect in order to answer the following relevant questions:

1. Does the toxic substance accumulate in the organism?
2. What will be the long-term concentration in the organism when uptake rate, excretion rate and biochemical *decomposition rate* are considered?
3. What is the *chronic effect* of this concentration?
4. Does the toxic substance accumulate in one or more organs?
5. What is the transfer between various parts of the organism?
6. Will *decomposition* products eventually cause *additional effects*?

Detailed answers to these questions may require a model of the processes taking place in the organism, and a translation of the concentrations in various parts of the organism into effects. This implies, of course, that the intake = (uptake by the organism) * (efficiency of uptake) is known. Intake may either be from water or air, which may also be expressed (at steady state) by concentration factors, which are the ratios between the concentration in the organism and in the air or water.

However, if all the processes mentioned above were to be taken into consideration for just a few organisms, the model would easily become too complex, contain too many parameters to calibrate, and require more detailed knowledge than it is possible to provide. Because toxicology and ecotoxicology are still in their infancy, we often do not even have all the relationships needed for a detailed model. Therefore, most models in this class will not consider too many details of the partition of the toxic substances in organisms and their corresponding effects, but rather be limited to the simple accumulation in the organisms and their effects. Usually, accumulation is rather easy to model and the following simple equation is often sufficiently accurate:

$$dC/dt = (ef * Cf * F + em * Cm * V)/W - Ex * C = (INT)/W - Ex * C \qquad (8.2)$$

where C is the concentration of the toxic substance in the organism; *ef* and *em* are the efficiencies for the *uptake* from the food and medium, respectively (water or air), Cf and Cm are the concentration of the toxic substance in the food and medium, respectively; F is the amount of food uptake per day; V is the volume of water or air taken up per day; W is the body weight either as dry or wet matter; and Ex is the *excretion coefficient* (1/day). As can be seen from the equation, INT covers the total intake of toxic substance per day.

This equation has a numerical solution, and the corresponding plot is shown in Fig. 8.10:

$$C/C(\max) = (INT * (1 - \exp(Ex * t)))/(W * Ex) \qquad (8.3)$$

where $C(\max)$ is the steady-state value of C:

$$C(\max) = INT/(W * Ex) \qquad (8.4)$$

Synergistic and *antagonistic effects* have not been touched on so far. They are rarely considered in this type of model for the simple reason that we do not know much

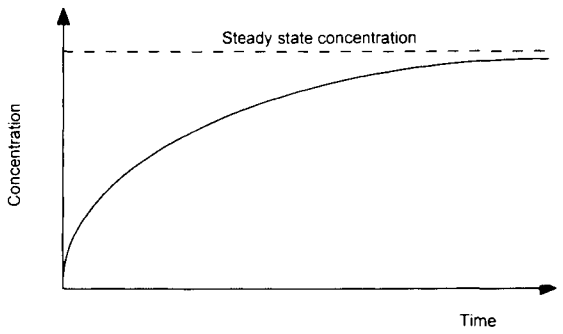

Fig. 8.10. Concentration of a toxic substance in an organism versus time.

about these effects. If we have to model combined effects of two or more toxic substances, we can only assume additive effects, unless we can provide empirical relationships for the combined effect.

In principle, a complete solution of an ecotoxicological problem requires four (sub)models, of which the fate model may be considered to be the first model in the chain (see Fig. 8.11). As can be seen from the figure, the four components are (see Morgan, 1984):

1. A fate or exposure model which, as already stressed, should be as simple as possible and only as complex as necessary.

2. An effect model, translating the concentration into an effect; see type 5 above and the different levels of effects presented in Section 8.1.

3. A model for *human perception* processes.

4. A model for *human evaluation* processes.

The first two submodels are in principle "objective", predictive models, corresponding to the structural model types (1)–(5) described above, or the classes described from an application point of view, described in Section 8.1. They are based on physical, chemical and biological processes. They are very similar to other environmental models and founded upon mass transfer, mass balances, physical, chemical and biological processes.

Submodels (3) and (4) are different from the generally applied environmental management models and are only touched on briefly below. A risk assessment component, associated with the fate model, comprises human perception and evaluation processes (see Fig. 8.11). These submodels are explicitly value-laden, but must of course build on objective information concerning concentrations and effects. They are often considered in the ERA-procedure by decision on the assessment factor.

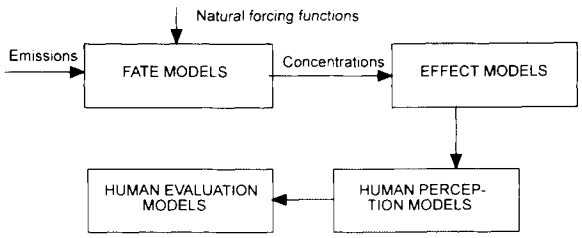

Fig. 8.11. The four submodels of a total ecotoxicological model.

Factors that may be important to consider in this context are:

1. Magnitude and *time constant* of *exposure*.
2. Spatial and temporal distribution of concentration.
3. Environmental conditions determining the process rates and effects.
4. Translation of concentrations into magnitude and duration of effects.
5. *Spatial* and *temporal distribution* of effects.
6. *Reversibility* of effects.

The uncertainties relating to the information on which the model is based and the uncertainties related to the development of the model, are crucial in risk assessment. In addition to the discussion of the assessment factor where the focus in Section 8.2 and partly in Section 8.3 was on the effects on the *trophic levels*, the uncertainty of risk assessment may be described by the following five categories:

1. Good direct knowledge of and statistical evidence for the important components (state variables, processes and interrelations of the variables) of the model is available.
2. Good knowledge of and statistical evidence for the important *submodels* are available, but the aggregation of the submodels is less certain.
3. No good knowledge of the model components for the considered system is available, but good data are available for the same processes from a similar system and it is estimated that these data may be applied directly or with minor modifications to the model development.
4. Some, but insufficient, knowledge is available from other systems. Attempts are made to use these data without the necessary transferability. Attempts are made to eliminate gaps in knowledge by the use of additional experimental data as far as possible within the limited resources available for the project.
5. The model is, to a large extent or at least partly, based on the subjective judgment of experts.

Acknowledgement of uncertainty is of great importance and may be taken into consideration, either qualitatively or quantitatively. Another problem is: where to take the uncertainty into account? Should the economy or the environment benefit from the uncertainty? The *ERA* procedure presented in Section 8.2 has definitely facilitated the possibility of considering the environment more than the economy.

Until 10–15 years ago, researchers had developed very little understanding of the processes by which people actually perceive the exposures and effects of toxic chemicals, but these processes are just as important for risk assessment as the exposures and effects processes themselves. The characteristics of risk and effect are of importance for the perceptions of people. These characteristics may be summarized in the following:

- **Characteristics of risk:**

  Voluntary or involuntary?
  Are the levels known to the people exposed or to science?
  Is it novel, or old and familiar?
  Is it common or dreaded (for instance does it involve cancer)?
  Does it involve death?
  Are mishaps controllable?
  Are future generations threatened?
  Global, regional or local?
  Function of time? How (e.g., increasing or decreasing)?
  Can it easily be reduced?

- **Characteristics of effects:**

  Immediate or delayed?
  On many or a few people?
  Global, regional or local?
  Involve death?
  Are effects of mishaps controllable?
  Observable immediately?
  How are they function of time?

A factor analysis was performed by Slovic et al. (1982) which shows, among other results, an unsurprising correlation between *people's perception* of dreaded and unknown risks. Broadly speaking, there are two methods of selecting the risks we will deal with.

The first may be described as the *'rational actor model'*, involving people who look systematically at all the risks they face and make choices about which they will live with and at what levels. For decision making this approach would use some single, consistent, objective functions and a set of decision rules.

The second method may be called the *'political/cultural model'*. This involves interactions between culture, social institutions and political processes for the identification of risks and determination of those that people will live with and at what level.

Both methods are unrealistic as they are both completely impractical in their pure form. Therefore we must select a strategy for risk abatement founded on a workable alternative based on the philosophy behind both methods.

Several risk management systems are available, but no attempt will be made here to evaluate them. However, some recommendations should be given for the development of risk management systems:

1. Consider as many of the characteristics listed above as possible and include the human perceptions of these characteristics in the model.
2. Do not focus too narrowly on certain types of risk. This may lead to *suboptimal solutions*. Attempt to approach the problem as broadly as possible.
3. Choose strategies that are pluralistic and adaptive.
4. Benefit–cost analysis is an important element of the risk management model, but it is far from being the only important element and the uncertainty in evaluation of benefit and cost should not be forgotten. The variant of this analysis applicable to environmental risk management may be formulated as follows:

$$\text{net } \textit{social benefit} = \text{social benefits of the project} - \text{"environmental" costs of the project} \tag{8.5}$$

5. Use multi-attribute utility functions, but remember that in general people have trouble thinking about more than two or three (four at the most) attributes in each outcome.

The application of the estimation methods presented in Section 8.5 renders it feasible to construct ecotoxicolgical models, even if our knowledge of the parameters is limited. The estimation methods obviously have a high uncertainty, but a great safety factor (assessment factor) helps in accepting this uncertainty. On the other hand, our knowledge about the effects of toxic substances is very limited—particularly at the ecosystem, organism and organ levels. It must not be expected, therefore, that models with effect components will give more than a first rough picture of what is known today in this area.

8.4 An Overview: The Application of Models in Ecotoxicology

Some toxic substance models are reviewed in Table 8.2 to give an impression of the types of model available today. Most models reflect the proposition that good knowledge of the problem and ecosystem can be used to make reasonable simplifications. Model characteristics shown in the table are state variables and/or processes considered in the model. The model class is according to the classification 1 to 5

Table 8.2. Examples of toxic substance models

Toxic substance (Model class)	Model characteristics	Reference
Cadmium (1)	Food chain similar to a eutrophication model	Thomann et al. (1974)
Mercury (6)	6 state variables: water, sediment, suspended matter, invertebrates, plant and fish	Miller (1979)
Vinyl chloride (3)	Chemical processes in water	Gillett et al. (1974)
Methyl parathion (1)	Chemical processes in water and benzothiophenemicrobial degradation, adsorption, 2-4 trophic levels	Lassiter (1978)
Methyl mercury (4)	A single trophic level: food intake, excretion, metabolism growth	Fagerstrøm & Aasell (1973)
Heavy metals (3)	Concentration factor, excretion, bioaccumulation	Aoyama et al. (1978)
Pesticides in fish DDT & methoxychlor (5)	Ingestion, concentration factor, adsorption on body, defecation, excretion, chemical decomposition, natural mortality	Leung (1978)
Zinc in algae (3)	Concentration factor, secretion hydrodynamical distribution	Seip (1978)
Copper in sea (5)	Complex formation, adsorption sublethal effect of ionic copper	Orlob et al. (1980)
Radionuclides in sediment (3)	Photoplysis, hydrolysis, oxidation, biolysis, volatilization and resuspension	Onishi & Wise (1982)
Metals (2)	A thermodynamic equilibrium model	Felmy et al. (1984)
Sulphur deposition (3)	Box model to calculate deposition of sulphur	McMahon et al. (1976)
Radionuclides (3)	Distribution of radionuclides from a nuclear accident release	ApSimon et al. (1980)
Sulphur transport (3)	Long-range transmission of sulphur pollutants. Use of pseudospectral model	Prahm and Christensen (1976)
Lead (5)	Hydrodynamics, precipitation, toxic effects of free ionic lead on algae, invertebrates and fish	Lam and Simons (1976)
Radionuclides (3)	Hydrodynamics, decay, uptake and release by various aquatic surfaces	Gromiec & Gloyna (1973)
Radionuclides (2)	Radionuclides in grass, grains, vegetables, milks, eggs, beef and poultry are state var.	Kirschner & Whicker (1984)
SO_2, NO_x and heavy metals (5)	Threshold model for accumulation effect of on sprucefir pollutants. Air and soil in forests	Kohlmaier et al. (1984)
Toxic environmental chemicals (5)	Hazard ranking and assessment from physico-chemical data and a limited number of laboratory tests	Bro-Rasmussen & Christiansen (1984)
Heavy metals (3)	Adsorption, chemical reactions, ion exchange	Several authors
Polycyclic aromatic hydrocarbons (3)	Transport, degradation, bioaccumulation	Bartell et al. (1984)
Persistent toxic organic substances (3)	Groundwater movement, transport and accumulation of pollutants in groundwater	Uchrin (1984)
Cadmium, PCB (2)	Hydraulic overflow rate (settling), sediment interactions, steady-state food chain submodel	Thomann (1984)

continued

Table 8.2 (*continuation*)

Toxic substance (Model class)	Model characteristics	Reference
Hydrophobic organics (3)	Gas exchange, sorption/desorption, hydrolysis compounds, photolysis, hydrodynamics	Schwarzenbach & Imboden (1984)
Mirex (3)	Water–sediment exchange processes, adsorption, volatilization, bioaccumulation	Halfon (1984)
Toxins (aromatic hydrocarbons, Cd) (3)	Hydrodynamics, deposition, resuspension, volatilization, photooxidation, decomposition, adsorption, complex formation (humic acid)	Harris et al. (1984)
Heavy metals (2)	Hydraulic submodel, adsorption	Nyholm et al. (1984)
Oil slicks (3)	Transport and spreading, influence of surface tension, gravity and weathering processes	Nihoul (1984)
Acid rain (soil) (3)	Aerodynamic, deposition	Kauppi et al. (1984)
Acid rain (3)	C, N and S cycles and their influence on acidity	Arp (1983)
Persistent organic chemicals (5)	Fate, exposure and human uptake	Mackay (1991)
Chemicals, general (5)	Fate, exposure, ecotoxicity for surface water and soil	Matthies et al. (1987)
Toxicants, general (4)	Effect on populations of toxicants	de Luna & Hallam (1987)
Chemical hazard (5)	Basin-wide ecological fate	Morioka & Chikami (1986)
Pesticides (4)	Effects on insect populations	Schaalje et al. (1989)
Insecticides (2)	Resistance	Longstaff (1988)
Mirex and Lindane (6)	Fate in Lake Ontario	Halfon (1986)
Pesticides (3)	Degradation in soil	Liu et al. (1988)
Pesticides (3)	Degradation in soil	Liu et al. (1988)
Pesticides (3)	Leaching to groundwater	Carsel et al. (1985)
Acid rain (5)	Effects on forest soils	Kauppi et al. (1986)
Acid rain (5)	Cation depletion of soil	Jørgensen et al. (1995a)
pH, Calcium and Aluminium (4)	Survival of fish populations	Breck et al. (1988)
Photochemical smog (5)	Fate and risk	Wratt et al. (1992)
Nitrate (3)	Leaching to groundwater	Wuttke et al. (1991)
Oil spill (5)	Fate	Jørgensen et al. (1995)
Toxicants (4)	Effects on populations	Gard (1990)
Chromium (2)	Distribution and accumulation in mussels	Mogensen & Jørgensen (1979)
Pesticides (3)	Loss rates	Jørgensen et al. (1995)
TCDD (3)	Photodegradation	Jørgensen et al. (1995)
Toxicants (4)	Effects general on populations	Gard (1990)
Pesticides and Surfactants (3)	Fate in rice fields	Jørgensen et al. (1997b)
Toxicants (3)	Migration of dissolved toxicants	Monte (1998)
Growth promoters (3)	Fate, agriculture	Jørgensen et al. (1998)
Toxicity (3)	Effect on eutrophication	Legovic (1997)
Pesticides (3)	Mineralization	Fomsgaard et al. (1997)
Mecoprop (3)	Mineralization in soil	Fomsgaard et al. (1999)

given above and is indicated in the table in brackets after the toxic substance. There are only five Type 4 models included in the table. Ecological modelling has been approached from two sides: population dynamics and biogeochemical flow analysis. As the second approach has been most in focus in environmental management, it is natural also to approach the toxic substance problems from this angle. The few Class 4 models are population dynamic models, with a few additional equations to account for the influence of toxic substances on *natality* and *mortality*. If these relations are available, it should be fairly easy to construct this type of model.

The most difficult part of modelling the effect and distribution of toxic substances is to obtain the relevant knowledge about the behaviour of toxic substances in the environment, and to use this knowledge to make the feasible simplifications. It gives the modeller of ecotoxicological problems the particular challenge of selecting the right, balanced complexity, and there are many examples of quite simple ecotoxicological models which can solve the focal problem.

It can be seen from the overview in Table 8.2 that most ecotoxicological models have been developed during the last decade. Before around 1975, toxic substances were hardly associated with environmental modelling at all, as the problems seemed to be straightforward. The many pollution problems associated with toxic substances could easily be solved simply by eliminating the source of the toxic substance. During the 1970s, it was acknowledged that the environmental problems associated with toxic substances were very complex because of the interaction of many sources and many simultaneously, interacting processes and components. Several accidental releases of toxic substances into the environment reinforced the need for models. The result has been that several ecotoxicological models have been developed in the period from the 1970s until today. Although Table 8.2 gives a comprehensive survey of the ecotoxicological models available, this list should not be considered to be complete or even almost complete as the table is not a result of a thorough literature review. The aim of the table is to give an idea of the spectrum of available models, to demonstrate that all five types of model have been developed and to help the reader to find a reference to a specific problem of modelling toxic substances.

8.5 Estimation of Ecotoxicological Parameters

Slightly more than 100,000 chemicals are produced in such an amount that they threaten or may threaten the environment. They cover a wide range of applications: household chemicals, detergents, cosmetics, medicines, dye stuffs, pesticides, intermediate chemicals, auxiliary chemicals in other industries, additives to a wide range of products, chemicals for water treatment and so on. They are (almost) indispensable in modern society and all fulfil more or less essential needs in the industrialized world, which has increased the production of chemicals about 40-fold during the last four decades. A proportion of these chemicals inevitably reaches the environment either during their production, their transportation from industry to end user, or

during their application. In addition, the production or use of chemicals may cause more or less unforeseen waste or by-products, e.g., *chloro-compounds* from the use of chlorine for *disinfection*. As we would like to have the benefits of using the chemicals but cannot accept the harm they may cause, this conflict raises several urgent questions which we have already discussed. These questions cannot be answered without models, and we cannot develop models without knowing the most important *parameters*, at least within some ranges. OECD has compiled a review of the properties that we should know for all chemicals. We need to know the *boiling point and melting point* in order to know in which form (solid, liquid or gas) the chemical will be found in the environment. We must know the distribution of the chemicals in the five spheres: hydrosphere, atmosphere, lithosphere, biosphere and *technosphere*. This will require knowledge about their *solubility* in water, the *partition coefficient* water/lipids, *Henry's constant*, the *vapour pressure*, the *rate of degradation* by *hydrolysis*, *photolysis*, chemical oxidation and microbiological processes and the *adsorption* equilibrium between water and soil—all as a function of the temperature. We need to discover the interactions between living organisms and the chemicals, which implies that we should know the biological concentration factor (*BCF*), the magnification through the food chain, the uptake rate and the excretion rate by the organisms and where in the organisms the chemicals will be concentrated, not only for one organism but for a wide range of organisms. We must also know the effects on a wide range of different organisms. This means that we should be able to find the LC_{50} and LD_{50} values, the *MAC* and *NEC* values (for the abbreviations and the definitions used see Appendix 2), the relationship between the various possible *sublethal effects* and concentrations, the influence of the chemical on fecundity and the *carcinogenic* and *teratogenic properties*. We should also know the effect on the ecosystem level: how the chemicals affect populations and their development and interactions, i.e., the entire network of the ecosystem.

Table 8.3 gives an overview of the most relevant physical–chemical properties of organic compounds and their interpretation with respect to the behaviour in the environment, which should be reflected in the model.

Among other inputs, however, *ERA*s also require information about the properties of the chemicals and their interactions with living organisms. It is maybe not necessary to know the properties to the very high degree of accuracy that can be provided by measurements in a laboratory, but it would be beneficial to know the properties with sufficient accuracy to make it possible to utilize the models for management and for risk assessments. Therefore estimation methods have been developed as an urgently needed alternative to measurements. To a great extent, they are based on the structure of the chemical compounds, the so-called *QSAR* and *SAR methods*, but it may also be possible to use allometric principles to transfer rates of interaction processes and concentration factors between a chemical and one or a few organisms to other organisms. This chapter focuses on these methods and attempts to give a brief overview of how these methods can be applied and what approximate accuracy they can offer. A more detailed overview of the methods can be found in Jørgensen et al. (1997a).

Table 8.3. Overview of the most relevant *environmental properties* of organic compounds and their interpretation

Property	Interpretation
Water solubility	High water solubility corresponds to high mobility
K_{ow}	High K_{ow} means that the compound is lipophilic. This implies that it has a high tendency to *bioaccumulate* and be sorbed to soil sludge and sediment. BCF and K_{oc} are correlated with K_{ow}.
Biodegradability	This is a measure of how fast the compound is decomposed to simpler molecules. A high biodegradation rate implies that the compound will not accumulate in the environment, while a low biodegradation rate may create environmental problems related to the increasing concentration in the environment and the possibilities of a synergistic effect with other compounds.
Volatilization, vapour	High rate of volatilization (high vapour pressure) implies that the pressure compound will cause an air pollution problem
Henry's constant (*He*)	H determines the distribution between the atmosphere and the hydrosphere. See also Chapter 3
pK	If the compound is an acid or a base, pH determines whether the acid or the corresponding base is present. As the two forms have different properties, pH becomes important for the properties of the compounds.

It may be interesting here to discuss the obvious question: why is it sufficient to estimate a property of a chemical in an ecotoxicological context with 20%, or sometimes with 50% or higher, uncertainty? Ecotoxicological assessment usually gives an uncertainty of the same order of magnitude, which means that the indicated uncertainty may be sufficient from a modelling viewpoint, but can results with such an uncertainty be used at all? The answer in most cases is "yes", because in most cases we want to ensure that we are far from a harmful or very harmful level. We use a safety factor of 10–1000 (most often 50–100) (see also Section 8.2 on risk assessment). When we are concerned with very harmful effects such as, e.g., the complete collapse of an ecosystem or a health risk for a large human population, we will inevitably select a very high *safety factor*. In addition, our lack of knowledge about synergistic effects and the presence of many compounds in the environment at the same time force us to apply a very high safety factor. In such a context we will usually go for a concentration in the environment which is magnitudes lower than corresponding to a slightly harmful effect or considerably lower than the *NEC*. This is analogous to civil engineers constructing bridges. They make very sophisticated calculations (develop models), that account for wind, snow, temperature changes and so on and afterwards they multiply the results by a safety factor of 2–3 to ensure that the bridge will not collapse. They use safety factors because the consequences of a bridge collapse are unacceptable.

The collapse of an ecosystem or a health risk to a large human population is also completely unacceptable, so we should use safety factors in ecotoxicological modelling to account for the uncertainty. Due to the complexity of the system, the simultaneous presence of many compounds and our present knowledge—or rather

lack of knowledge—we should use a safety factor of 10–100 or even sometimes 1000. If we use safety factors that are too high, the risk is only that the environment will be less contaminated at possibly a higher cost. Besides there are no alternatives to the use of safety factors. We can increase our ecotoxicological knowledge step by step, but it will take decades before it may be reflected in considerably lower safety factors. A measuring program of all processes and components is an impossibility due to the high complexity of the ecosystems. Of course, this does not imply that we should not use the information on measured properties available today. Measured data will almost always be more accurate than estimated data. Furthermore, the use of measured data within the network of estimation methods will improve the accuracy of estimation methods. Fortunately, several handbooks on ecotoxicological parameters are available; references to the most important were given in Section 8.2. Estimation methods for the physical–chemical properties of chemical compounds were already applied 40–60 years ago as they were urgently needed in chemical engineering. They are to a great extent based on contributions to a focal property by molecular groups and the molecular weight: the boiling point, the melting point and the vapour pressure as function of the temperature are examples of properties that were frequently estimated in chemical engineering by these methods. In addition, a number of auxiliary properties results from these estimation methods, such as the critical data and the molecular volume. These properties may not have a direct application as ecotoxicological parameters in environmental risk assessment, but are used as intermediate parameters which may be used as a basis for the estimation of other parameters.

The *water solubility*, the *partition coefficient* octanol–water, K_{ow}, and *Henry's constant* are crucial *parameters* in our network of estimation methods, because many other parameters are well correlated with these two parameters. The three properties can fortunately be found for a number of compounds, or be estimated with reasonably high accuracy using knowledge of the chemical structure, i.e., the number of various elements, the number of rings and the number of functional groups. In addition, there is a good relationship between water solubility and K_{ow} (see Fig. 8.12). Particularly in the last decade many good estimation methods for these three core properties have been developed.

During the last couple of decades several correlation equations have been developed based on a relationship between the water solubility, K_{ow} or Henry's constant on the one hand, and physical, chemical, biological and ecotoxicological parameters for chemical compounds on the other. The most important of these parameters are: the adsorption isotherms soil–water, the rate of the chemical degradation processes (*hydrolysis*, *photolysis* and *chemical oxidation*), the biological concentration factor (*BCF*), the ecological magnification factor (EMF), the uptake rate, excretion rate and a number of ecotoxicological parameters. Both the ratio of concentrations in the sorbed phase and in water at equilibrium, K_a, and BCF may often be estimated with a relatively good accuracy from expressions like K_a, K_{oc} or $BCF = a \log K_{ow} + b$. K_{oc} is the ratio between the concentration in soil consisting of 100% organic carbon and in water at equilibrium between the two phases.

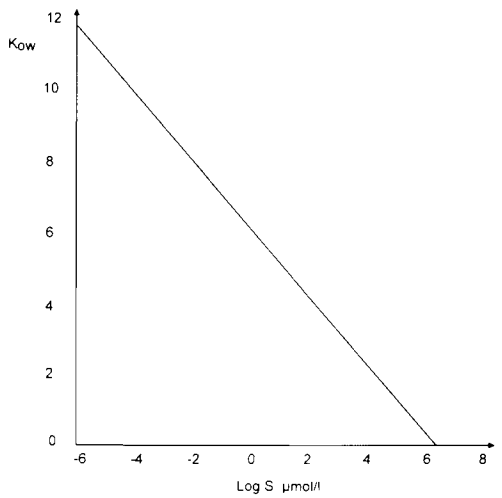

Fig. 8.12. Relationship between water *solubility* (µmol l) and octanol–water *distribution coefficient*.

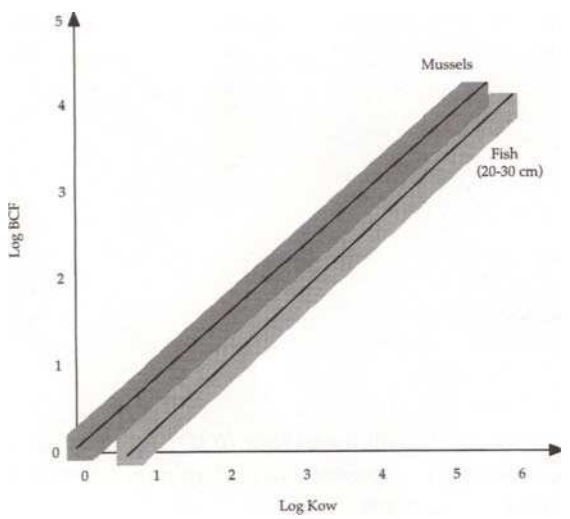

Fig. 8.13. Two applicable relationships for the octanol-water distribution coefficient and the biological concentration factor for fish and mussels.

Numerous expressions with different a and b values have been published (see Jørgensen et al., 1991; Jørgensen, 1994). Some of these relationships are shown in Table 8.4 and Fig. 8.13.

The biodegradation in waste treatment plants is often of particular interest, in which case the *%ThOD* may be used. It is defined as the 5-day BOD as a percentage of the theoretical *BOD*. It may also be indicated as the BOD_5-fraction. For instance,

Table 8.4. Regression equations for estimation of *concentration*, *bioconcentration* and *ecological magnification factors*

Indicator	Relationship	Correlation coefficient	Range (Indicator)
K_{ow}	$\log CF = -0.973 + 0.767 \log K_{ow}$	0.76	2.0×10^{-2}–2.0×10^{6}
K_{ow}	$\log CF = 0.7504 + 1.1587 \log K_{ow}$	0.98	7.0–1.6×10^{4}
K_{ow}	$\log CF = 0.7285 + 0.6335 \log K_{ow}$	0.79	1.6–1.4×10^{4}
K_{ow}	$\log CF = 0.124 + 0.542 \log K_{ow}$	0.95	4.4–4.2×10^{7}
K_{ow}	$\log CF = -1.495 + 0.935 \log K_{ow}$	0.87	1.6–3.7×10^{6}
K_{ow}	$\log CF = -0.70 + 0.85 \log K_{ow}$	0.95	1.0–1.0×10^{7}
K_{ow}	$\log CF = 0.124 + 0.542 \log K_{ow}$	0.90	1.0–5.0×10^{7}
S (µg/l)	$\log BCF = 3.9950 - 0.3891 \log S$	0.92	1.2–3.7×10^{7}
S (µg/l)	$\log BCF = 4.4806 - 0.4732 \log S$	0.97	1.3–4.0×10^{7}
S (µmol/l)	$\log BCF = 3.41 - 0.508 \log S$	0.96	2.0×10^{-2}–5.0×10^{3}

Table 8.4. (*Continued*)

Animal	Number of chemicals	References
Fish species	36	Kenaga and Goring (1978)
Mosquito fish	9	Metcalf et al. (1975)
Mosquito fish	11	Lu and Metcalf (1975)
Trout	8	Neely et al. (1974)
Fish species	26	Kenaga and Goring (1978)
Fathead minnow	59	Veith et al. (1979)
Fathead minnow, bluegill	59	Lassiter (1975)
Fish species	13	Kenaga and Goring (1978)
Fish species	50	Kenaga and Goring (1978)
Mosquito fish	9	Metcalf et al. (1975)
Fish species	36	Kenaga and Goring (1978)
Mosquito fish, whole	15	Lu and Metcalf (1975)

a BOD_5-fraction of 0.7 will mean that BOD_5 corresponds to 70% of the theoretical BOD. It is, however, also possible to find an indication of BOD_5 percentage removal in an activated sludge plant.

The biodegradation is, however, in some cases very dependent on the concentration of microorganisms (see also the discussion of biodegradation in Chapter 3). Therefore it may be beneficial to indicate it as *rate coefficient* relative to the biomass of the active microorganisms in the unit mg/(g dry wt 24 h), which in many cases will be more informative and correct.

In the microbiological decomposition of *xenobiotic compounds* an acclimatization period from a few days to 1–2 months should be foreseen before the optimum biodegradation rate can be achieved. We distinguish between primary and ultimate biodegradation. Primary, biodegradation is any biologically induced transformation which changes the molecular integrity. Ultimate biodegradation is the biologically

mediated conversion of an organic compounds to inorganic compounds and products associated with complete and normal metabolic decomposition.

The biodegradation rate is expressed by a wide range of units:

1. as a first-order rate constant (1/24 h)
2. as *half life time* (days or hours)
3. mg per g sludge per 24 h (mg/(g 24 h))
4. mg per g bacteria per 24 h (mg/(g 24 h))
5. ml of substrate per bacterial cell per 24 h (ml/(24 h cells))
6. mg *COD* per g biomass per 24 h (mg/(g 24 h))
7. ml of substrate per gram of volatile solids inclusive microorganisms (ml/(g 24 h))
8. BOD_x/BOD_8, i.e., the biological oxygen demand in x days compared with complete degradation (–), called the *BOD_x-coefficient*.
9. BOD_x/COD, i.e., the biological oxygen demand in x days compared with complete degradation, expressed by means of COD (–)

The *biodegradation rate* in water or soil is difficult to estimate because the number of microorganisms varies by several orders of magnitudes from one type of aquatic ecosystem to the next and from one type of soil to the next.

Artificial intelligence has been used as a promising tool to estimate this important parameter. However, a (very) rough, first estimation can be made on the basis of molecular structure and biodegradability. The following rules can be used to set up these estimations:

1. Polymer compounds are generally less biodegradable than monomer compounds. 1 point for a molecular weight > 500 and ≤ 1000, 2 points for a molecular weight > 1000.
2. Aliphatic compounds are more biodegradable than aromatic compounds. 1 point for each aromatic ring.
3. Substitutions, especially with halogens and nitro groups, will decrease the biodegradability. 0.5 points for each substitution, although 1 point if it is a halogen or a nitro group.
4. Introduction of double or triple bond will generally mean an increase in the biodegradability (double bonds in aromatic rings are of course not included in this rule). 1 point for each double or triple bond.
5. Oxygen and nitrogen bridges (–O– and –N– (or =)) in a molecule will decrease the biodegradability. 1 point for each oxygen or nitrogen bridge.
6. Branches (secondary or tertiary compounds) are generally less biodegradable than the corresponding primary compounds. 0.5 point for each branch.

Find the number of points and use the following classification:

- ≤ 1.5 points: the compound is readily biodegraded. More than 90% will be biodegraded in a biological treatment plant.
- 2.0–3.0 points: the compound is biodegradable. Probably about 10–90% will be removed in a biological treatment plant. BOD_5 is 0.1–0.9 of the theoretical oxygen demand.
- 3.5–4.5 points: the compound is slowly biodegradable. Less than 10% will be removed in a biological treatment plant. $BOD_{10} \leq 0.1$ of the *theoretical oxygen demand.*
- 5.0–5.5 points: the compound is very slowly biodegradable. It will hardly be removed in a biological treatment plant and a 90% *biodegradation* in water or soil will take ≥ 6 months.
- ≥ 6.0 points: the compound is refractory. The *half life time* in soil or water is counted in years.

Several useful methods for estimating biological properties are based upon the similarity of chemical structures. The idea is that if we know the properties of one compound, it may be used to find the properties of similar compounds. For example, if we know the properties of phenol, which is called the parent compound, it may be used to give more accurate estimation of the properties of monochloro-phenol, dichloro-phenol, trichloro-phenol and so on and for the corresponding cresol compounds. Estimation approaches based on chemical similarity generally give more accurate estimation, but are also more cumbersome to apply, as they cannot be used generally in the sense that each estimation has a different starting point, namely the compound (the parent compound) with known properties.

Allometric estimation methods presume (Peters, 1983) that there is a relationship between the value of a biological parameter and the size of a considered organism. These estimation methods were presented in Section 2.9, as they are closely related to the energy balances of organisms. The toxicological parameters, LC_{50}, LD_{50}, MAC, EC and NEC can be estimated from a wide spectrum of physical and chemical parameters, although these estimation equations generally are more inaccurate than the estimation methods for physical, chemical and biological parameters. Both molecular connectivity and chemical similarity usually offer better accuracy for estimating toxicological parameters.

The various estimation methods can be classified into two groups:

A. General estimation methods based on an equation of general validity for all types of compounds, although some of the constants may be dependent on the type of chemical compound or may be calculated by adding contributions (increments) based on chemical groups and bonds.

B. Estimation methods valid for a specific class of chemical compounds, e.g., aromatic amines, phenols, aliphatic hydrocarbons, and so on. The property of at

least one key compound is known. Based on the structural differences between the key compounds and all other compounds of the considered type (e.g., two chlorine atoms have substituted hydrogen in phenol to get 2,3-dichloro-phenol) and the correlation between the structural differences and the differences in the considered property, the properties for all compounds of the considered class can be found. These methods are therefore based on chemical similarity.

Methods of Class B are generally more accurate than methods of Class A, but they are more cumbersome to use as for each type of chemical, it is necessary to find the right correlation for each property. Furthermore, the properties required should be known for at least one key component which may be difficult when a series of properties are needed. If estimation of the properties for a series of compounds belonging to the same chemical class is required, it is tempting to use a suitable collection of Class B methods.

Methods belonging to Class A form a network which facilitates the possibility of linking the estimation methods together in a computer software system such as WINTOX (Jørgensen et al., 1997). The software is easy to use and can rapidly provide estimations. Each relationship between two properties is based on the average result obtained from a number of different equations found in the literature. However, there is a price to pay for using such "easy to go" software. The accuracy of the estimations is not as good as with the more sophisticated methods based on similarity of chemical structure, but in many contexts, particularly modelling, the results found by *WINTOX* can offer sufficient accuracy. In addition, it is always useful to obtain a first intermediate guess.

The software also makes it possible to start the estimations from the properties of the chemical compound already known. The accuracy of the estimation obtained from using the software can be improved considerably by knowing a few key parameters, e.g., the boiling point and Henry's constant. As it is possible to get software which is able to estimate *Henry's constant* and K_{ow} with generally higher accuracy than WINTOX, a combination of separate estimations of these two parameters prior to the use of WINTOX can be recommended. Another possibility would be to estimate a couple of key properties using chemical similarity methods and then use these estimations as known values in WINTOX. These methods for improving the accuracy will be discussed in the next section. The network of WINTOX as an example of these estimation networks is illustrated in Fig. 8.14. As it is a network of Class A methods, it should not be expected that the accuracy of the estimations would be as high as it is possible to obtain by the more specific Class B methods. With WINTOX it is, however, possible to estimate the most pertinent properties directly and relatively from the structural formula.

WINTOX is based on average values of results obtained by the simultaneous use of several estimation methods for most of the parameters. This implies increased accuracy of the estimation, mainly because it gives a reasonable accuracy for a wider range of compounds. If several methods are used in parallel, a simple average of the parallel results have been used in some cases, while a weighted average is used in

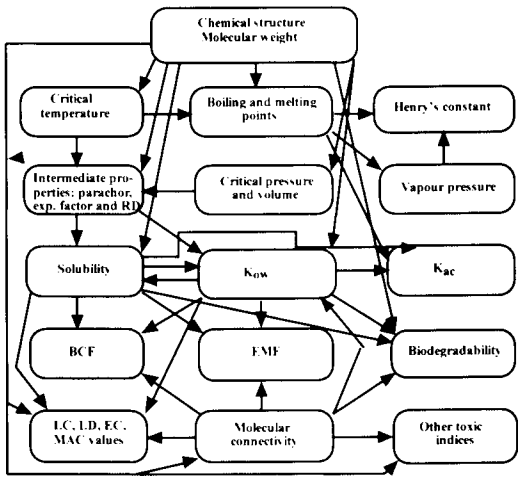

Fig. 8.14. The network of estimation methods in WINTOX is shown. An arrow represents a relationship between two or more properties.

other cases where it has been found beneficial for the overall accuracy of the program. When parallel estimation methods yield the highest accuracy for *different* classes of compounds, the use of weighting factors seems to offer a clear advantage. It is generally recommended that as many estimation methods as possible be applied for a given case study to increase the overall accuracy. If the estimation by *WINTOX* can be supported by other recommended estimation methods, it is strongly recommended that this be done.

8.6 Ecotoxicological Case Study I: Modelling the Distribution of Chromium in a Danish Fjord

This case study has been presented in previous publications, see, e.g., Jørgensen (1990c). It is an *FTE-model* combining a fate model Type AII (a specific ecosystem is considered) with an effect model Type BI (focus on the organisms level). The structure of the model is according to Class 2 (see Section 8.3), as it is simplified by focusing on a steady-state situation, although the spatial distribution is considered. Only one trophic level is considered. This is an illustrative case study, because:

1. The case study shows what can be achieved by a simple model.

2. It has been possible to validate the prognosis set-up eight years previously. *Validation* of models is not only important but absolutely necessary for the development of reliable models. Here it has even been possible to validate the

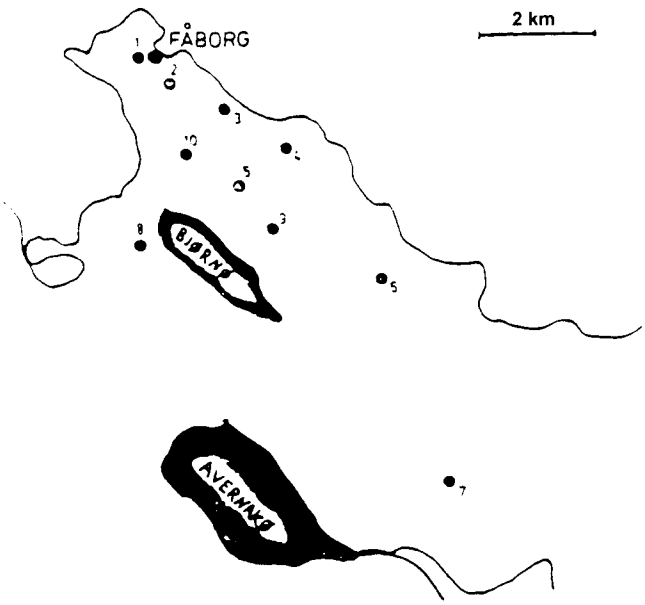

Fig. 8.15. *Fåborg Fjord* showing sampling stations 1–10. The point close to sampling station 1 indicates the discharge point.

model predictions. Unfortunately, we have only very few cases of prognosis validations. Therefore it has been considered significant to include this case study, because *a prognosis validation* is carried out.

3. The model development clearly shows how important it is to know the system and its processes if the *right* model with the *right* simplifications is to be selected.

A map of the system, Fåborg Fjord, is shown in Fig. 8.15. The numbers show sampling stations; station 1 is of particular importance as it is close to the discharge point.

For decades, a tanning plant has discharged waste water with a high concentration of chromium(III) into the fjord. In 1958 production was expanded significantly resulting in a pronounced increase in the chromium concentration of the sediment (see Mogensen and Jørgensen, 1979; for further details see also Mogensen, 1978).

It was the aim of this investigation to set up a model for the distribution of chromium in the fjord based on analysis of chromium in phytoplankton, zooplankton, fish, benthic fauna, water (dissolved as well as suspended) and sediment. During the first phase of the investigation it was already clear that the phytoplankton, zooplankton and fish were hardly contaminated by chromium, while the sediment and the benthic fauna clearly showed a raised concentration of chromium. This was easy to explain: *chromium(III)* precipitates as hydroxide by contact with seawater which has a pH of 8.1 compared with 6.5–7.0 for waste water.

Model Description

The overall analysis showed that the important processes are:

1. Settling of the precipitated *chromium(III) hydroxide* and other insoluble chromium compounds.
2. Diffusion of the chromium, mainly as suspended matter, throughout the fjord is caused mainly by tides. This implies that an eddy diffusion coefficient has to be found.
3. *Bioaccumulation* from sediment to benthic fauna.

Process (1) and (2) can be combined in one *submodel*, while process 3 requires a separate submodel.

The distribution model is based on the following simple *chromium(III)* transport equation (see for instance Rich, 1973) and the equations of *advection* and *diffusion* processes, presented in Chapter 3, which have been expanded to include settling:

$$\partial C/\partial t = D * \partial^2 C/\partial X^2 - Q * \partial C/\partial X - K * (C - C_0)/h \tag{8.6}$$

where C is the concentration of total chromium in water (in mg/l); C_0 is the *solubility* of chromium(III) in seawater at pH = 8.1 (in mg/l); Q is the inflow to the fjord = outflow by *advection* (m^3/24 h); D is the eddy *diffusion coefficient* considering the tide (m^2/24 h); X is the distance from the discharge point (in m); K is the settling rate (in m/24 h); h is the mean depth (in m).

For a tidal fjord such as *Fåborg Fjord* with only insignificant *advection* Q may be set to 0. Since the tanning plant has discharged an almost constant amount of chromium(III) during the last two decades, we can consider the stationary situation:

$$\partial C/\partial t = 0 \tag{8.7}$$

Equation (8.6) therefore takes the form:

$$D * \partial^2 C/\partial X^2 = K * (C - C_0)/h \tag{8.8}$$

This differential equation of second order has an analytical solution. C_u, the total discharge of chromium in g per 24 h, is known. This information is used together with F, the cross sectional area (m^2), to state the boundary conditions. The following expression is obtained as an analytical solution:

$$C - C_0 = (C_u / F) * \sqrt{h / D * K} * \exp[-\sqrt{(K / h \& D)} * X] + IK \tag{8.9}$$

F is known only approximately in this equation due to the non-uniform geometry of the fjord. The total annual discharge of chromium is 22,400 kg. Both the consumption of chromium by the tanning factory and the analytical determinations of

the waste water discharged by the factory confirm this figure. h is about 8 m on average. IK is an integration constant.

Equation (8.9) may be transformed into:

$$Y = K * (C - C_0) = (C_0/F) * \sqrt{(h * K / D)} * \exp[-\sqrt{K / h * D)} * X + K * IK \quad (8.10)$$

Y is, as seen, the amount of chromium (g) settled per 24 h and per m^2. The equation gives Y as a function of X.

Y is, however, known from the *sediment analysis*. A typical chromium profile for a sediment core is shown in Fig. 8.16. As we know that the increase in the chromium concentration took place about 25 years before the model was built, it is possible to find the sediment rate in mm or cm per year: 75 mm/25 y = 3 mm/y. Furthermore, as we know the concentration of chromium in the sediment, we can calculate the amount of chromium settled per year, or 24 h, and per m^2, and this is Y. The Y-values found by this method are plotted versus X in Fig. 8.17.

A non-linear regression analysis was used to fit the data to an equation of the following form:

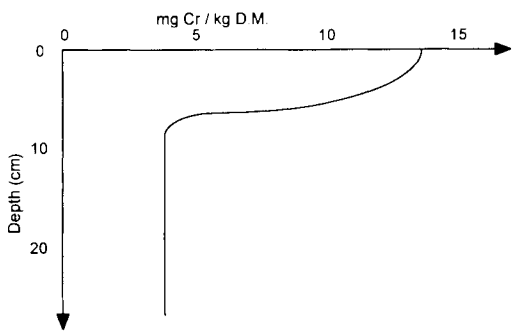

Fig. 8.16. Typical chromium profile of sediment core.

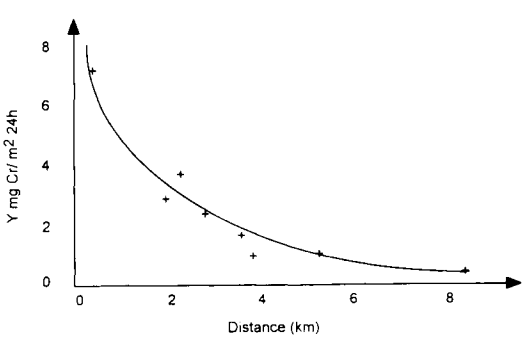

Fig. 8.17. Y, found by *sediment analysis*, is plotted versus X.

$$Y = a * \exp(-bX + c) \tag{8.11}$$

a, b and c are constants, which are found by the regression analysis.

Table 8.5 shows $Y = f(X)$. Table 8.6 gives the estimations of a, b and c found by the statistical analysis. Table 8.7 shows the result of the statistical analysis and, as can be seen, the model found with the values of a, b and c from Table 8.6 has a very high probability. The F-value found is 114.5, while an F-value with a probability of 0.9995 is only 30.4.

Table 8.8 translates the constants a, b and c into parameters of the model. D is found on the basis of an average value for K, 1.6 m/24 h. This value is found from the definition of Y. Y is known as shown above. Furthermore C_0 (the solubility of chromium(III) hydroxide) is known from the solubility constant and pH = 8.1 to be 0.2 mg/m^3, and as C is measured for all stations, K may be found from:

$$K = Y/(C - C_0) \tag{8.12}$$

Table 8.5. Y versus X

Station no.	g Cr/m^2 year	Y mg Cr m^2 day	X Distance from discharge point (m)
1	2.55	7.0	500
2	2.39	6.5	500
3	1.47	4.0	1500
4	0.35	1.0	2750
5	0.78	2.1	2750
6	0.14	0.38	5250
7	0.03	0.082	8500
8	0.20	0.55	3250
9	0.06	0.16	3500
10	0.58	1.6	2000

Table 8.6. Estimations of a, b and c

	Estimate	Asymptotic st. error
a	0.009909	0.00084
b	0.000723	0.00015
c	-0.000081	0.00045

Table 8.7. Statistical analysis

	Degree of freedom	Sum of squares	Mean square
Model	3	0.00011337	0.00003779
Residual	6	0.00000233	0.00000033
Total	9		
	F = 114.5		

The settling rates found by this method are shown in Table 8.9.

As can be seen from Table 8.9, the settling rate is approximately the same at three of the five stations. Stations 6 and 7 are given a lower value. It should be expected that the settling rate will decrease with increasing distance from the discharge point. But it should not be forgotten that the determination of the chromium concentration in the water is not very accurate because the concentration is low. K should be compared with settling rates of phytoplankton and detritus (see Tables 2.9 and 2.10). It is expected that the settling rate for *chromium(III) hydroxide* will be higher than the settling for phytoplankton and detritus, which is confirmed by the results in Table 8.9.

The value for the diffusion coefficient found from the settling rate corresponds to 4.4 m^2/s: a reasonable value compared with other D-values from similar situations (estuaries). The value for F is based on a width slightly more than the width of the inner fjord, but as a weighted average for the inner and outer fjord it seems a reasonable value.

Table 8.8. *Parameters*

From the regression analysis we have:

$$\frac{Cu}{F}\cdot\left(\frac{hK}{D}\right)^{1/2} = 0.00990 = a$$

and

$$\left(\frac{K}{h\cdot D}\right)^{1/2} = 0.000723 = b$$

which gives

$$Cu\cdot h/F = a/b = 13.7$$

$F = 35{,}800\ m^2$, which seems a reasonable average value of the cross-sectional area. From analysis of C at stations 2, 5, 6, 7 and 8 (see Table 8.10), we get an estimation of K since

$$Y = \frac{gCr}{m^2\ day} = K\,(C - C_0\ (C_0 \text{ is found to be } 0.2\ mg\ m^{-3})\ m^{-2}day$$

Table 8.9. *Settling rates*

Station	mg Cr/m^2 day	$C - C_0$ (mg m^{-3})	K (m day^{-1})
2	6.5	2.5	2.6
5	2.1	0.9	2.3
6	0.4	0.6	0.7
7	0.1	0.2	0.5
8	0.6	0.3	2.0

Integration from 0 to infinity over a half circle area gives a result of 22 t of *chromium(III)*, i.e., almost all the chromium discharged may be explained by the model, assuming that the distribution takes place over a half circle area.

All in all, it may be concluded that the *distribution model* gives acceptable results. The high concentrations of chromium in the sediment give reliable determinations, which again are the basis of the distribution model. The use of sediment analysis as demonstrated is, therefore, recommended for the development of a distribution model for a component that settles readily.

The second *submodel* focuses on the chromium contamination of the benthic fauna. It may be shown (Jørgensen, 1979) that *under steady-state conditions* the relation between the concentration of a contaminant in the n'th link in the *food chain* and the corresponding concentration in the $(n-1)$'th link can be expressed using the following equation:

$$C_n = (MY(n) * C_{n-1} * YT(n))/(MY(n) * YF(n) - RESP(n) + EXC(n)) = K' * C_{n-1} \quad (8.13)$$

where $MY(n)$ = the maximum growth rate for the n'th link of the food chain (1/day); Cn = the chromium concentration in the n'th link of the food chain (mg/kg); C_{n-1} = the chromium concentration in the $(n-1)$'th link of the food chain (mg/kg); $YT(n)$ = the utility factor of chromium in the food for the n'th link of the food chain (–); $YF(N)$ = the utility factor of the food in the n'th link of the food chain (–); $RESP(n)$ = the respiration rate of the n'th link of the food chain (1/day); $EXC(n)$ = the excretion rate of chromium for the n'th link of the food chain (1/day).

For some species present in Fåborg Fjord these parameter values can be found in the literature (see, for instance, Mogensen and Jørgensen, 1979, 1991 and 2000). The mussel *Mytilus edulis* was found on almost all the stations and the following parameters are valid ($YT(n)$ and $YF(n)$ are found for other species):

$MY(n) = 0.03$ 1/day
$YT(n) = 0.07$
$YF(n) = 0.66$
$RESP(n) = 0.001$ 1/day
$EXC(n) = 0.04$ 1/day

The use of these values implies that $K' = 0.036$ for *Mytilus edulis*. In other words, the concentration of chromium in *Mytilus edulis* should be expected to be 0.036 times the concentration in the sediment.

Twenty-one mussels from *Fåborg Fjord* were analyzed and by statistical analysis it was found that the relation between the concentration in the sediment and in the mussels is linear:

$$C_n = C_{n-1} * K' \quad (8.14)$$

where K' was found to be 0.015 ± 0.002. The discrepancy from the theoretical value is fully acceptable when it is considered that the parameters are found in the literature and they may not be exactly the same values for all environments for all

Table 8.10. *Validation of the prognosis*

Item	Observed value (mg/kg dry matter)	Range (mg kg dry matter)	Predicted value (mg/kg dry matter)
Cr in sediment	65	57–81	70
Cr in mussels	2.2	1.4–4.5	2.5
mg Cr/m^2 day	0.59	0.44–0.83	0.67

possible conditions. In general, biological parameters can only be considered approximate values. The relatively low standard deviation of the observed K' value, however, confirms the relation used.

It is proposed that one should use the highest K' value = 0.036 when the model is used for environmental management, because in this way the uncertainty of the K'-value is used "to the benefit of the environment".

The model was utilized as a management tool and the acceptable level of the chromium concentration in the sediment of the most polluted area was assessed to be 70 mg per kg dry matter. That would correspond to a chromium concentration of $70 \times 0.036 = 2.5$ mg per kg dry biomass in mussels, or about 2.5 times the concentration found in uncontaminated areas of the open sea. This was considered the NOEC and accepted by the environmental authorities of the district (council).

The *distribution model* was then used to assess the total allowable discharge of chromium (kg/y) if the chromium concentration in the sediment was to be reduced to 70 mg per kg dry matter in the most polluted areas (stations 1 and 2). It was found that the total discharge of chromium should be reduced to 2000 kg or less per year to achieve a reduction of about 92%.

Consequently, the environmental authorities required the tanning plant to reduce its chromium discharge to ≤2000 kg per year. The tanning plant has complied with the standards since 1980.

A few samples of *sediment* (4) and mussels (7) taken in 1987–88 have been analyzed and used to validate this prognosis. The results are given in Table 8.10. Settled chromium in mg/m^2 day was found on the basis of the previously determined *sedimentation rate* (see above). The prognosis validation was fully acceptable as the deviation between prognosis and observed average values for chromium in mussels is approximately 12%.

8.7 Ecotoxicological Case Study II: Contamination of Agricultural Products by Cadmium and Lead

Agricultural products are contaminated with *lead* and *cadmium* originating from air pollution, the application of sludge from municipal waste water plants as a soil conditioner, and from the use of fertilizers.

The *uptake* of *heavy metals* from municipal sludge by plants has previously been modelled (see Jørgensen, 1975, 1976b). This model can briefly be described as follows. Depending on the soil composition it is possible to find a distribution coefficient for various heavy metal ions, i.e., the fraction of the heavy metal that is dissolved in the soil–water relative to the total amount. The distribution coefficient was found by examining the dissolved heavy metals relative to the total amount for several different types of soil. Correlation between pH, the concentration of *humic substances*, clay and sand in the soil on the one hand, and the distribution coefficient on the other, was also determined. The uptake of heavy metals was considered a first-order reaction of the dissolved heavy metal.

This model does not, however, consider:

1. the direct uptake from atmospheric fallout onto the plants; or
2. the other sources of contamination such as fertilizers and the long-term release of heavy metal bound to the soil and the non-harvested parts of the plants.

It was the objectives of the model presented here to include these sources in a model for lead and cadmium contamination of plants; it is a fate model Type A3 (see Section 8.1). Published data on lead and cadmium contamination in agriculture are used to calibrate and validate the model which is intended to be used for a more generally applicable risk assessment for the use of fertilizers and sludge that contains cadmium and lead as contaminants. The structure of the model is according to Type 3 (see Section 8.3).

The basis for the model is the lead and cadmium balance for average agricultural land in Denmark. Figures 8.18 and 8.19 give the balances, modified from Andreasen (1985), and Knudsen and Kristensen (1987) to account for the changes of the mass

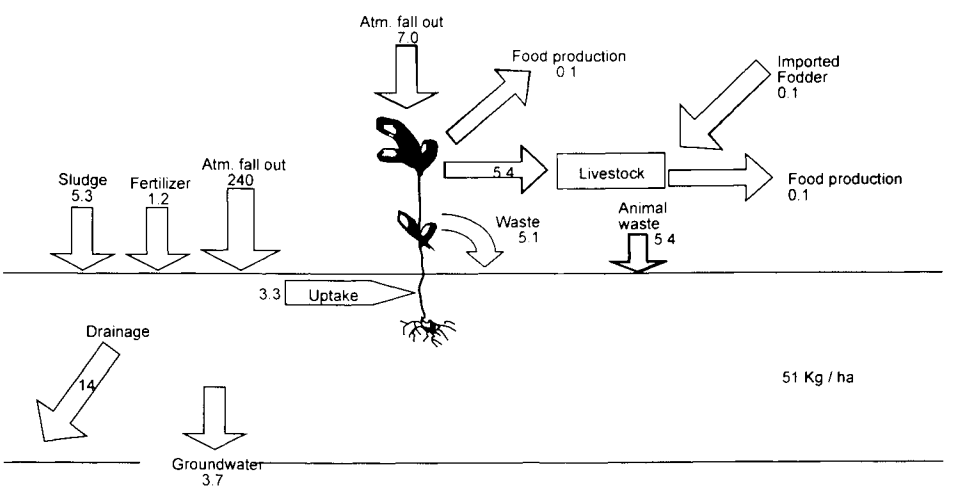

Fig. 8.18. *Lead* balance of average Danish agriculture land. All rates are g Pb/ha year.

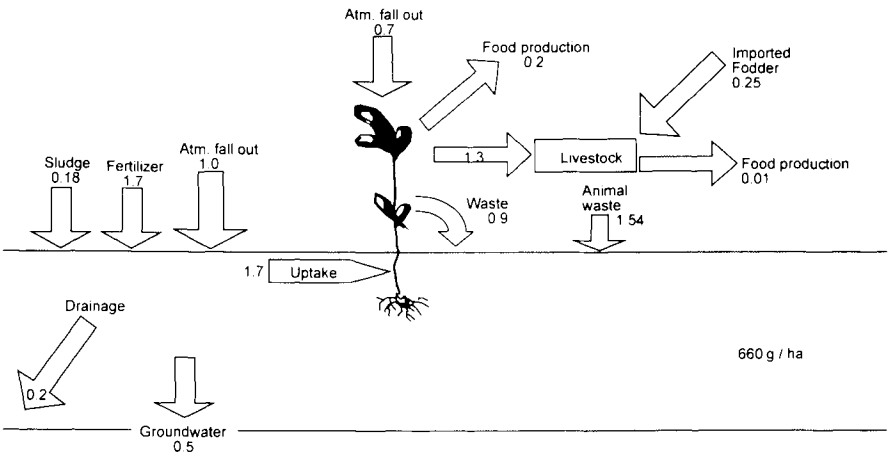

Fig. 8.19. *Cadmium* balance of average Danish agriculture land. All rates are g Cd/ha year.

balances in 1999. The atmospheric fallout of lead has gradually be reduced in the last 15 years due to the reduction of lead concentration in gasoline, while the most important source of cadmium contamination is fertilizer. The latter can only be reduced by using less contaminated sludge and phosphorus ore for the production of phosphorus fertilizer.

It is seen that the amounts of lead and cadmium from domestic animals and plant residues after harvest are not insignificant contributions.

The Model

Figure 8.20 shows a conceptual diagram of the *Cd-model.* The *STELLA* software was applied. As can be seen, it has four state variables: Cd-bound, Cd-soil, Cd-detritus and Cd-plant. An attempt was made to use one or two state variables for cadmium in the soil, but to get an acceptable accordance between the data and the model output three state variables were needed. This can be explained by the presence of several soil components that bind the heavy metal differently; see Christensen (1981; 1984), EPA, Denmark (1979), Hansen and Tjell (1981), Jensen and Tjell (1981) and Chubin and Street (1981). Cd-bound covers the cadmium bound to minerals and to more or less refractory material; Cd-soil covers the cadmium bound by adsorption and ion exchange; and Cd-detritus is the cadmium bound to organic material with a wide range of biodegradability.

The forcing functions are: airpoll, Cd-air, Cd-input, yield and loss.

The atmospheric fallout is known, and the allocation of this source to the soil (airpoll) and to the plants (Cd-air), is according to Hansen and Tjell (1981) and Jensen and Tjell (1981). Cd-input covers the heavy metal in the fertilizer and, as seen

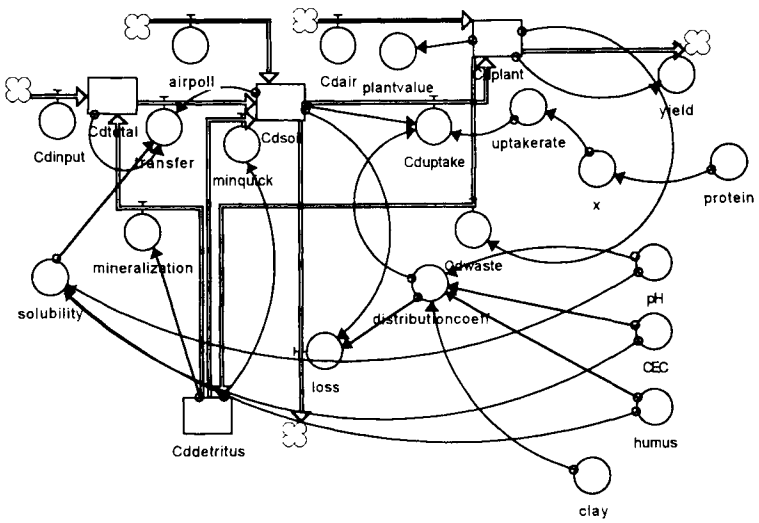

Fig. 8.20. Conceptual diagram of the model. The model has been developed on a Macintosh Plus by use of the software *STELLA*. Boxes show state variables, double-line arrows give flows, circles give functions and single-line arrows show feed-back mechanisms.

from the equations in Table 8.11, this comes as a pulse at day 1 and afterwards with a frequency of every 180 days. The yield corresponds to the part of the plant that is harvested, which is also expressed as a pulse function at day 180, and afterwards with an occurrence of every 360 days. In Table 8.11, it is 40% of the plant biomass.

The loss covers transfer to the soil and groundwater below the root zone. It is expressed as a first-order reaction with a rate coefficient dependent on the *distribution coefficient* that is found from the soil composition and pH, according to the correlation found by Jørgensen (1975). Furthermore the rate constant is dependent on the hydraulic conductivity of the soil. In Table 8.11 the constant 0.01 reflects the dependence of the hydraulic conductivity.

The transfer from Cd-bound to Cd-soil indicates the slow release of cadmium due to a slow decomposition of the more or less refractory material to which cadmium is bound. The cadmium uptake by plants is expressed as a first-order reaction, where the rate is dependent on the distribution coefficient, as only dissolved cadmium can be taken up. It is further dependent on the plant species. As will be seen, the uptake is a step function that here (grass) is 0.0005 during the growing season and zero after the harvest and until the next growing season starts. Cd-waste covers the transfer of plant residues to detritus after harvest. It is therefore a pulse function, which here is 60% of the plant biomass, as the remaining 40% has been harvested.

Cd-detritus covers a wide range of biodegradable matter and the mineralization is therefore accounted for in the model by two mineralization processes: one for Cd-soil and one for Cd-total.

Table 8.11. Model equations

```
Cd-detritus = Cd-detritus + dt * (Cd-waste - mineralization - minquick)
INIT(Cd-detritus) = 0.27
Cd-plant = Cd-plant + dt * (Cduptake - yield - Cd-waste + Cd-air)
INIT(Cd-plant) = 0.0002
Cd-soil = Cd-soil + dt * (-Cduptake - loss + transfer + minquick + airpoll)
INIT(Cd-soil) = 0.08
Cdtotal = Cdtotal + dt * (Cd-input - transfer + mineralization)
INIT(Cdtotal) = 0.19
airpoll =0.0000014
Cd-air = 0.0000028 + STEP(-0.0000028,180) + STEP(+0.0000028,360) + STEP(-0.0000028,540) +
STEP(+0.0000028,720) + STEP(-0.0000028,900)
Cd-input = PULSE(0.0014,1,180)
Cduptake = distributioncoeff * Cd-soil * uptake rate
Cd-waste = PULSE(0.6 * Cd-plant,180,360) + PULSE(0.6 * Cd-plant,181,360)
CEC = 33
clay = 34.4
distributioncoeff =0.0001 * (80.01-6.135 * pH-0.2603 * clay-0.5189 * humus-0.93 * CEC)
humus = 2.1
loss = 0.01 * Cd-soil * distributioncoeff
mineralization = 0.012 * Cd-detritus
minquick = IF TIME_180 THEN 0.01 * Cd-detritus ELSE 0.0001 * Cd-detritus
pH = 7.5
plantvalue = 3000 * Cd-plant/14
protein = 47
solubility = 10 ^ (+6.273-1.505 * pH+0.00212 * humus+0.002414 * CEC) * 112.4 * 350
transfer = IF Cd-soil<solubility THEN 0.00001 * Cdtotal ELSE 0.000001 * Cdtotal
uptake rate = x +STEP(-x,180) + STEP(x,360) + STEP(-x,540) + STEP(x,720)+STEP(-x,900)
x = 0.002157 * (-0.3771+0.04544 * protein)
yield = PULSE(0.4 * Cd-plant,180,360) + PULSE(0.4 * Cd-plant,181,360)
```

Model Results

Data from Jensen and Tjell (1981) and Hansen and Tjell (1981) was used for calibration and validation of the model. It was in this phase of the modelling procedure that it was revealed that three *state variables* for *heavy metal* in soil were needed to achieve acceptable results. It was particularly difficult to get the correct values for heavy metal concentrations in the second and third years after municipal sludge had been used as a soil conditioner. This use of models may be called experimental mathematics or modelling, where simulations with different models are used to deduce which model structure should be preferred. The results of experimental mathematics must, of course, be explained by examination of the processes involved and here can be referred to the references given above.

The results of the *validation* phase are shown in Figs 8.21 and 8.22 and, as can be seen, the accordance between observations and model predictions is reasonably

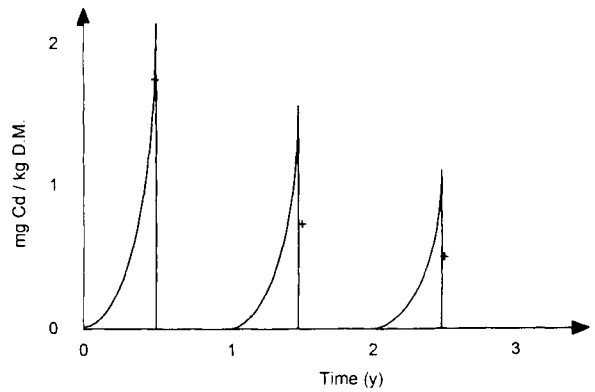

Fig. 8.21. The model was validated by use of the cadmium concentration as a function of time (y) for lead. + Gives the observations and the solid line gives the corresponding model predictions.

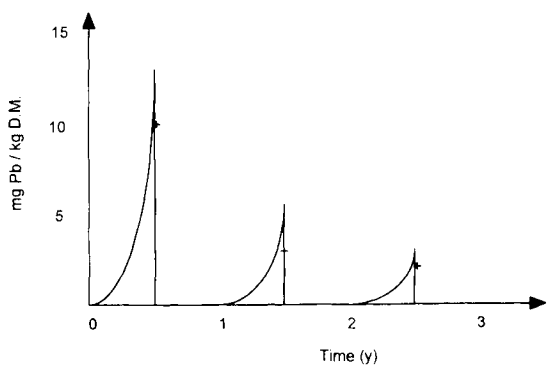

Fig. 8.22. The model was validated using the lead concentration as a function of time (y) for salad plants. + Indicates the observations and the full line gives the corresponding model predictions.

good. As seems apparent from the validation, the developed model can explain the observations. A wider use of the model would require that still more data from experiments with many plant species be used to test the model. It may be concluded from these results, however, that the model structure must account for at least three state variables for the heavy metal in soil to cover the ability of different soil components to bind the heavy metal by various processes.

The model has been calibrated and validated on the basis of three years' experiments and measurements and it was clear from the model exercises that the atmospheric fallout and heavy metal in the plant residues were significant, although these were not considered in the model published in 1976. Translocation of the heavy metal to various parts of the plant was not considered in the model and this would be a natural next step to include in the model, as it is important to distinguish heavy metal concentrations in various parts of the plants.

The problem modelled is very complex and many processes are involved. On the other hand, an ecotoxicological management model should be fairly simple and not involve too many parameters. The model can obviously be improved, but it gives at least a first rough picture of the important factors in the contamination of agricultural crops. Usually, it is not possible to get very accurate results with toxic substance models but, on the other hand, as we want to use quite large safety factors, the need for high accuracy is not pressing.

8.8 Ecotoxicological Case Study III: A Mercury Model for Mex Bay, Alexandria

Mex Bay is located west of Alexandria and suffers from serious pollution problems due to the discharge of waste water from many heavy industries, such as a cement plant, tanneries, an oil refinery and a chlorine alkali plant. The bay's most serious pollution problem is probably the mercury contamination of fish. The concentration of mercury in most fish caught in the bay exceeds the limit for human food set by WHO (1 ppm). Figure 8.23 shows a map of *Mex Bay*. The surface area is 29 km^2 and the mean depth is 10 m.

A comprehensive investigation of the *mercury* pollution of the bay has been carried out at Alexandria University. The results, which that are the basis for the development of the model, are published in Aboul Dahab (1985), Aboul Dahab et al., (1984), El-Gindy et al., (1985), El-Rayis et al., (1984) and Halim et al., (1984).

The Model

A static model is used to describe the spatial distribution of mercury contamination of the bay. The model is based on a mass balance for the bay. The model combines the fate of a specific case (Type A2) with an effect on the organism level (the

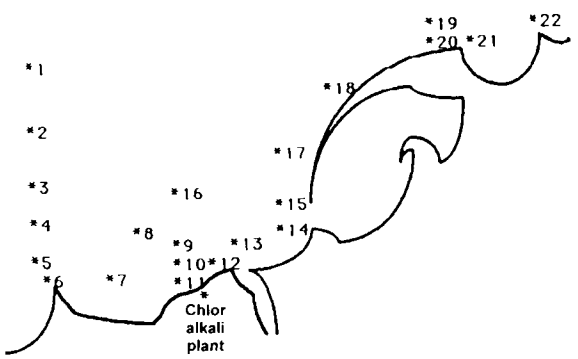

Fig. 8.23. Map of Mex Bay.

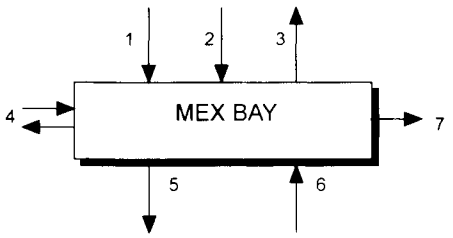

Fig. 8.24. The model is developed on the basis of the mass balance principles applied to the seven processes (see text for explanation).

concentration of mercury in tuna fish which is the maximum allowable concentration to be used for human consumption according to WHO (effect level B1). The structure of the model is Type 2, as the time variation is not considered. The distance from the discharge point is considered the independent variable, as in Ecotoxicological Case Study Number 1 (see Section 8.6).

The principles are given in Fig. 8.24 where the following processes are indicated:

1. Discharge of municipal and industrial waste water.
2. Atmospheric fallout—dry and wet deposition.
3. *Volatilization.*
4. Exchange with the open sea.
5. *Sedimentation.*
6. Release from the sediment.
7. *Fishery.*

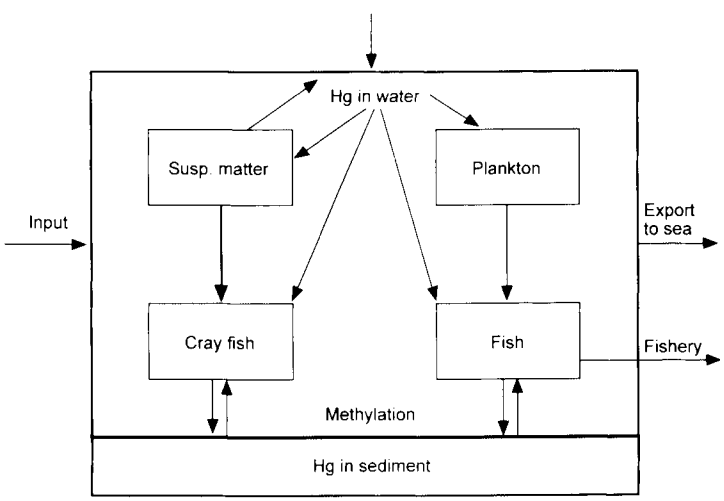

Fig. 8.25. The total model consists of five submodels.

The model has five submodels which are interrelated as shown in the conceptual diagram in Fig. 8.25.

Submodel 1 deals with the mercury concentration in water. It is a Class 2 model and describes the mercury concentration as a function of the distance from the outlet (see also Fig. 8.23). The change in mercury concentration with time is the result of dispersion – advection – settling + methylation (see also the chromium model in Section 8.6). In this case, we obtain the following equation:

$$\frac{\partial Hgt}{\partial t} = 0 = D\frac{\partial Hgt}{\partial x^2} \cdot \left(\frac{Q}{AE}\right)\frac{\partial Hgt}{\partial x} = \left(\frac{SR}{Depth}\right)Hgt + (M \cdot MC) \cdot Hgts \tag{8.15}$$

where Q is the flow of water from The Umum Drain = 7.6×10^6 (m^3/day); AE is the width of the bay multiplied by the depth = $BB \times$ Depth (m^2); *Depth* is the mean depth of the bay = 10 m; M is the *methylation rate* (day^{-1} or less); SR the settling rate in water is calculated (m/day); MC, modification coefficient is the amount of organic carbon divided by the highest value of organic carbon in the bay; and D, the *diffusion coefficient* = 10^9 (m^2/day) or less.

As the discharge of mercury has been almost constant for several years, we are able to transform the partial differential equation to a differential equation. Furthermore, we are not interested in daily fluctuations but in the general pollution picture. We get (compare with Ecotoxicological Case Study Number 1):

$$\begin{aligned} D\frac{d^2 Hgt}{dx^2} - \left(\frac{Q}{AE}\right)\frac{dHgt}{dx} + \left(\frac{SR}{Depth}\right)Hgt - (M \cdot MC) \cdot Hgts = 0 \\ \frac{d^2 Hgt}{dx^2} - \left(\frac{Q}{D \cdot AE}\right)\frac{dHgt}{dx} + \left(\frac{SR}{D \cdot Depth}\right)Hgt - \left(\frac{M \cdot MC}{D}\right)Hgts = 0 \end{aligned} \tag{8.16}$$

Submodel 2 is a Class 2 model and considers the concentration of *suspended matter* in water. It describes the concentration of suspended matter as a function of the distance from the outlet. The concentration of suspended matter is the result of: *dispersion – advection – settling*:

$$\frac{\partial TSM}{\partial t} = 0 = D\frac{\partial TSM}{\partial x^2} - \left(\frac{Q}{AE}\right)\frac{\partial TSM}{\partial x} - \left(\frac{SR}{Depth}\right)TSM \tag{8.17}$$

where Q is the flow of water from The Umum Drain = 7.6×10^6 (m^3/day); AE is the width of the bay multiplied by the depth = $BB \times$ Depth (m^2); *Depth* is the mean depth of the bay = 10 m; SR, the settling rate in water is calculated (m/day); D, the diffusion coefficient = 10^9 (m^2/day) or less; TSM is the amount of total suspended matter.

It is again possible to transform a partial differential equation into a differential equation, as the discharge of suspended matter has been constant for a longer period. Furthermore, we are not interested in the changes on a day-to-day basis, but on the general pollution picture of the *Mex Bay*:

$$D\frac{d^2TSM}{dx^2}-\left(\frac{Q}{AE}\right)\frac{dTSM}{dx}+\left(\frac{SR}{Depth}\right)TSM=0$$
$$\frac{d^2TSM}{dx^2}-\left(\frac{Q}{D\cdot AE}\right)\frac{dTSM}{dx}+\left(\frac{SR}{D\cdot Depth}\right)TSM \tag{8.18}$$

Submodel 3 describes the concentration of mercury in phytoplankton. The model distinguishes between *organic mercury* and *inorganic mercury* in phytoplankton. They are both described simply as a concentration factor × the concentration in water.

Submodel 4 deals with mercury in the sediment. The concentration in the sediment is a result of settling (from submodel 1) and *methylation* (also described in *submodel* 1). As the mercury concentration in the sediment is a function of these two processes, which are considered constant with the time (see again submodel 1), the concentration in the sediment is considered a constant at a given station—it is only dependent on the distance from the outlet and the depth.

Submodel 5 has a Class 3 structure. It considers the mercury in fish and distinguishes between inorganic and organic mercury as a function of time. The mercury concentration of fish, *HgF*, is determined by:

1. the uptake from water: = *CF* * Hg in water * d*w*/d*t*
2. the uptake from food: $a * w^b$ * Hg in food * *eff*
3. the excretion: *excretion coefficient* * Hg in fish

where *CF* is the concentration factor (fish/water), *w* is the weight of the fish, which implies that d*w*/d*t* is the growth of the fish, *a* and *b* are characteristic constants describing the food uptake by the fish, *eff* is the efficiency of the *mercury uptake* from the food (it is different for inorganic and organic mercury). The change in *mercury* concentration of the fish is determined by:

$$dHgF/dt = \text{uptake from water} + \text{uptake from food} - \text{excretion} \tag{8.19}$$

The growth of the fish is found by:

$$dw/dt = a * w^b - r * w^c \tag{8.20}$$

where a and b are constants mentioned above, while r and c are other constants. According to several investigations, $b = 0.68$ and $c = 0.8$.

For each station the mercury concentration of the sediment and the phytoplankton is determined by use of *submodels* 3 and 4. A *probability generator* deterines in which of the stations the "average" filter feeders (*Sardina pilchardus*), the "average" benthic invertebrates (*Penaeus kerat-hurus*) and the "average" Pelagic fish (*Boops boops*) are at a given day.

The station determines the *mercury* concentration of the food for these three species. Their concentrations are currently determined by the above equations and the concentration of carnivorous predators is determined by the use of the same set of equations, but now using the mercury concentration of their *average* food sources. The ratio of the three species which comprise the food is determined comparing an analysis of the stomach contents of the fish with general knowledge of the preferred food items of the species. The state variables and forcing functions of the model are listed in Tables 8.12 and 8.13.

At this stage, the model has only been calibrated. Submodels 1 and 2 are second-order differential equations and the concentration of mercury, *Hgt*, and suspended matter *TSM* at $x = 0$ and $dHgt/dx$ and $dTSM/dx$ at $x = 0$ have therefore been included in the calibration. Values based upon the measurements are used as initial guesses. The initial guesses of the settling rates are based on sediment analyses according to the method used in Ecotoxicological Case Study Number 1.

The chlorine alkali plant began production in 1950 and the settling rates found based on the sediment profiles are listed in Table 8.14. Figures 8.26 and 8.27 show the model results compared with the measured values for Submodels 1 and 2. Figure 8.28 gives the results of the mercury content of the fish species *Euthynnus alletteratus*. The accord between model results and measured values is acceptable. As can be seen, the tuna fish will exceed a mercury concentration of 1 mg/kg at a weight of 350 g.

Results of a simulation for *tuna fish* corresponding to 90% reduction of the mercury originating from waste water are also shown in Fig. 8.28. This reduction gives satisfactory low mercury concentration in the tuna fish and these results should be used in environmental management.

The model applied in this case study is fairly simple compared with the complex biological and hydrodynamical processes responsible for the mercury concentrations of the fish species which are the most central state variables. Yet an acceptable accordance between measured values and model values is found, although *submodel* 1 does not give an acceptable fit for the relationship between mercury concentration and the distance from the outlet, probably due to a too simple description of the hydrodynamics.

The model is an illustration of what can be achieved with a simple model, resulting from considerations of where simplification can be made and what the most essential processes and state variables are. If the experience gained by developing this model and the chromium model presented in Section 8.6 is used to set up a procedure for developing a management model for the control of heavy metal pollution in aquatic ecosystems, the following procedure can be recommended:

Table 8.12. *State variables*

State variable		Unit	Comments
1	Salinity	‰	Measured for all stations and in different depths
2	Hg–inorganic	µg/l	Hg–inorganic
3	Hg–organic	µg/l	Hg–organic
4	Hg–total dissolved	µg/l	Hg–total dissolved is the sum of Hg–inorganic and Hg–organic
5	Hg–particulate	µg/l	Hg–particulate
6	Hg–total	µg/l	Hg–total is the sum of Hg–total dissolved and Hg–particulate
7	Inorganic Hg plankton	µg/kg WW	Hg inorg. in plankton
8	Total Hg–plankton	µg/kg WW	Hg total in plankton
9	Inorganic Hg–Pelagic fish	µg/kg WW	five different forms of Pelagic fish were examined
10	Total Hg–Pelagic fish	µg/kg WW	Is measured in all the five species in muscle (flesh)
11	Inorganic Hg–Benthic fish	µg/kg WW	Two species of benthic fish were examined
12	Total Hg–Benthic fish	µg/kg WW	
13	Inorganic Hg–Filter feed fish	µg/kg WW	Two species of filter feed fish were examined
14	Total Hg–Filter feed fish	µg/kg WW	Is measured in muscle (flesh)
15	Inorganic Hg–Carn. fish	µg/kg WW	Two species of Carn. fish were examined
16	Total Hg–Carn. fish	µg/kg WW	Is measured in muscle
17	Inorganic Hg–Benthic invertebrates	µg/kg WW	Two species of benthic invertebrates were examined
18	Total Hg–Benthic invertebrates	µg/kg WW	
19	Suspended matter	µg/l	
20	Suspended matter	µg C l	Use of equation
21	Leachable Hg–sediment	µg/g DM	
22	Organic Hg–sediment	µg/g DM	
23	Total Hg–sediment	µg/g DM	
24–28	Hg *f*(weight(time)) in pelagic-, benthic-, carnivorous fish and benthic invertebrates		

1. A relationship between the concentration in water and/or sediment is developed using *Fick's second law.* This *submodel* probably has the lowest accuracy of the submodels included and if higher accuracy is required further research into the hydrodynamics of the system should be implemented in order to improve this submodel.

Table 8.13. *Forcing functions*

Forcing function		Unit	Comments
1	Wind	km/h	Monthly mean scalar wind speed is measured as an average over 20 years. Alexandria Meteorological station
2	Effluent 1	m^3/day	Umum Drain has a flow of 7×10^6 m^3/day
3	Effluent 2	m^3/day	Industrial waste water from Chlorine Alkali Plant has a flow of 35×10^3 m3/day (Aboul Dahab, 1985)
4	Effluent 1 Hg–inorganic	µg/l	The inorganic Hg of Umum Drain is measured as dissolved reactive mercury
5	Effluent 1 Hg–organic	µg/l	The organic Hg of Umum Drain is measured as dissolved organic
6	Effluent 1 Hg–particulate	µg/l	The particulate Hg of Umum Drain is measured as particulate
7	Effluent 1	µg/l	The suspended matter of Umum Drain is suspended matter measured
8	Effluent 2 Hg–inorganic	µg/l	The inorganic Hg of the Chlorine Alkali effluent is measured as dissolved reactive
9	Effluent 2 Hg–organic	µg/l	The organic Hg of the Chlorine Alkali effluent is measured as dissolved organic
10	Effluent 2 Hg–particulate	µg/l	The particulate Hg of the Chlorine Alkali effluent is measured
11	Effluent 2 suspended matter	µg/l	The suspended matter of the Chlorine Alkali effluent is measured as particulate
12	Sea water temp.	°C	Water temperature is measured at different depths
13	Atm. fallout	µg Hg/m^2 day	*f*(wind)
14	Sediment comp.	% sand	% mud is measured
15	Aerobic/anaerobic conditions in sediment are determined		
16	Open sea Hg	µg/l	Station 1 = open sea
17	Open sea salinity	‰	Station 1 = open sea
18	Open sea (susp m.)	µg/l	Station 1 = open sea
19	Settling rate (net)	mm/year	Is determined by means of sediment analysis
20	Density	kg/l	Salinity and temperature are measured. Density is *f*(salinity, temp.)
21	Air temperature	°C	Air temperature is measured
22	Depth	*m*	Depths are measured for all stations
23	Precipitation	mm/day	Tables available

2. The parameters in this relationship are found using determinations of the heavy metal concentrations in water and sediment. The concentration profiles of heavy metal in sediment are of particular interest, as they may be used to determine the net annual sedimentation and the settling rate.

Table 8.14. *Settling rate*

Station	SR (cm/year)	SR (g/m^2 day)
7	0.81	24.4
8	–	–
9	0.93	25.8
10	0.93	25.8
11	0.93	25.8
12	0.81	24.4
13	0.81	24.4
14	0.81	24.4
15	0.70	19.4
16	0.81	24.4
17	0.93	25.8
18	0.93	25.8
Average		24.6

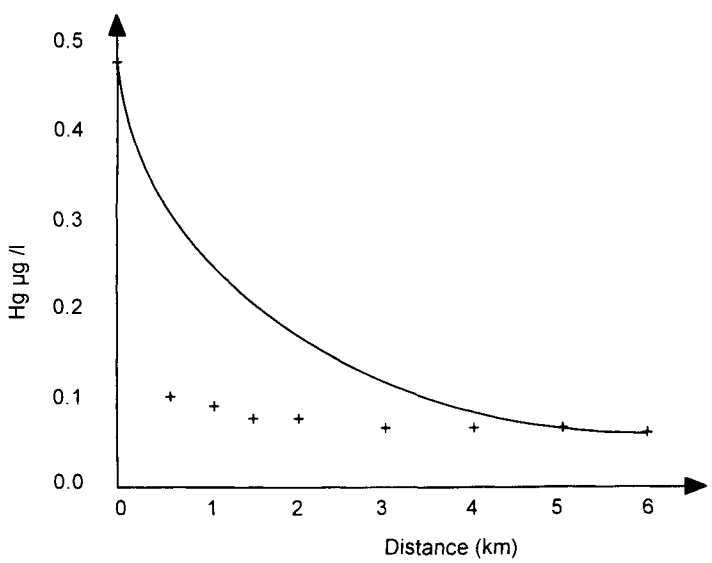

Fig. 8.26. Results of Submodel 1. Hg as function of distance. (A) Measured values. (B) Model results.

3. The concentration of heavy metal in those species with high level contamination can be determined using *concentration factors* and a description of *bioaccumulation.* If a description of the concentration as *f*(weight) is required, submodel 5 (this example) can be applied.

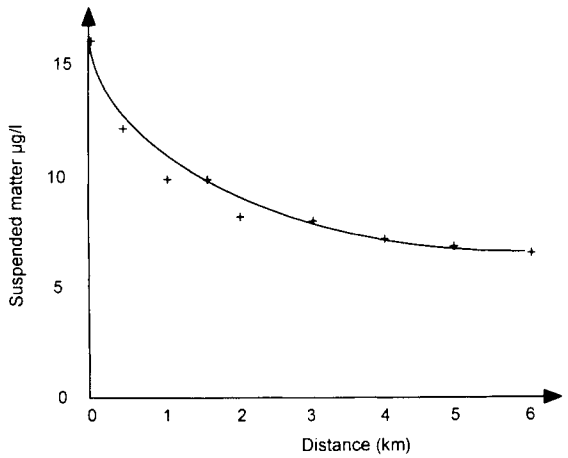

Fig. 8.27. Results of *submodel* 2. Total suspended matter as function of distance. A: measured values. B: model results.

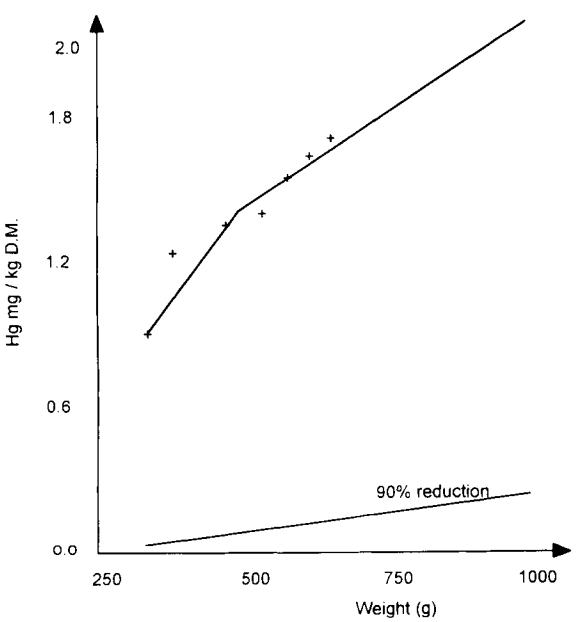

Fig. 8.28. *Mercury* concentration in *Euthynnus alletteratus* (µg/kg) as a function of weight. The solid line without text represents the model results and + indicates the measured values for fish of different weights. The curve 90% reduction corresponds to the simulated results obtained by a reduction of the total mercury input from waste water to *Mex Bay*. Notice that at present the *WHO standard* of 1 mg/kg D.M. is exceeded at a weight = 375 g, while it is not the case by 90% reduction.

8.9 Fugacity Fate Models

These A1-type *fate models* (see Section 8.1) are applied mainly to compare two or more chemicals in order to be able to select the least environmentally harmful one or to point out particularly hazardous chemicals. These models have a wide application in environmental chemistry. They were originally developed mainly by *Mackay* (Mackay, 1991), but today a wide spectrum of different models are available, developed by different authors (see *SETAC*, 1995).

These models are based on the concept of *fugacity*, $f = c/Z$, where c is the concentration in the considered phase and Z is the fugacity capacity (measured in mol/m^3 Pa or moles/l atm). Fugacity is defined as the escaping tendency, has the unit of pressure (atmosphere or Pa) and is identical to the partial pressure of ideal gases. By equilibrium between two phases, the fugacity of the two phases are equal. If the two Zs are known, it is possible to calculate the concentrations in the two phases. If there is no equilibrium, the rate of transfer from one phase to the other is proportional to the difference in fugacity.

If the equation for ideal gases can be applied, we have $pV = nRT$, where n is the number of moles. R the gas constant = 8.314 Pa m^3/mole K and T is the absolute temperature. This leads to $p = c * R * T$ and:

$$c = p/RT = f/(RT) \tag{8.21}$$

By acceptable approximation (application of the equation for ideal gases and the activity is equal to the concentration) the *fugacity capacity* in air

$$Z_a = 1/RT \tag{8.22}$$

At equilibrium between water and air, the *fugacity* is the same in the two phases, as already mentioned:

$$c_a Z_a = c_w Z_w \tag{8.23}$$

where w is used as the index for water.

Based on *Henry's law* (see Chapter 3) $p = He \cdot y$, where as used above $p = c_a RT$ and $y = c_w/(c_w + [H_2O])$, we can find the distribution between air and water. The concentration of water in water is with good approximation $1000/18 >> c_w$, which means that we get $p = c_a RT = He\, y = He\, c_w/(c_w + [H_2O]) = He\, c_w\, 18/1000$. Equation (8.23) yields

$$c_a/c_w = Z_a/Z_w = 18He/1000RT \tag{8.24}$$

This implies that $Z_w = 1000/18He$.

Similarly, the distribution between water and soil (index s) can be applied to find the fugacity capacity of soil:

$$c_s/c_w = Z_s/Z_w = K_{ac} \tag{8.25}$$

Z_s is therefore found as $Z_w * K_{ac} = 1000\ K_{ac}/18He$. In a parallel manner Z_o, the fugacity capacity for octanol can be found as $1000\ K_{ow}/18\ He$ and the fugacity capacity for biota, Z_b as $1000\ BCF/18\ He$. Table 8.15 gives an overview of the found fugacity capacities in mole/l atm. $R = 0.0820$ atm l/(moles K) when these units are applied. If m^3 is used as volume unit and Pa as unit for pressure, we get 1 atm = 101,325 Pa and 1 l = 1/1000 m^3. This implies that R has the unit J/mole K corresponding to the value $0.082 \times 101\ 325/1000 = 8.3$ J/(moles K). Figure 8.29 shows a conceptual diagram of the most simple *fugacity model*.

Multimedia models are applied on four levels. An equilibrium distribution (level 1) is found from the known fugacity capacities and equal fugacities in all spheres. If advection and chemical reactions must be included in one or more phases, but the equilibrium is still valid, we have Level 2. The fugacities are still the same in all phases. Level 3 presumes steady state but no equilibrium between the phases. Transfer between the phases is therefore taking place. The transfer rate is proportional to the fugacity difference between two phases. Level 4 is a dynamic version of Level 3, which implies that all concentrations and possibly also the emissions are changed over time.

Table 8.15. *Fugacity capacity* in moles/l atm. (If the unit moles m^3 Pa is required divide by 101.325.)

Phase	mol l atm.
Atmosphere	$1\ RT\ (R = 0.0820)$
Hydrosphere	$1000\ He\ 18$
Lithosphere (soil)	$1000\ K_{oc}\ 18\ He$
Octanol	$1000\ K_{ow}\ 18\ He$
Biota	$1000\ BCF\ 18\ He$

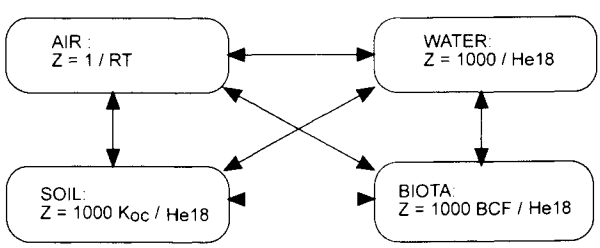

Fig. 8.29. Conceptual diagram of the *fugacity model*. At steady state the fugacities in the four compartment are the same. The concentration can easily be found as $c = fZ$. The Z values are shown in the diagram.

If the total emission in all phases is denoted M, we have:

$$M = \Sigma c_i V_i = f \Sigma Z_i V_i \tag{8.26}$$

where c_i, V_i and Z_i are concentration, volume and fugacity capacity of sphere number i. Levels 1 and 2 are usually sufficient to calculate the environmental risk of a chemical. For Level 1 calculations the fugacity capacities are found from Table 8.15 and Eq. (8.26) is applied to find f, because the total emission and the volumes of the spheres are known. The concentrations are then easily determined from $c_i = f Z_i$. The amounts in the spheres are found from the concentrations times the volumes of the spheres. Example 8.1 illustrates these calculations.

Example 8.1

A chemical compound has a molecular weight of 200 g/mole and a water solubility of 20 mg/l, which gives a vapour pressure of 1 Pa. The distribution coefficient octanol–water is 10,000 and the K_{ac} = 4000. How will an emission of 1000 moles be distributed in a region with an atmosphere of 6×10^8 m^3, a hydrosphere of 6×10^6 m^3, a lithosphere of 50.000 m^3 with a specific gravity of 1.5 kg/l and an organic carbon content of 10%. Biota (fish) is estimated to be 10 m^3 (specific gravity 1.00 kg/l and a lipid content of 5%. The temperature is presumed to be 20°C.

Solution

Fugacity capacities:
$Z_a = 1/RT = 1/8.314 * 293 = 0.00041$ mol/m^3 Pa
$Z_w = (20/200)/1 = 0.1$ moles/m^3 Pa
$Z_s = 0.1\times0.1\times4000 = 40$ moles/m^3 Pa
$Z_{biota} = 0.1\times0.05\times10.000 = 50$ moles/m^3 Pa
$\Sigma Z_i V_i = 0.00041\times6\times10^8 + 0.1\times6\times10^6 + 40\times50.000 + 10\times50 = 2846500$ moles/Pa
$f = M/\Sigma Z_i V_i = 1000/2846500 = 3.51\times10^{-4}$

Concentrations:
$c_a = f Z_a = 3.51\times10^{-4} \times 0.00041 = 1.44\times10^{-7}$ moles/m^3
$c_w = f Z_w = 3.51\times10^{-4} \times 0.1 = 3.51\times10^{-5}$ moles/m^3
$c_s = f Z_s = 3.51\times10^{-4} \times 40 = 1.404\times10^{-2}$ moles/m^3
$c_{biota} = f Z_{biota} = 3.51\times10^{-4} \times 50 = 1.755\times10^{-2}$ moles/m^3

Amounts:
$M_a = c_a V_a = 1.44\times10^{-7}$ mol/m^3 $\times$ 6×10^8 m^3 = 86 moles
$M_w = c_w V_w = 3.51\times10^{-5}$ mol/m^3 $\times$ 6×10^6 m^3 = 211 moles
$M_s = c_s V_s = 1.404\times10^{-2}$ mol/m^3 $\times$ 50.000 m^3 = 702 moles
$M_{biota} = c_{biota} V_{biota} = 1.755\times10^{-2}$ mol/m^3 $\times$ 10 m^3 = 0.2 moles

The sum of the four amounts is 999.2, which is in good accordance with the total emission of 1000 moles.

Fugacity models, Level 2, presume a steady-state situation, but with a continuous *advection* to and from the phases and a continuous reaction (decomposition) of the chemical considered. Steady state implies that input = output + decomposition. The following equation is therefore valid:

$$E + \Sigma Gin_i \times c_{i\,\mathrm{ind}} = \Sigma Gout_i \times c_i + \Sigma V_i c_i k_i \tag{8.27}$$

where E is the emission and Gin_i is the advection into phase i, $c_{i\,\mathrm{ind}}$ is the concentration in the inflow, $Gout_i$ is the outflow by advection, c_i is the concentration in phase i and $V_i c_i k_i$ is the reaction of the considered component in phase i. As $c_i = fZ_i$, we get the following equation:

$$E + \Sigma Gin_i c_{i\,\mathrm{ind}} = f(\Sigma Gout_i Z_i + \Sigma V_i c_i k_i) \tag{8.28}$$

f is therefore the total amount of the component going into phase i divided by $(\Sigma Gout_i Z_i + \Sigma V_i Z_i k_i)$. We can often presume that $Gin_i = Gout_i$ is denoted G_i. The concentration in the phase is as usual $f Z_i$. The amount is correspondingly the concentrations in the phase multiplied by the volume. The turnover rate of the compound in phase i is $f(G_i Z_i + V_i c_i k_i)$. Example 8.2 illustrates these calculations.

Example 8.2

In an area consisting of 10,000 m^3 atmosphere, 1000 m^3 of water, 100 m^3 of soil and 10 m^3 of biota the same chemical compound as mentioned in Example 8.1 is emitted. This means that the same *fugacity capacities* can be applied:

Fugacity capacities:

$Z_a = 1/RT = 1/8.314 * 293 = 0.00041$ moles/m^3 Pa
$Z_w = (20/200)/1 = 0.1$ moles/m^3 Pa
$Z_s = 0.1 \times 0.1 \times 4000 = 40$ moles/m^3 Pa
$Z_{biota} = 0.1 \times 0.05 \times 10{,}000 = 50$ moles/m^3 Pa

10,000 m^3/24 h of air with a contamination corresponding to a concentration of 0.01 moles/m^3 and 10 m^3/24 h of water with a concentration of the chemical on 1 mole/m^3 is flowing into the area by advection. Within the area an emission of 500 moles/24 h takes place. *Decomposition* of the chemical takes place with a rate coefficient for air, water, soil and biota of 0.001 1/24 h; 0.01 1 24 h and 0.1 1/24 h (soil and biota), respectively. What will the concentration of the chemical be as a result of a steady-state situation in the various spheres?

Solution

The total amount of chemical entering the area is 500 + 100 + 10 = 610 moles/24 h.

The following table summarizes the calculations:

Phase	Volume	Z_i	G_iZ_i	$V_iZ_ik_i$	c_i	M_i	Conv. rate
Air	10,000	0.00041	4.1	0.0041	0.00055	5.5	5.48
Water	1000	0.1	1.0	1.0	0.134	134	2.67
Soil	100	40	0	400	53.5	5350	534.8
Biota	10	50	0	50	66.9	669	66.9
			5.1	451			609.9

f is the total in-flowing amount of the chemical divided by $(\Sigma G_i Z_i + \Sigma V_i Z_i k_i) = 610/456.1 = 1.337$. The concentrations are found as $c_i = fZ_i$. The total conversion/24 h is 609.9 moles, in good accordance with the total input of 610 moles.

Transfer rates between two phases by *diffusion* are expressed by the following equation (models per unit of area and time):

$$N = D * \Delta f \tag{8.29}$$

where N is the rate of transfer, D is the diffusion coefficient and Δf is the difference in *fugacity*. D is the total resistance for the transfer consisting of the resistances of the two phases in series. Notice that D may be found as $K * Z$, where K is the transfer coefficient and Z is the fugacity capacity defined above.

The so-called 'unit world model' consists of six compartments: air, water, soil, sediment, suspended sediment and biota. This simplified model aims to identify the partition between these six compartments of toxic substances emitted to the environment. The volumes and densities of the unit world and the definition of *fugacity capacities* are given in Table 1, Appendix 3. The average *residence time*, *tr*, due to reactions may be found using the following equation:

$$tr = M/E \tag{8.30}$$

and the overall rate constant, K, is E/M or $1/tr$.

The third level is devoted to a steady-state, non-equilibrium situation, which implies that the fugacities are different in each phase. Equation (8.29) is used to account for the transfer. The D values may be calculated from quantities such as interface areas, mass transfer coefficients (as indicated above D is the product of the transfer coefficient and the fugacity capacity: $D = K * Z$), release rate of chemicals into phases such as biota or sediment, and Z values, or by using the estimation methods presented in Section 8.5.

Level 4 involves a dynamic version of Level 3, where emissions and thus concentrations, vary with time. This implies that differential equations must be applied for each compartment to calculate the change in concentrations with time, for instance:

$$V_i * dC_i/dt = E_i - V_i * C_i * k_i - \sum D_{ij} * \Delta f_{ij} \quad (8.31)$$

This model level is similar in concept to the *EXAMS model* (see Mackay et al., 1992).

Levels 1 or 2 are usually sufficient, but if the environmental management problem requires the prediction of:

1. the time taken for a substance to accumulate to a certain concentration in a phase after emission has started, or
2. the length of time for the system to recover after the emission has ceased,

then the fourth level must be applied.

This approach has been widely used and a typical example is given by Mackay (1991). It concerns the *distribution* of *PCB* between air and water in the Great Lakes. Here *He* is 49.1 and the distribution coefficient for air/water (= $He/R * T$) was therefore 0.02. The unit for *C* is mole/m^3. The fugacity capacity for water = $1/He$ was 0.0204 and the fugacity capacity for air = $1/R * T$ = 0.000404. The distribution coefficient between water and suspended matter in the water was estimated to be 100,000. As the concentration of suspended matter in the Great Lakes was 2×10^{-6} on a volume basis (approximately 4 mg/l, the density being 2000 g/l), the fraction dissolved was 1/(1 + 0.2) = 0.833.

PCB concentration in water of the *Great Lakes* was 2 ng/l, and in the air 2 ng/m^3. The *fugacity* can be calculated in water and air as *C/Z* and it was found that the fugacity in water is (2000×0.83317/0.0204) / (2/0.000404), ≈ 17 times higher than in air, which implies that volatilization will occur. If it is assumed that the *transfer coefficient* in water is 10^{-5} m/s and in air 10^{-3} m/s, the volatilization rate can be calculated from the traditional two-resistance model, using the relation:

$$D = K * Z \quad (8.32)$$

to find the overall *diffusion coefficient, D*.

$$1/D = 1/10^{-5}\times0.0204 + 1/10^{-3}\times0.000404 \quad (8.33)$$

D is found to be 1.36×10^{-7}. *N*, the *transfer rate* is calculated by the use of (8.29):

$$N = D\,(f_w - f_a) = D(2.8\times10^{-7} - 1.53\times10^{-8}) \quad (8.34)$$

N is thus found be to be 35.9×10^{-15} mol/m^2/s.

It can be shown that the transfer with precipitation is negligible compared with the volatilization rate, while the washout of particles and dry deposition are important processes. If these processes are considered, the net flux to the atmosphere becomes about 75% of the flux found above.

Many *fugacity models* have been developed since the mid-1980s with the common idea of answering the following pertinent questions: where would a given chemical compound released to the environment do most harm? What concentrations are we talking about and what effects should be expected?

PROBLEMS

1. Corresponding values of lead in sediment and lead in lobster are observed as follows (unit mg/kg dry matter):

Lead in lobster	Lead in sediment
23	450
44	980
12	306
89	2200
78	1921

   - Steady state can be considered. It may be estimated that lobsters are approximately 20 cm long, while *Mytilus edulis* are about 4 cm long. The concentration of lead in the water is negligible.
   - Are these results consistent with the results in Section 8.6? BCF for *Mytilus edulis* is 1230. Which concentration factor would be expected for lobsters? Which sediment concentration will be required to ensure that the lobsters will have 2 mg/kg dry matter of lead or less?

2. A chemical compound has a molecular weight of 320 g/mole and a water solubility of 1 mg/l, which gives a vapour pressure of 2 Pa. Find an approximate value for the octanol–water distribution coefficient and for the distribution between water and soil with 4% organic carbon.
   - How will an emission of 2000 moles be distributed in a region with 6,000,000 m^3 air, 500,000 water m^3, 80,000 m^3 of soil (4% organic carbon, specific gravity of 2 kg/l and 20 m^3 biota (specific gravity 1.00 kg/l and a lipid content of 8%)? Room temperature is presumed.

3. A chlorophenol has a solubility in water of 1.2 mg l^{-1}. Find the approximate concentration factor for mussels (length about 5 cm) using the methods presented in this chapter.

4. The water solubility of nitrobenzene is 1.27 g/l at room temperature.
   - (a) Estimate the concentration factor for fish of length 20–30 cm.
   - (b) Estimate the concentration factor for blue mussels of length 5 cm.
   - (c) Estimate the ratio between nitrobenzene adsorbed to activated sludge and dissolved in water in an activated sludge plant.
   - (d) Do you estimate nitrobenzene to be readily biodegradable, slowly biodegradable, very biodegradable or refractory? Explain your answers from the molecular formula.
   - (e) On the basis of your answers to questions (c) and (d), where would you expect to find nitrobenzene after an activated sludge plant: in the treated water, in the sludge or would it be decomposed?

5. A considerable amount of polyaromatic hydrocarbons, PAH, has been dumped on a rubbish dump. The environmental department of the city fears that the ground water will be contaminated.
   - (a) Calculate the % of PAH adsorbed to the soil and in equilibrium with PAH in soil water. The soil is known to contain 10% carbon. Assume that $\log K_{ow} = 5.5$.
   - (b) Henry's constant for the mixture of PAH is 0.002 atm. What is the concentration in air in equilibrium with soil water containing 80 mg/l? Is it expected that PAH will be removed relatively rapidly by evaporation?
   - (c) The biodegradation can be described by a first-order reaction with a rate constant of 0.005 l/24 h. Is this biodegradation in accordance with the expected biodegradation of PAH (assume that it consists of 3–4 aromatic rings)?
   - (d) If the initial concentration is 80 mg/l what would the concentration be after 180 days, if we assume that biodegradation is the only removal process?

6. Explain why the concentration of most micropollutants in an organism increase with time (and weight of the organism).

7. DDT has been banned and in many countries at least partly replaced by chlordane. Estimate the difference in physical–chemical properties between the two pesticides based on their chemical structure. What difference is expected in the bioaccumulation and persistence of these two substances?

8. What is the expected difference in environmental behaviour between phenoxyacetic acid containing the COOH group and the corresponding sodium salt containing COONa? What would be the difference between the two forms in relation to accumulation in soil and evaporation? Use the results to indicate how pH will influence these properties for phenoxyacetic acid?

9. What would be the difference in biodegradability of a branched alkylsulphonate (carbon chain with 12 C-atoms, 7 branches) and a completely linear alkylsulphonate with the same number of carbon atoms. Use the rules presented in the text to indicate the difference semi-quantitatively.

10. Log K_{ow} for atrazine is 2.75. Estimate the distribution between soil with 1.8% organic carbon and water for atrazine. What would be the estimated ratio of the concentration in carrots with 0.6% lipid to the concentration in soil grown in atrazine contaminated soil?

11. The following contaminants have been found in the soil of an industrial site: benzene, toluene, chloropyrifos and phenol. Evaluate the potential for these four compounds to contaminate the ground water. The following properties are available for the four compounds:

Compound	Vapour pressure (mm Hg)	Water solubility (mg/l)	log (Soil sorption coeff.) (–)
Benzene	76	1780	3.3
Toluene	10	515	3.5
Phenol	0.2	67,000	2
Chloropyrifos	0.00002	2	4.1

12. Indicate by an x in Table I below in which classes the eight compounds in the table belong. Class 1 covers the compounds that are decomposed at least 10% in a biological treatment plant and eventually after adaptation significantly more than 10%. Class 2 comprises compounds that are 1–10% biodegraded in a biological treatment plant, while Class 3 means that the compounds are not biodegraded (<1%) in a biological treatment plant.

    – Are the compounds that are not biodegraded (Classes 2 and 3) accumulated in the water or in the sludge phase?

Table I

Compound	Class 1	Class 2	Class 3
Ethyleneglycol			
1,3 dichloranthracene			
2,3,4-trinitrophenol			
DDT			
PCB			
Glycerine			
Dioxin			
Pentachlorphenol			

13. Hexachlorobenzene has an octanol/water partition coefficient of 106,18. Find the approximate concentration factor for 25–30 cm length fish.
    - Also find BCF for blue mussels (length approximately 5 cm) presuming the same % fat tissue.
    - Finally, find the concentration of hexachloro-benzene in soya beans with a lipid content of 8.5% cultivated in soil with 2% organic carbon and with a concentration of hexachloro-benzene of 12 mg/kg dry matter.
14. It is found that a dioxin has a BCF value for 25 cm fish of 12,000. The fat content of the fish used for the experiment is 7%.
    - What would be the BCF for a fish with 1% fat content?
    - What would be the BCF for a fish of the length 1 m with a fat content of 2%?

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CHAPTER 9

Recent Developments in Ecological and Environmental Modelling

9.1 Introduction

Models of ecosystems attempt to capture the characteristics of ecosystems. However, ecosystems differ from most other systems by being extremely adaptive, having both the ability of self-organization and a large number of feedback mechanisms. The real challenge to modelling is: how can we construct models that are able to reflect these characteristics? Some recent developments have attempted to answer this question. Section 9.2 will focus on the characteristics of ecosystems and Section 9.3 is devoted to development of what are termed structurally dynamic models or variable parameter models—sometimes also called the fifth generation of models. Section 9.4 presents three illustrative examples of structurally dynamic models which will probably be used increasingly in the coming years in our endeavour to make better prognoses, because reliable prognoses can only be made by models with a correct description of ecosystem properties. If our models do not properly describe adaptation and possible shifts in species composition, the prognoses will inevitably be less incorrect.

Another recent discussion within ecosystem theory and ecological modelling concerns the possibility of ecosystems showing chaotic and catastrophic behaviour. Chaos theory has raged like a steppe fire throughout all the sciences during the last two decades. It has resulted in new insights, particularly into the behaviour of systems. It is therefore obvious to try to use chaos theory in modelling and the results of the considerations will be presented in Section 9.5; Section 9.6 will show the application of catastrophe theory in modelling.

Finally, Section 9.7 gives an overview of some new tools in modelling such as the application of *artificial intelligence*, *object oriented models*, *individual based models* and *fuzzy models*.

Many of these developments are almost routine in modelling, but as they have only been developed and used comprehensively in ecological modelling in the last decade, we still consider them to be "recent developments" or "current trends" in modelling. Hopefully, the reader will peruse this last chapter of the book with particular interest and hence will become just as enthusiastic for modelling as the authors.

9.2 Ecosystem Characteristics

Ecology deals with *irreducible systems* (Wolfram, 1984a,b; Jørgensen, 1990a,b; 1992a,b). We cannot design simple experiments to reveal a relationship which can be transferred in all its detail from one ecological situation and one ecosystem to different situation in another ecosystem. This is possible with, for instance, Newton's laws of gravity because the relationship between forces and acceleration is reducible. The relationship between force and acceleration is linear, but the growth of living organisms is dependent on many *interacting* factors, which again are functions of time. Feedback mechanisms will simultaneously regulate all the factors and rates; they also interact and are functions of time, too (Straskraba, 1980).

Table 9.1 shows the *hierarchy* of the *regulation mechanisms* that are operating at the same time. From this example the complexity alone clearly prohibits the reduction to simple relationships that can be used repeatedly.

An ecosystem has so many interacting components that it is impossible ever to be able to examine all these relationships; even if we could, it would be impossible to separate one relationship and examine it carefully to reveal its details because it works differently in nature (where it interacts with many other processes) from when

Table 9.1. The *hierarchy* of regulating *feedback mechanisms* (Jørgensen, 1988)

Level	Explanation of regulation process	Exemplified by phytoplankton growth
1.	Rate by concentration in medium	Uptake of phosphorus in accordance with phosphorus concentration
2.	Rate by needs	Uptake of phosphorus in accordance with intracellular concentration
3.	Rate by other external factors	Chlorophyll concentration in accordance with previous solar radiation
4.	Adaptation of properties	Change of optimal temperature for growth
5.	Selection of other species	Shift to better fitted species
6.	Selection of other food web	Shift to better fitted food-web
7.	Mutations, new sexual recombinations and other shifts of genes	Emergence of new species or shifts of species properties

we examine it in a laboratory (where the relationship is separated from the other ecosystem components). Compare also with Section 2.11 on quantum theory and modelling.

This observation—that it is impossible to separate and examine processes in real ecosystems—corresponds with that of the examinations of organs which are separated from the organisms in which they work. Their functions are completely different when separated from their organisms and examined in, e.g., a laboratory from when they are placed in their right context and in "working" condition.

These observations are indeed expressed in ecosystem ecology. A well known phrase is: "everything is linked to everything" or "the whole is greater than the sum of the parts" (Allen, 1988). It implies that it may be possible to examine the parts by reduction to simple relationships, but when the parts are put together they will form a whole which behaves differently from the sum of the parts. This statement requires a more detailed discussion of how an ecosystem works.

Allen (1988) claims that the latter statement is correct, because of the evolutionary potential hidden within living systems. The ecosystem contains within itself the possibility of becoming something different, i.e., of adapting and evolving. The evolutionary potential is linked to the existence of microscopic freedom, represented by *stochasticity* and non-average behaviour, resulting from the diversity, complexity and variability of its elements.

Underlying the taxonomic classification is the microscopic diversity, which only adds to the complexity to such an extent that it is completely impossible to cover all the possibilities and details of the observed phenomena. We attempt to capture at least a part of the reality by the use of models. It is not possible to use one or a few simple relationships, but a model seems to be the only useful tool when we are dealing with irreducible systems. However, one model is so far from reality that we need many models; we need many models simultaneously to capture a more complete image of reality. This seems to be our only possibility of dealing with the very complex living systems.

This has been acknowledged by holistic ecology or systems ecology, while the more reductionistic ecology attempts to understand ecological reactions by analysis of one or at the most a few processes, which are related to one or two components. The results of analyses are expanded to be used in the more *reductionistic* approaches as a basic explanation of observations in real ecosystems, but such an extrapolation is often not valid and leads to false conclusions.

Both analyses and syntheses are needed in ecology; the analysis is a necessary foundation for the synthesis, but may lead to wrong scientific conclusions to stop at the analysis. Analysis of several interacting processes may give a correct result of the processes under the conditions analyzed, but the conditions in ecosystems are constantly changing and even if the processes were unchanged (which they very rarely are), it is not possible to review the analytical results of so many simultaneously working processes. Our brain simply cannot review what will happen in a system where, let us say, only six interacting processes are working simultaneously.

Reductionism does not consider that:

1. the basic conditions determined by the external factors for our analysis are constantly changing (one factor is typically varied by an analysis, while all the others are assumed constant) in the real world and the analytical results are therefore not necessarily valid in the system context.
2. the interaction of all the other processes and components may change the processes and the properties of all biological components significantly in the real ecosystem and the analytical results are therefore not valid at all.
3. a direct overview of the many processes simultaneously working is not possible and wrong conclusions may in any case be the result even if it is attempted.

The conclusion is, therefore, that we need a tool to provide an overview of and synthesize the many interacting processes. In the first instance, the synthesis may just "put together" the various analytical results, but afterwards we need to make changes to account for an additional effect resulting from the fact that the processes are working together and thereby become more than the sum of the parts, in other words they show a synergistic effect—a symbiosis. It was mentioned in Chapter 6 how important the indirect effects are compared with the direct effects in an ecological network.

Modelling can meet our need for a synthesizing tool. It is our only hope for a further synthesis of our knowledge to attain a *system-understanding* of ecosystems which will enable us to cope with the environmental problems threatening the survival of mankind.

A massive scientific effort is needed to teach us how to cope with ecological complexity, or even with complex systems in general.

- Which tools should we use to attack these problems?
- How do we use the tools with most efficiency?
- Which general laws are valid for complex systems with many feedbacks and particularly for living systems?
- Have all hierarchically organized systems with many hierarchically organized feedbacks and regulations the same basic laws?
- What do we need to add to these laws for living systems?

Ulanowicz (1986) calls for holistic descriptions of ecosystems. Holism is taken to mean a description of the system level properties of an ensemble, rather than simply an exhaustive description of all the components. It is thought that by adopting a holistic viewpoint, certain properties become apparent and other behaviours are made visible that otherwise would be undetected.

It is clear, however, from this discussion that the complexity of ecosystems has set the limitations for our understanding and for the possibilities of proper management. We cannot capture the complexity as such in *all* its details, but we can understand how ecosystems are complex and we can set up a realistic strategy for

how to get sufficient knowledge about the system—not knowing all the details, but still understanding and knowing the mean behaviour and the important reactions of the system. This means that we can only try to reveal the basic properties *behind* the complexity.

We have no other choice than to "go holistic". The results from the more reductionistic ecology are essential in our effort "to go to the root" of the system properties of ecosystems, but we need systems ecology, which consists of many new ideas, approaches and concepts, in order to follow the path to the roots of the basic system properties of ecosystems. The idea may also be expressed in another way: we cannot find the properties of ecosystems by analysing all the details, because there are simply too many, but by trying to reveal the system properties of ecosystems by examining the entire systems.

- **The number of *feedbacks* and regulations is extremely high and makes it possible for living organisms and populations to survive and reproduce in spite of changes in external conditions.**

These regulations correspond to Levels 3 and 4 in Table 9.1. Numerous examples can be found in the literature. If the actual properties of the species are changed, the regulation is called adaptation. Phytoplankton, for instance, is able to regulate its chlorophyll concentration according to the solar radiation. If more chlorophyll is needed because the radiation is insufficient to guarantee growth, more chlorophyll is produced by the phytoplankton. The digestion efficiency of the food for many animals depends on the abundance of the food. The same species may be of different sizes in different environments, depending on what is most beneficial for survival and growth. If nutrients are scarce, phytoplankton becomes smaller and *vice versa*. In this latter case the change in size is a result of a selection process, which is made possible because of the distribution in size.

Furthermore, the feedbacks are constantly changing, i.e., the adaptation itself is adaptable in the sense that if a regulation is not sufficient, another regulation process higher in the hierarchy of feedbacks (see Table 9.1) will take over. The change in size within the same species is, for instance, limited. When this limitation has been reached, other species will take over. This implies that not only the processes and the components but also the feedbacks can be replaced if it necessary for achieving a better utilization of the available resources.

Three different concepts have been used to explain the functioning of ecosystems.

1. *The individualistic or Gleasonian concept* assumes that populations respond independently to an external environment.

2. *The superorganism or Clementsian concept* views ecosystems as organisms of a higher order and defines succession as ontogenesis of this super-organism, see

e.g., self-organization of ecosystems (Margalef, 1968). Ecosystems and organisms differ, however, in one important aspect. Ecosystems can be dismantled without destroying them; they are just replaced by others, such as agro-ecosystems or human settlements or other succession states. Patten (1991) has pointed out that the indirect effects in ecosystems are significant compared with the direct ones, while in organisms the direct linkages will be most dominant. An ecosystem has more linkages than an organism, but most of them are weaker. It makes the ecosystem less sensitive to the presence of *all* the existing linkages. It does not imply that the linkages in ecosystems are insignificant and do not play a role in ecosystem reactions. The ecological network is of great importance in an ecosystem, but the many and indirect effects give the ecosystem buffer capacities to deal with minor changes in the network. The description of ecosystems as super-organisms seems therefore insufficient.

3. *The hierarchy theory* (Allen and Starr, 1982) insists that the higher-level systems have emergent properties that are independent of the properties of their lower-level components. This compromise between the two other concepts seems consistent with our observations in nature.

   The hierarchical theory is a very useful tool for understanding and describing such complex "medium number" systems as ecosystems (O'Neill et al., 1986).

During the last decade a debate has arisen on whether *"bottom-up"* (limitation by resources) or *"top-down"* (control by predators) effects primarily control the system dynamics. The conclusion of this debate seems to be that both effects control the dynamics of the system. Sometimes the effect of the resources may be most dominant, sometimes the higher levels control the dynamics of the system and sometimes both effects determine the dynamics of the system. This conclusion is nicely presented in "Plankton Ecology" by Sommer (1989).

The ecosystem and its properties emerge as a result of many simultaneous and parallel focal-level processes, as influenced by even more remote environmental features. This means that the ecosystem itself will be seen by an observer to be factorable into levels. Features of the immediate environment are enclosed in entities of yet larger scale and so on. This implies that the environment of a system includes historical factors as well as immediately cogent ones (Patten, 1991). The history of the ecosystem and its components is therefore important for the reactions and further development of the ecosystem. This is one of the main ideas behind Patten's indirect effect: that the indirect effect accounts for the "history", while the direct effect only reflects the immediate effect. The importance of the history of the ecosystem and its components emphasizes the need for a dynamic approach and supports the idea that we will never observe the same situation in an ecosystem twice. The history will always be "between" two similar situations. Therefore, as mentioned above, the equilibrium models may fail in their conclusions, particularly when we want to look into reactions at the system level.

- **Ecosystems show a high degree of heterogeneity in space and in time**

An ecosystem is a very dynamic system. All its components and particularly the biological ones are steadily moving and their properties are steadily modified, which is why an ecosystem will never return to the same situation again.

Furthermore, every point is different from any other point and offers different conditions for the various life forms.

This enormous heterogeneity explains why there are so many species on earth. There is an ecological niche for "everyone" and "everyone" may be able to find a niche where he or she is best fitted to utilize the resources.

Ecotones, the transition zones between two ecosystems, offer a certain variability in life conditions, which often results in a particular richness of species diversity. Studies of ecotones have recently drawn much attention from ecologists, because *ecotones* have pronounced gradients in the external and internal variables, which give a clearer picture of the relationship between external and internal variables.

Margalef (1991) claims that ecosystems are anisotropic, meaning that they exhibit properties with different values, when measured along axes in different directions. This means that the ecosystem is not homogeneous in relation to properties concerning matter, energy and information, and that the entire dynamics of the ecosystem works towards increasing the differences.

These variations in time and space make it particularly difficult to model ecosystems and to capture their essential features. However, the hierarchy theory (see Section 6.3) applies these variations to develop a natural hierarchy as a framework for ecosystem descriptions and theory. The strength of the hierarchy theory is that it facilitates the study and modelling of ecosystems.

- **Ecosystems and their biological components, the species, evolve steadily and in the long-term perspective toward higher complexity**

Darwin's theory describes the competition among species and states that the species that are best fitted to the prevailing conditions in the ecosystem will survive. Darwin's theory can, in other words, describe the changes in ecological structure and species composition, but cannot be directly applied quantitatively, e.g., in ecological modelling (see, however the next Section).

All species in an ecosystem are confronted with the question: how is it possible to survive or even grow under the prevailing conditions? The prevailing conditions are considered as *all* factors influencing the species, i.e., all external and internal factors including those originating from other species. This explains co-evolution, as any change in the properties of one species will influence the *evolution* of the other.

All natural external and internal factors of ecosystems are dynamic—the conditions are steadily changing and there are always many species waiting in the wings, ready to take over, if they are better fitted to the emerging conditions than the species dominating under the present conditions. There is a wide spectrum of species representing different combinations of properties available for the ecosystem. The question is, which of these species are best able to survive and grow under the

present conditions and which species are best able to survive and grow under the conditions one time step further and two time steps further and so on? The necessity in Monod's sense is given by the prevailing conditions—the species must have genes or maybe phenotypes (meaning properties) that match these conditions in order to be able to survive. But the natural external factors and the genetic pool available for the test may change randomly or by chance.

Steadily, new *mutations* (misprints are produced accidentally) and *sexual re-combinations* (the genes are mixed and shuffled) emerge and give new material to be tested by the question: which species are best fitted under the conditions prevailing just now?

These ideas are illustrated in Fig. 9.1. The *external factors* are steadily changed, some even relatively quickly, partly at random, such as meteorological or climatic factors. The species of the system are selected among the species available and represented by the genetic pool, which again is slowly but surely changed randomly or by chance. The selection in Fig. 9.1 includes Level 4 of Table 9.1. It is a selection of the organisms that possess the properties best fitted to the prevailing organisms according to the frequency distribution. What is called ecological development is the change over time in nature caused by the dynamics of the external factors, giving the system sufficient time for the reactions.

Evolution, on the other hand, is related to the genetic pool. It is the result of the relationship between the dynamics of the external factors and the dynamics of the genetic pool. The external factors steadily change the conditions for survival and the genetic pool steadily comes up with new solutions to the problem of survival.

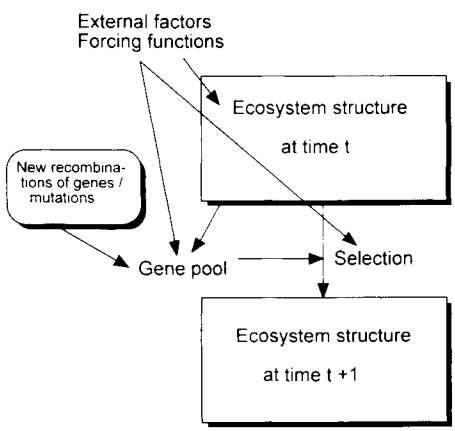

Fig. 9.1. *Conceptualization* of how the external factors steadily change the species composition. The possible shifts in species composition are determined by the gene pool, which is steadily changed due to mutations and new sexual re-combinations of genes. The development is, however, more complex. This is indicated by (1) arrows from "structure" to "external factors" and "selection" to account for the possibility that the species can modify their own environment (see below) and thereby their own selection pressure; (2) an arrow from "structure" to "gene pool" to account for the possibility that the species can to a certain extent change their own gene pool.

The species are continuously tested against the prevailing conditions (external as well as internal factors) and the better they are fitted, the better they are able to maintain and even increase their biomass. The specific rate of population growth may even be used as a measure for the fitness (see, e.g., Stenseth, 1986). But the property of fitness must of course be inheritable to have any effect on the species composition and the ecological structure of the ecosystem in the long run.

Natural selection has been criticized for being a tautology: fitness is measured by survival, and survival of the fittest therefore means survival of the survivors. However, the entire Darwinian theory including the above-mentioned three assumptions cannot be conceived as a tautology, but may be interpreted as follows: the species offer different solutions to survival under given prevailing conditions and the species that have the best combinations of properties to match the conditions also have the highest probability of survival and growth.

- **Man-made changes in external factors, i.e., anthropogenic pollution, have created new problems, because new genes fitted to these changes do not develop overnight, while most natural changes have occurred many times previously and the genetic pool is therefore prepared and fitted to meet the natural changes. The spectrum of genes is able to meet most natural changes, but not all the man-made changes, because they are new and untested in the ecosystem.**

Evolution moves towards increasing *complexity* in the long term. The fossil records have shown a steady increase in species diversity. There may be destructive forces (e.g., man-made pollution or natural catastrophes) for a shorter time but the probability that

1. new and better genes are developed and
2. new ecological niches are utilized

will increase with time. The probability will even increase faster and faster—again excluding the short time perspective—as the probability is roughly proportional to the amount of genetic material on which the mutations and new sexual recombinations can be developed.

It is equally important to note that a biological structure is more than an active non-linear system. In the course of its evolution, the biological structure is continuously changed so that its structural map is itself modified. The overall structure thus becomes a representation of all the information received. Biological structure represents through its complexity a synthesis of the information with which it has been in communication (Schoffeniels, 1976).

Evolution is possibly the most discussed topic in biology and ecology and millions of pages have been written about evolution and its ecological implications. Today the facts of evolution are taken for granted and interest has shifted to more subtle classes of fitness/selection, i.e., towards an understanding of the complexity of evolutionary processes. One of these classes concerns traits that influence not only the fitness of the individuals possessing them, but also the entire population. These traits overtly

include social behaviours, such as aggression or cooperation, and activities that through some modification of the biotic and *abiotic environment* feedback to affect the population at large, e.g., pollution and resource depletion.

It can be shown that many types of selections actually take place in nature and that many observations support the various selection models that are based on these types of selection. Kin selection has been observed with bees, wasps and ants (Wilson, 1978). Prairie dogs endanger themselves (altruism) by conspicuously barking to warn fellow dogs of an approaching enemy (Wilson 1978) and a parallel behaviour is observed for a number of species.

Co-evolution explains the interactive processes among species. It is difficult to observe a co-evolution, but it is easy to understand that it plays a major role in the entire evolution process. The co-evolution of herbivorous animals and plants is a very good example. The plants will develop a better spreading of seeds and a better defence against herbivorous animals. In the latter case, this will create a selection of herbivorous animals that are able to cope with the defence. Therefore the plants and the herbivorous animals will co-evolve. Co-evolution means that the evolution process cannot be described as *reductionistic*, but that the entire system is evolving. A holistic description of the evolution of the system is needed.

Darwinian and *neo-Darwinian theories* have been criticized from many sides. It has for instance been questioned whether the selection of the fittest can explain the relatively high rate of evolution. Fitness may here be measured by the ability to grow and reproduce under the prevailing conditions. This implies that the question raised according to Darwinian theories (see the discussion above) is: which species have the properties that give the highest ability for growth and reproduction? We shall not go into the discussion in this context—it is another very comprehensive theme—but will just mention that the complexity of the evolution processes is often overlooked in this debate. Many interacting processes in evolution may explain the relatively high rate of evolution observed.

Having presented some main features of ecosystems, the next crucial question is obviously: how can we account for these properties in modelling? Some preliminary results on how to consider Levels 4–6 of dynamics (see Table 9.1) will be presented in the next section.

9.3 Structurally Dynamic Models

If we follow the modelling procedure proposed in Fig. 2.2, we will attain a model that describes the processes in the focal ecosystem, but the *parameters* will represent the properties of the state variables as they are in the ecosystem *during* the examination period. They are not necessarily valid for another period, because we know that an ecosystem can regulate, modify and change them if needed as a response to the change in the prevailing conditions determined by the forcing functions and the interrelations between the state variables. Our present models have rigid structures and a fixed set of parameters, reflecting that no changes or replacements of the

components are possible. However, we need to introduce parameters (properties) that can change according to changing forcing functions and general conditions for the state variables (components) to optimize continuously the ability of the system to move away from thermodynamic equilibrium. We may hypothesize therefore that Levels 5 and 6 in the regulation hierarchy (Table 9.1) can be accounted for in our model by a current change of parameters according to an ecological goal function. The idea is currently to test if a change of the most crucial parameters produces a higher goal function of the system and, if this is the case, to use that set of parameters.

The type of model that can account for the change in species composition as well as for the ability of the species (i.e., the biological components of our models) to change their properties (i.e., to adapt to the prevailing conditions imposed on the species) are sometimes called structurally dynamic models to indicate that they are able to capture structural changes. They may also be called the next or fifth generation of ecological models to underline that they are radically different from previous modelling approaches and can do more, i.e., describe changes in species composition.

It could be argued that the ability of ecosystems to replace present species with other (Level 6 in Table 9.1), better fitted species, can be considered by constructing models encompassing *all* actual species for the entire period that the model attempts to cover. This approach has two essential disadvantages, however. First of all, the model becomes very complex as it will contain many state variables for each *trophic level*. This implies that the model will contain many more parameters which have to be calibrated and validated and, as presented in Sections 2.5 and 2.6, this will introduce a high uncertainty to the model and will render the application of the model very case specific (Nielsen, 1992a,b). Also, the model will still be rigid and not have the property of the ecosystems' continuously changing parameters even without changing the species composition (Fontaine, 1981).

Several goal functions have been proposed, as shown in Table 9.2, but only very few models have been developed which account for change in species composition or for the ability of the species to change their properties within some limits.

Bossel (1992) uses what he calls six basic *orientors* or requirements to develop a system model that can describe the system performance properly. The six orientors are:

1. *Existence*. The system environment must not exhibit any conditions which may move the state variables out of its safe range.

2. *Efficiency*. The exergy gained from the environment should exceed over time the exergy expenditure.

3. *Freedom of action*. The system reacts to the inputs (forcing functions) with a certain variability.

4. *Security*. The system has to cope with the different threats to its security requirement with appropriate but different measures. These measures either

Table 9.2. *Goal functions* proposed

Proposed for	Objective function	Reference
Several systems	Maximum useful power or energy flow	Odum and Pinkerton (1955)
Several systems	Minimum entropy	Glansdorff and Prigogine (1971)
Networks	Maximum ascendency	Ulanowicz (1980)
Several systems	Maximum exergy	Mejer and Jørgensen (1979)
Ecological systems	Maximum persistent organic matter	Whittaker and Woodwell (1971); O'Neill et al. (1975)
Ecological systems	Maximum biomass	Margalef (1968)
Economic systems	Maximum profit	Various authors

aim at internal changes in the system itself or at particular changes in the forcing functions (external environment).

5. *Adaptability.* If a system cannot escape the threatening influences of its environment, the one remaining possibility consists in changing the system itself to cope better with the environmental impacts.
6. *Consideration of other systems.* A system must respond to the behaviour of other systems. The fact that these other systems may be of importance to a particular system may have to be considered with this requirement.

Bossel (1992) applies maximization of a benefit or satisfaction index based upon balancing weighted surplus *orientor* satisfactions on a common satisfaction scale. The approach is used to select the model structure of continuous dynamic systems and is able to account for the ecological structural properties as presented in Table 9.1. The approach seems very promising, but has unfortunately not been applied to ecological systems except in three cases.

Straskraba (1979) uses a maximization of biomass as the governing principle. The model computes the biomass and adjusts one or more selected parameters to achieve the maximum biomass at every instance. The model has a routine which computes the biomass for all possible combinations of parameters within a given realistic range. The combination that gives the maximum biomass is selected for the next time step and so on.

Exergy has been used most widely as a goal function in ecological models, and a few of the available case studies will be presented and discussed in this section. Exergy has two pronounced advantages as goal function compared with entropy and maximum power: it is defined far from thermodynamic equilibrium and it is related to the state variables, which are easily determined or measured. As exergy is not a generally used thermodynamic function, we need first to present this concept.

Exergy expresses energy with a built-in measure of quality like energy. Exergy accounts for natural resources and can be considered as fuel for any system that converts energy and matter in a metabolic process (Schrödinger, 1944). Ecosystems consume energy, and an exergy flow through the system is necessary to keep the

system functioning. Exergy measures the distance from the "inorganic soup" in energy terms, as will be further explained below.

Exergy, Ex, is defined by the following equation:

$$Ex = T_0 \cdot NE = T_0 \cdot I = T_0 \cdot (S_{eq} - S) \tag{9.1}$$

where T_0 is the temperature of the environment, I is the thermodynamic information, defined as NE, NE is the negentropy of system, i.e., = $(S_{eq} - S)$ = the difference between the entropy for the system at thermodynamic equilibrium and the entropy at the present state.

It can be shown that exergy differences can be reduced to differences of other, better known, thermodynamic potentials which may facilitate the computations of exergy in some relevant cases.

As can be seen, the exergy of the system measures the contrast—it is the difference in free energy if there is no difference in pressure, as may be assumed for an ecosystem—against the surrounding environment. If the system is in equilibrium with the surrounding environment the exergy is zero.

Since the only way to move systems away from equilibrium is to perform work on them, and since the available work in a system is a measure of the ability, we have to distinguish between the system and its environment or thermodynamic equilibrium alias the inorganic soup. Therefore it is reasonable to use the available work, i.e., the exergy, as a measure of the distance from thermodynamic equilibrium.

Let us turn to the translation of *Darwin's theory* into thermodynamics (see Section 9.2), applying exergy as the basic concept. Survival implies maintenance of the biomass, and growth means increase of biomass. It costs exergy to construct biomass and biomass therefore possesses exergy, which is transferable to support other exergy (energy) processes. Survival and growth can therefore be measured by use of the thermodynamic concept exergy, which may be understood as *the free energy relative to the environment* (see Eq. 9.1).

Darwin's theory may therefore be reformulated in thermodynamic terms as follows:

- **The prevailing conditions of an ecosystem steadily change and the system will continuously select the species and thereby the processes that can contribute most to the maintenance or even growth of the exergy of the system.**

Ecosystems are open systems and receive an inflow of solar energy. This carries low entropy, while the radiation from the ecosystem carries high *entropy*.

If the power of the *solar radiation* is W and the average temperature of the system is T_1, then the *exergy gain* per unit of time, ΔEx is (Erikson et al., 1976):

$$\Delta Ex = T_1 \cdot W\,(1/T_0 - 1/T_2), \tag{9.2}$$

where T_0 is the temperature of the environment and T_2 is the temperature of the sun. This exergy flow can be used to construct and maintain structure far away from equilibrium.

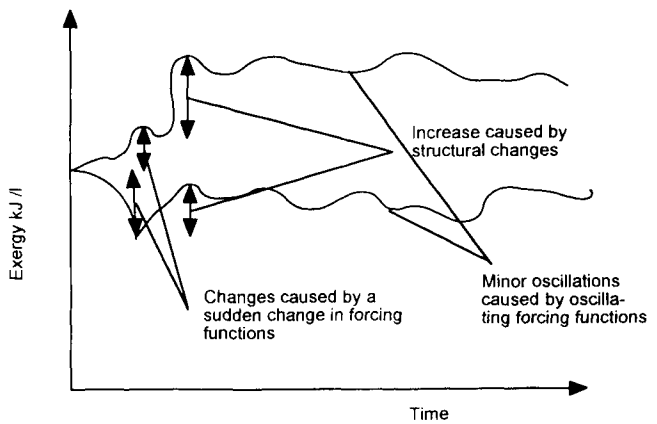

Fig. 9.2. Exergy response to increased and decreased nutrient concentration.

Notice that the thermodynamic translation of Darwin's theory requires that populations have the properties of reproduction, inheritance and variation. The selection of the species that contribute most to the exergy of the system under the prevailing conditions requires that there are enough individuals with different properties for a selection to take place; this means that the reproduction and the variation must be high and that once a change has taken place due to better fitness it can be conveyed to the next generation.

Notice also that the change in exergy is not necessarily ≥ 0; it depends on the changes of the resources of the ecosystem. The proposition claims, however, that the ecosystem attempts to reach the highest possible exergy level under the given circumstances and with the available genetic pool ready for this attempt (Jørgensen and Mejer, 1977; 1979). Compare Fig. 9.2, where the reactions of exergy for a lake ecosystem to an increase and a decrease in nutrient concentrations are shown. It is not possible to measure exergy directly, but it is possible to compute it if the composition of the ecosystem is known. Mejer and Jørgensen (1979) have shown by the use of thermodynamics that the following equation is valid for the components of an ecosystem:

$$Ex = RT \sum_{i=1}^{i=n} (C_i \cdot \ln(C_i / C_{eq,i}) - (C_i - C_{eq,i})) \tag{9.3}$$

where R is the gas constant, T the temperature of the environment (Kelvin), while C_i represents the i'th component expressed in a suitable unit, e.g., for phytoplankton in a lake C_i could be milligrams of a focal nutrient in the phytoplankton per litre of lake water, $C_{eq,i}$ is the concentration of the i'th component at thermodynamic equilibrium, which can be found in Morowitz (1968) and n is the number of components. $C_{eq,i}$ is, of course, a very small concentration of organic components, corresponding to the probability of forming a complex organic compound in an inorganic soup (at

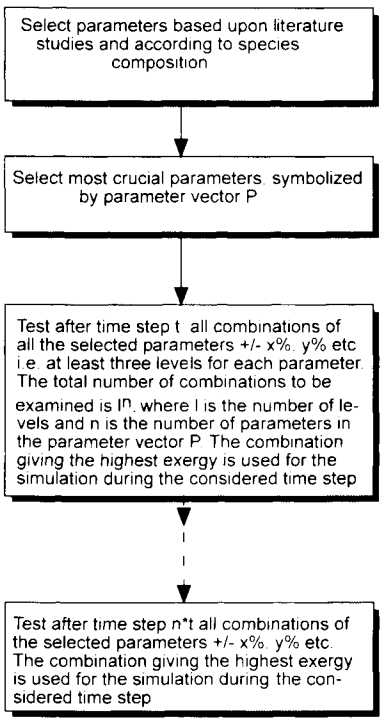

Fig. 9.3. The procedure used for the development of structurally dynamic models.

thermodynamic equilibrium). Morowitz (1968) has calculated this probability and found that for proteins, carbohydrates and fats the concentration is about 10^{-86} μg/l, which may be used as the concentration at thermodynamic equilibrium.

The idea of the new generation of models presented here is continuously to find a new set of parameters (limited for practical reasons to the most crucial, i.e., sensitive parameters) better fitted for the prevailing conditions of the ecosystem. "Fitted" is defined in the Darwinian sense by the ability of the species to survive and grow, which may be measured by the use of exergy (see Jørgensen, 1982, 1986, 1988, 1990; Jørgensen and Mejer, 1977, 1979; Mejer and Jørgensen, 1979; Jørgensen et al., 1995c). Figure 9.3 shows the proposed modelling procedure, which has been applied in the cases presented in Section 9.4.

Exergy has previously been tested as a "goal function" for ecosystem development; see for instance Jørgensen (1986) and Jørgensen and Mejer (1979). However in all these cases the model applied did not include the "elasticity" of the system, obtained by the use of variable parameters, and therefore the models did not reflect real ecosystem properties. A realistic test of the exergy principle would require the application of *variable parameters*.

Exergy is defined as the work the system can perform when it is brought into equilibrium with the environment or another well-defined reference state. If we presume a reference environment for a system at thermodynamic equilibrium, meaning that all the components are: (1) inorganic, (2) at the highest possible oxidation state signifying that all free energy has been utilized to do work, and (3) homogeneously distributed in the system, meaning no gradients, then the situation illustrated in Fig. 9.4 is valid. Szargut (1998) and Szargut et al. (1988) distinguish between *chemical exergy* and *physical exergy*. The chemical energy embodied in organic compounds and biological structure contributes most to the *exergy* content of ecological systems.

Temperature and pressure differences between systems and their reference environments are small in contribution to overall exergy and for present purposes can be ignored. We will compute an *exergy index* based entirely on chemical energy: $\Sigma_i(\mu_c - \mu_{c,o})N_i$, where i is the number of exergy-contributing compounds, c, and μ_c is the chemical potential relative to that at a reference inorganic state, $\mu_{c,o}$. Our (chemical) exergy index for a system will be taken with reference to the same system at the same temperature and pressure, but in the form of an inorganic soup without life, biological structure, information, or organic molecules.

As $(\mu_c - \mu_{co})$ can be found from the definition of the chemical potential, replacing activities by concentrations we obtain the following expression for *chemical exergy*:

$$Ex = RT \sum_{i=0}^{n} c_i \ln c_i / c_{ieq} \qquad [ML^2 T^{-2}] \tag{9.4}$$

R is the gas constant, T is the temperature of the environment and system (Fig. 9.4), c_i is the concentration of the i'th component expressed in suitable units, $c_{i,eq}$ is the concentration of the i'th component at thermodynamic equilibrium, and n is the

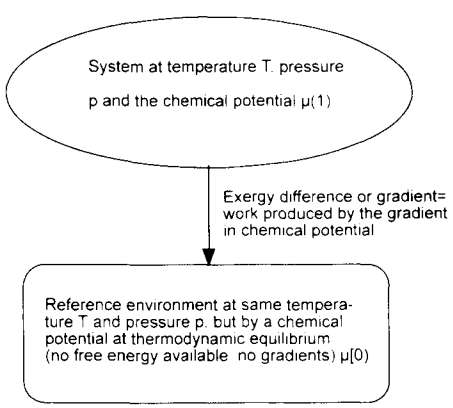

Fig. 9.4. Illustration of the concept of exergy used to compute the *exergy index* for an ecological model. Temperature and pressure are the same for the both the system and the reference state which implies that only the difference in chemical potential can contribute to the exergy.

number of components. The quantity $c_{i,eq}$ represents a very small, but non-zero, concentration (except for $i = 0$, which is considered to cover the inorganic compounds), corresponding to a very low probability of forming complex organic compounds spontaneously in an inorganic soup at thermodynamic equilibrium. The chemical exergy contributed by components in an open system with through-flow is (Mejer and Jørgensen, 1979):

$$Ex = RT\sum_{i=0}^{n}[c_i \ln(c_i / c_{i,eq}) - (c_i - c_{i,eq})] \quad [ML^2 T^{-2}] \tag{9.5}$$

The problem in applying these equations is related to the magnitude of $c_{i,eq}$. Contributions from inorganic components are usually very low and can in most cases be neglected. Shieh and Fen (1982) have suggested that the exergy of structurally complicated material be measured on the basis of elemental composition. For our purposes this is unsatisfactory because compositionally similar higher and lower organisms would have the same exergy, which is at variance with our intent to account for the exergy embodied in information. The problem of assessing $c_{i,eq}$ has been discussed and a possible solution proposed by Jørgensen et al. (1992b, 1997) and Jørgensen et al. (1995c, 2000). The essential arguments are repeated here. The chemical potential of dead organic matter, indexed $i = 1$, can be expressed from classical thermodynamics (e.g., Russel and Adebiyi, 1993) as:

$$\mu_1 = \mu_{1,eq} + RT \ln c_1 / c_{1,eq} \qquad [ML^2 T^{-2} \text{ moles}^{-1}] \tag{9.6}$$

where μ_1 is the chemical potential. The difference $\mu_1 - \mu_{1,eq}$ is known for detritus organic matter, which is a mixture of carbohydrates, fats and proteins. Generally, $c_{i,eq}$ can be calculated from the definition of the probability, $P_{i,eq}$, of finding component i at thermodynamic equilibrium, which is:

$$P_{i,eq} \equiv c_{i,eq} \sum_{i=0}^{n} c_{i,eq} \qquad [1, \text{dimensionless}] \tag{9.7}$$

If this probability can be determined, then in effect the ratio of $c_{i,eq}$ to the total concentration is also determined. As the inorganic component, c_0, is very dominant at thermodynamic equilibrium, Eq. (9.5) can be approximated as:

$$P_{i,eq} \approx c_{i,eq} / c_{0,eq} \qquad [1] \tag{9.8}$$

By a combination of Eqs. (9.4) and (9.6), we get:

$$P_{1,eq} = [c_1 / c_{0,eq}] \exp[-(\mu_1 - \mu_{1,eq}) / RT] \qquad [1] \tag{9.9}$$

For biological components, $i = 2, 3, ..., n$ ($i = 0$ covers inorganic compounds, and $i = 1$ detritus), $P_{i,eq}$, is the probability of producing organic matter, $P_{1,eq}$, and in addition

the probability, $P_{i.a}$, of assembling the genetic information to determine amino acid sequences. Organisms use 20 different amino acids, and each gene determines a sequence of about 700 amino acids (Li and Grauer, 1991). $P_{i.a}$ can be found from the number of permutations among which the characteristic amino acid sequence for the considered organism has been selected. This means that the following two equations are available to calculate P_i:

$$\begin{aligned} P_{i.eq} &= P_{1.eq} P_{i.a} \quad (i \geq 2) \qquad [1] \\ P_{i.a} &= 20^{-700g} \qquad\qquad\qquad [1] \end{aligned} \tag{9.10}$$

where g is the number of genes. Equation (9.6) can be reformulated to:

$$c_{i.eq} \approx P_{i.eq}\, c_{0.eq} \qquad [\text{moles L}^{-3}] \tag{9.11}$$

and Eqs. (9.3) and (9.9) combined to yield for *exergy*:

$$Ex \approx RT \sum_{i=0}^{n} [c_i \ln(c_i / P_{i.eq}, c_{0.eq})) - (c_i - P_{i.eq}\, c_{0.eq})] \quad [\text{ML}^2\,\text{T}^{-2}] \tag{9.12}$$

This equation may be simplified by use of the following approximations (based upon $P_{i.eq} << c_i$, $P_{i.eq} << P_0$, and $1/P_{i.eq} >> c_i$ and $1/P_{i.eq} >> c_{0.eq}/c_i$): $c/c_{0.eq} \approx 1$, $c_i \approx 0$, $P_{i.eq}$ $c_{0.eq} \approx 0$, and the inorganic component can be omitted. The significant contribution comes from $1/P_{i.eq}$ (Eq. 9.8). We obtain:

$$Ex \approx -RT \sum_{i=1}^{n} c_i \ln(P_{i.eq}) \quad [\text{ML}^2\,\text{T}^{-2}] \tag{9.13}$$

where the sum starts from 1 because $P_{0.eq} \approx 1$.

Expressing $P_{i.eq}$ as in Eq. (9.8) and $P_{1.eq}$ as in (9.7), we arrive at the following expression for an *exergy index:*

$$Ex / RT = \sum_{i=1}^{n} [c_i \ln(c_1 / c_{0.eq}) - (\mu_1 - \mu_{1.eq}) \sum_{i=1}^{n} c_i / RT - \sum_{i=2}^{n} c_i \ln P_{i.a} \quad [\text{moles L}^{-3}]$$

As the first sum is minor compared with the other two (use for instance $c_i/c_{0.eq} \approx 1$), we can write:

$$Ex / RT = (\mu_1 - \mu_{1.eq}) \sum_{i=1}^{n} c_i / RT - \sum_{i=2}^{n} c_i \ln P_{i.a} \quad [\text{moles L}^{-3}] \tag{9.14}$$

This equation can now be applied to calculate contributions to the exergy index by significant ecosystem components. If only detritus is considered, we know the free energy released is about 18.7 kJ/g. R is 8.4 J/mole, and the average molecular weight

of detritus is around 10^5. We get the following contribution of exergy by detritus per litre of water, when we use the unit g detritus exergy equivalent/litre:

$$Ex_1 = 18.7\, c_i \text{ kJ/l} \quad \text{or} \quad Ex_1/RT = 7.34\times10^5\, c_i \qquad [ML^{-3}] \tag{9.15}$$

A typical unicellular alga has on average 850 *genes*. We purposely use the number of genes and not the amount of DNA per cell, which would include unstructured and nonsense DNA. In addition, a clear correlation between the number of genes and complexity has been shown (Li and Grauer, 1991). Recently it has begun to be realized that nonsense genes play an important role in the repair of genes when they are damaged. With 850 genes, a sequence of 850 × 700 = 595,000 amino acids can be determined. This represents a contribution of exergy per litre of water, using g/l detritus equivalent as the concentration unit, of:

$$Ex_{algae}/RT = 7.34\times10^5\, c_i - c_i \ln 20^{-595,000} = 25.2\times10^5\, c_i \text{ g/l} \tag{9.16}$$

The contribution to exergy from a simple *prokaryotic cell* can be calculated similarly as:

$$Ex_{prokar}/RT = 7.34\times10^5\, c_i + c_i \ln 20^{529,000} = 17.2\times10^5\, c_i \text{ g/l} \tag{9.17}$$

Organisms with more than one cell will have DNA in all cells determined by the first cell. The number of possible microstates therefore becomes proportional to the number of cells. Zooplankton have approximately 100,000 cells and 15,000 genes per cell (see Table 9.3), each determining the sequence of approximately 700 amino acids. P_{zoopl} can therefore be found as:

$$-\ln P_{zoopl} = -\ln (20^{-15,000\times700}\times10^{-5}) \approx 315\times10^5 \tag{9.18}$$

As shown, the contribution from the numbers of cells is insignificant. $P_{i,a}$ values for other organisms can be found using data such as those in Table 9.3.

With this, an ecologically useful exergy index can be computed based on concentrations of chemical components, c_i, multiplied by *weighting factors*, β_i, reflecting the exergy contents of the various components due to their chemical energy and the information embodied in DNA:

$$Ex = \sum_{i=0}^{n} \beta_i c_i \tag{9.19}$$

Values for β_i based on detritus exergy equivalents are available for a number of different species and taxonomic groups. The unit, detritus exergy equivalents expressed in g/l, can be converted to kJ/l by multiplication by 18.7, which corresponds approximately to the average energy content of 1 g detritus (Morowitz, 1968). The index $i = 0$ for constituents covers inorganic components, but in most cases these will

Table 9.3. Approximate numbers of *non-repetitive genes*

Organisms	Number of *information genes*	*Conversion factor**
Detritus (reference)	0	1
Minimal cells	470	2.7
Bacteria	600	3.0
Algae	850	3.9
Yeast	2000	6.4
Fungi	3000	10.2
Sponges	9000	30
Moulds	9500	32
Trees	10000–30000	30–87
Jellyfish	10000	30
Worms	10500	35
Insects	10000–15000	30–46
Zooplankton	10000–15000	30–46
Fishes	100000–120000	300–370
Amphibians	120000	370
Birds	120000	390
Reptiles	130000	400
Mammals	140000	430
Humans	250000	740

Based on numbers of *information genes* and the *exergy* content of organic matter in the various organisms, compared with the exergy content of detritus (about 18 kJ g). For further details see Jørgensen (1997).

be neglected as contributions from detritus and living biota are much higher due to extremely low concentrations of these components in the reference system. Our exergy index therefore accounts for the chemical energy in organic matter plus the information embodied in living organisms. It is measured from the extremely small probabilities of forming living components spontaneously from inorganic matter. The weighting factors, β_i, may be considered as quality factors reflecting the extent to which different taxa contribute to overall exergy.

9.4 Four Illustrative Structurally Dynamic Case Studies

The use of exergy calculations to vary the parameters continuously has only been used in ten cases of ecological modelling. Four case studies will be shown here as an illustration of what can be achieved by this modelling approach: Søbygaard Lake; two population dynamic models with structural changes; and the development of a structurally dynamic model that can explain success and failure of *biomanipulation* of lakes.

The results from Søbygaard Lake (Jeppesen et al., 1989) are particularly suited to test the applicability of the approach to structurally dynamic models described.

Søbygaard Lake is a shallow lake (depth 1 m) with a short retention time (15–20 days). The nutrient loading was significantly reduced after 1982, namely for phosphorus from 30 g P/m^2 y to 5 g P/m^2 y. The reduced load did not, however, cause reduced nutrients and chlorophyll concentrations in the period 1982–1985 due to an internal loading caused by the storage of nutrients in the sediment (Jeppesen et al., 1989).

Yet radical changes were observed in the period 1985–1988. The recruitment of planktivorous fish was significantly reduced in the period 1984–1988 due to a very high pH caused by eutrophication. Because zooplankton increased, phytoplankton decreased in concentration (the summer average of chlorophyll A was reduced from 700 μg/l in 1985 to 150 μg/l in 1988). The phytoplankton population even collapsed in shorter periods due to extremely high zooplankton concentrations. Simultaneously the phytoplankton species increased in size. The growth rate decreased and a higher settling rate was observed (Kristensen and Jensen, 1987). In other words, the case study shows pronounced structural changes. The primary production was not, however, higher in 1985 than in 1988 due to a pronounced self-shading by the smaller algae in 1985. It was therefore very important to include the self-shading effect in the model; this was not the case in the first model version, which therefore gave incorrect figures for the primary production. Simultaneously a more sloppy feeding of the zooplankton was observed, as zooplankton was shifted from *Bosmina to Daphnia.*

The model applied has six state variables: N in fish, N in zooplankton, N in phytoplankton, N in detritus, N as soluble nitrogen and N in sediment. The equations are given in Table 9.4. As can be seen, only the nitrogen cycle is included in the model, but as nitrogen is the nutrient controlling the eutrophication, it may be sufficient to include only this nutrient.

The aim of the study is to describe by the use of a structurally dynamic model the continuous changes in the most essential parameters using the procedure shown in Fig. 9.5. The data from 1984–1985 were used to calibrate the model and the two parameters which it is intended to change from 1985 to 1988 received the following values by this calibration:

Maximum growth rate of phytoplankton: 2.2 day^{-1}

Settling rate of phytoplankton: 0.15 day^{-1}

The *state variable* fish-N was kept constant = 6.0 during the calibration period, but an increased fish mortality was introduced during the period 1985–88 to reflect the increased pH. The fish stock was thereby reduced to 0.6 mg N/l; notice the equation "mort = 0.08 if fish > 6 (may be changed to 0.6) else almost 0". A time step of $t = 5$ days and $x\% = 10\%$ was applied (see Fig. 9.5). This means that nine runs were needed for each time step to select the parameter combination giving the highest exergy. The results are shown in Fig. 9.5 and the changes in parameters from 1985 to 1988 (summer situation) are summarized in Table 9.5. The proposed procedure (Fig. 9.3) can simulate approximately the observed change in structure.

Table 9.4. Equations of the model for *Sobygaard Lake*

```
fish = fish + dt * (-mort + predation)
INIT(fish) = 6
na = na + dt * (uptake - graz - outa - mortfa - settl - setnon)
INIT(na) = 2
nd = nd + dt * (-decom - outd + zoomo + mortfa)
INIT(nd) = 0.30
ns = ns + dt * (inflow - uptake + decom - outs + diff)
INIT(ns) = 2
nsed = nsed + dt * (settl - diff)
INIT(nsed) = 55
nz = nz + dt * (graz - zoomo - predation)
INIT(nz) = 0.07
decom = nd* (0.3)
diff = (0.015)*nsed
exergy = total_n*(Structuralexergy)
graz = (0.55)*na*nz/(0.4+na)
inflow = 6.8*qv
mort = IF fish > 6 THEN 0.08*fish ELSE 0.0001*fish
mortfa =(0.625)*na*nz/(0.4+na)
outa = na*qv
outd = qv*nd
outs = qv*ns
pmax = uptake*7/9
predation = nz*fish*0.08/(1+nz)
qv = 0.05
setnon = na*0.15*(0.12)
settl = (0.15 )*0.88*na
Structuralexergy= (nd+nsed/total_n) * (LOGN(nd+nsed/total_n)+59) + (ns/total_n) *
(LOGN(ns/total_n) - LOGN(total_n)) + (na/total_n) * (LOGN(na/total_n)+60) + (nz/total_n) *
(LOGN(nz/total_n)+62) + (fish/total_n) * (LOGN(fish/total_n)+64)
total_n = nd+ns+na+nz+fish+nsed
uptake = (2.0-2.0*(na/9))*ns*na/(0.4+ns)
zoomo= 0.1 *nz
```

Table 9.5. *Parameter combinations* giving the highest *exergy*.

	Maximum growth rate (day^{-1})	Settling rate ($m\ day^{-1}$)
1985	2.0	0.15
1988	1.2	0.45

The maximum growth rate of phytoplankton is reduced by 50% from 2.2 day^{-1} to 1.1 day^{-1}, which is approximately according to the increase in size. It was observed that the average size was increased from a few 100 μm^3 to 500–1000 μm^3, which is a factor of 2–3 (Jeppesen et al., 1989). This would correspond to a specific growth reduction by a factor $f = 2^{2/3}$–$3^{2/3}$ (see also Section 2.9).

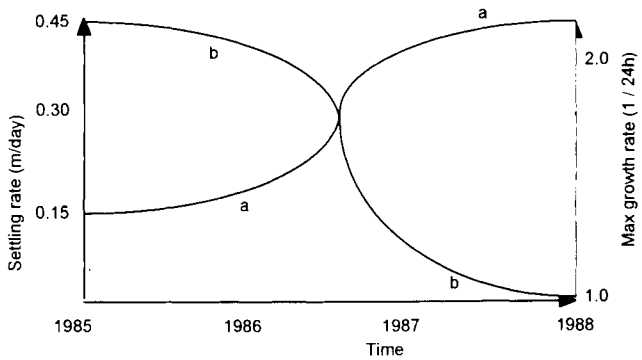

Fig. 9.5. The continuously changed parameters obtained from the application of a structurally dynamic modelling approach to *Søbygaard Lake* are shown. (a) Covers the settling rate of phytoplankton and (b) the maximum growth rate of phytoplankton.

This means that:

$$\text{growth rate in 1988} = \text{growth rate in 1985}/f, \tag{9.20}$$

where f is between 1.58 and 2.08, while in Table 9.5 2.0 is found by the use of the structurally dynamic modelling approach.

Kristensen and Jensen (1987) observed that the settling was 0.2 m day^{-1} (range 0.02–0.4) in 1985, while it was 0.6 m day^{-1} (range 0.1–1.0) in 1988. With the structurally dynamic modelling approach an increase was found from 0.15 day^{-1} to 0.45 day^{-1}, the factor being the same (three) but with slightly lower values. The phytoplankton concentration as chlorophyll-a was simultaneously reduced from 600 μg/l to 200 μg/l, which is approximately according to the observed reduction.

All in all, it may be concluded that the structurally dynamic modelling approach gave an acceptable result and that the validation of the model and the procedure in relation to structural changes was positive. The structurally dynamic modelling approach is of course never better than the model applied, and the model presented may be criticized for being too simple and not accounting for the structurally dynamic changes of zooplankton. For further elucidation of the importance of introducing a parameter shift, it has been tried running the 1985 situation with the parameter combination found to fit the 1988 situation and *vice versa*. These results are shown in Table 9.6; they show that it is of great importance to apply the right parameter set to given conditions. If the parameters from 1985 are used for the 1988 conditions a lower exergy is obtained and to a certain extent the model behaves chaotically while the 1988 parameters used on the 1985 conditions give a significantly lower exergy.

The structurally dynamic approach presented in Fig. 9.3 has also been applied to two models of population dynamics, which are presented below to illustrate the use of this approach in simple case studies. The two case studies confirm the applicability of the approach.

Table 9.6. *Exergy* and *stability* by different combinations of *parameters* and conditions.

Parameter	Conditions	
	1985	1988
1985	75.0 stable	39.8 (average) Violent fluctuations. Chaos
1988	38.7 stable	61.4 (average) Only minor fluctuations

The first case study deals with a simple two-level predator–prey system, using the following equations:

$$\begin{aligned} dx/dt &= b \cdot x(1-x/K) - s \cdot x \cdot y \quad \text{and} \\ dy/dt &= s \cdot y \cdot x^2/(k+x) - m \cdot x \end{aligned} \tag{9.21}$$

where x is the prey, y is the predator, b is the growth rate of the prey, K is the carrying capacity, s is the specific *predation rate*, k is a half-saturation constant, and m is the mortality coefficient for the predator. The procedure described in Fig. 9.3 was used on this model, starting with the following parameters:

$b = 2,$
$K = 100,$
$s = 0.25,$
$m = 0.2.$

It is known that random mutations will lead to an increase in b and K and a decrease in m, while the evolution of s will have no clear direction (see Allen, 1985). All the parameters were set to be changed up to 10% relatively for each ten days. The initial values for x and y were found by running the model to steady state and applying the corresponding x and y values as initial values. The starting exergy was $2400*R*T$. The result after 1000 time steps was a new system with exergy as much as ten times higher and the following parameters:

$b = 5$
$K = 150$
$s = 0.05$
$m = 0.05$

The second population dynamical case study focused on competition and the role of the width of the ecological niche versus the size of the resources available for the competing species. According to Allen (1975, 1976), it should be expected that a rich system will show an evolution toward specialization, meaning less competition and narrow ecological niches, while a poor system will lead to generalists; this implies more competition and wide ecological niches.

The model presented in Table 9.7 was used to simulate the competition of three species. The procedure in Fig. 9.3 was again applied to allow the model to change the parameters to values giving higher exergy. Up to a 10% change was allowed every ten days for *either* the competition factors *or* the carrying capacities. The change that gave the highest increase in exergy was realized. The model was run at five different combinations of the other parameters, giving five different utilizations of the carrying capacities at steady state. The results are summarized in Table 9.8, where the change in competition factors starting at 1.0 and the carrying capacities starting at 500 are given after 1000 time steps.

It was found that the competition factors (all 0.5 in the version for the model in Table 9.7 for all combinations of competitions) were mainly adjusted when the carrying capacities were high compared with the numbers of the three species. On the other hand, the *carrying capacities* were adjusted when the number of species was closer to the carrying capacities. These results are completely according to the *evolution* of the system that we expected: a rich system should reduce the competition factor and a poor system should increase the carrying capacities.

Table 9.7. Source code for the equations of the *competition model*

```
spec_1 = spec_1 + dt * (growth - mort)
INIT(spec_1) = 5
spec_2 = spec_2 + dt * (growth2 - mort_2)
INIT(spec_2) = 4
spec_3 = spec_3 + dt * (growth_3 - mort3)
INIT(spec_3) = 5
carrying_capacity = 500
carry_cap_2 = 500
carry_cap_3 = 500
growth = 0.44*spec_1*(1-((spec_1+0.5*spec_2+0.5*spec_3) /carrying_capacity))
growth2=0.38*spec_2*(1-(spec_2+0.5*spec_1+0.5*spec_3)/carry_cap_2)
growth_3 = 0.475*spec_3 * (1-(spec_3+0.5*spec_2+0.5*spec_1) / carry_cap_3)
mort = 0.4*spec_1
mort3 = 0.45*spec_3
mort_2 = 0.35*spec_2
sum = spec_2+spec_1+spec_3
```

Table 9.8. Results of the use of structurally dynamic approach on the *competition model*

Utilization of carrying capacity	Change in competition factors	Change in carrying capacity
60%	0	+300
32%	0	+300
11%	0.5	+200
3%	0.7	+50
0.5%	0.9	0

The *eutrophication* and remediation of a *lacustrine environment* do not proceed according to a linear relationship between nutrient load and vegetative biomass, but display rather a sigmoid trend with delay, as shown in Fig. 9.6. The *hysteresis reaction* is completely in accordance with observations (Hosper, 1989; Van Donk et al., 1989) and can be explained by structural changes (de Bernardi, 1989; Hosper, 1989; Sas, 1989; de Bernardi and Giussani, 1995). A lake ecosystem shows a marked buffering capacity to increasing nutrient level which can be explained by a current increasing removal rate of phytoplankton by grazing and settling. Zooplankton and fish abundance are maintained at relatively high levels under these circumstances. At a certain level of eutrophication it is not possible for zooplankton to increase the grazing rate further, and the phytoplankton concentration will increase very rapidly by slightly increasing concentrations of nutrients. When the nutrient input is decreased under these conditions a similar buffering capacity to variation is observed. The structure has now changed to a high concentration of phytoplankton and planktivorous fish which causes a resistance and delay to a change where the second and fourth trophic levels become dominant again.

Willemsen (1980) distinguishes two possible conditions:

1. A bream state characterized by turbid water, high *eutrophication*, low zooplankton concentration, absence of submerged vegetation and large amounts of bream, while pike is hardly found at all.
2. A pike state, characterized by clear water and low eutrophication. Pike and zooplankton are abundant and there are significant fewer breams.

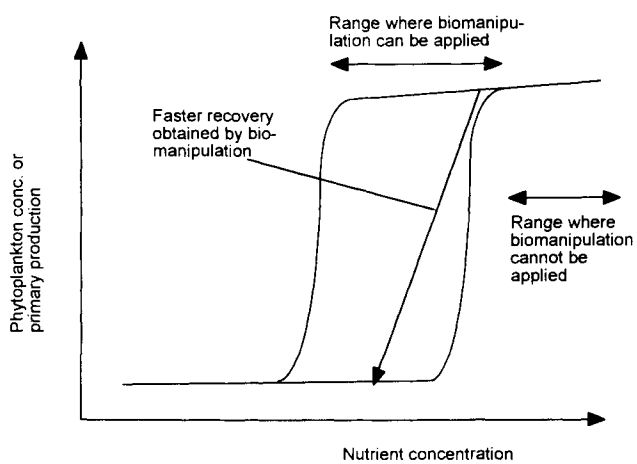

Fig. 9.6. The *hysteresis relation* between nutrient level and eutrophication measured by the phytoplankton concentration is shown. The possible effect of biomanipulation is shown. An effect of *biomanipulation* can hardly be expected above a certain concentration of nutrients, as indicated on the diagram. The biomanipulation can only give the expected results in the range where two different structures are possible.

The presence of two possible states in a certain range of nutrient concentrations may explain why *biomanipulation* has not always been used successfully. According to the observations referred to in the literature, success is associated with a total phosphorus concentration below 50 μg/l (Lammens, 1988) or at least below 100–200 μg/l (Jeppesen et al., 1990), while disappointing results are often associated with phosphorus concentration above this level of more than approximately 120 μg/l (Benndorf, 1987, 1990) with a difficult control of the standing stocks of planktivorous fish (Koschel et al., 1993).

Scheffer (1990) has used a mathematical model based on catastrophe theory to describe these shifts in structure. This model does not, however, consider the shifts in species composition, which is of particular importance for biomanipulation. The zooplankton population undergoes a structural change when we increase the concentration of nutrients, e.g., a dominance of *calanoid copepods* to small *caldocera* and *rotifers* according (de Bernardi and Giussani, 1995; Giussani and Galanti, 1995). Hence, a test of structurally dynamic models could be used to give a better understanding of the relationship between concentrations of nutrients and the vegetative biomass and to explain possible results of *biomanipulation*. This section refers to the results achieved by the development of structurally dynamic models with the aim of understanding the changes in structure and species compositions described above (Jørgensen and de Bernardi, 1998).

The applied model (based on information taken from Jørgensen et al., 1995b) has six state variables: dissolved inorganic phosphorus, phytoplankton (phyt), zooplankton (zoopl), planktivorous fish (fish 1), predatory fish (fish 2) and detritus (detritus). The forcing functions are the input of phosphorus, in P, and the through flow of water determining the retention time. The latter forcing function also determines the outflow of detritus and phytoplankton. The conceptual diagram is similar to Fig. 2.1, except that only phosphorus is considered as nutrient, as it is presumed that phosphorus is the limiting nutrient.

Simulations have been carried out for phosphorus concentrations in the inflowing water of 0.02, 0.04, 0.08, 0.12, 0.16, 0.20, 0.30, 0.40, 0.60 and 0.80 mg/l. For each of these cases the model was run for any combination of a phosphorus uptake rate of 0.06, 0.05, 0.04, 0.03, 0.02, 0.01 1/24 h and a grazing rate of 0.125, 0.15, 0.2, 0.3, 0.4, 0.5, 0.6, 0.8 and 1.0 1/24 h. When these two parameters were changed, simultaneous changes of phytoplankton and zooplankton mortalities were made according to *allometric principles* (see Peters, 1983). The parameters which are made variable to account for the dynamics in structure are therefore for phytoplankton growth rate (uptake rate of phosphorus) and mortality and for zooplankton growth rate and mortality.

The settling rate of phytoplankton was made proportional to the $(\text{length})^2$. Half of the additional sedimentation when the size of phytoplankton increases corresponding to a decrease in the uptake rate, was allocated to detritus to account for resuspension or faster release from the sediment. A sensitivity analysis has revealed that exergy is most sensitive to changes in these five selected parameters which also represent the parameters that change significantly by size. The 6 and 9 levels selected

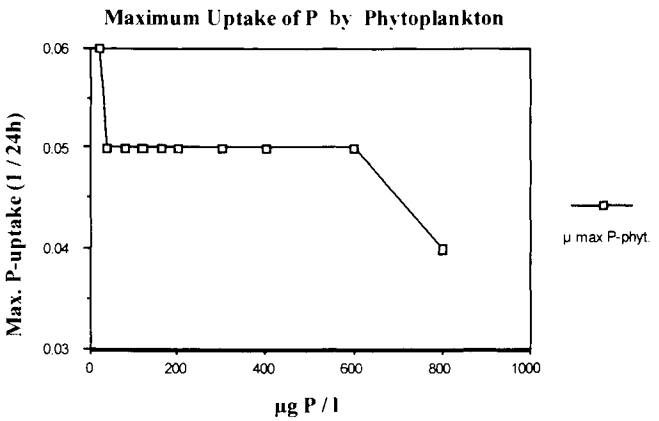

Fig 9.7. The maximum growth rate of phytoplankton obtained by the structural dynamic modelling approach is plotted versus phosphorus concentration.

above represent approximately the range in size for phytoplankton and zooplankton, respectively.

For each phosphorus concentration 54 simulations were carried out to account for all combinations of the two key parameters. Simulations over three years, 1100 days, were applied to ensure that either steady state, limit cycles or chaotic behaviour would be attained. This structurally dynamic modelling approach presumed that the combination with the highest exergy should be selected as representing the process rates in the ecosystem. If exergy oscillated even during the last 200 days of the simulation, the average value for the last 200 days was used to decide which parameter combination would give the highest exergy. The combinations of the two parameters, the uptake rate of phosphorus for phytoplankton and the grazing rate of zooplankton giving the highest exergy at different levels of phosphorus inputs are plotted in Figs. 9.7 and 9.8. The uptake rate of phosphorus for phytoplankton gradually decreases as the phosphorus concentration increases. As can be seen, the zooplankton grazing rate changes at a phosphorus concentration of 0.12 mg/l from 0.4 1/24 h to 1.0 1/24 h, i.e. from larger species to smaller species, which is according to expectations.

Figure 9.9 shows the exergy (called information on the diagram) with an uptake rate according to the results in Fig. 9.7 and a grazing rate of 1.0 1/24 h (information 1) and 0.4 1/24 h (information 2), respectively. Below a phosphorus concentration of 0.12 mg/l information 2 is slightly higher, while information 1 is significantly higher above this concentration. The phytoplankton concentration increases for both parameter sets with increasing phosphorus input, as shown Fig. 9.10, while the planktivorous fish shows significantly higher levels by a grazing rate of 1.0 1/24 h, when the phosphorus concentration is = 0.12 mg/l (= valid for the high exergy level). Below this concentration the difference is minor. The concentration of fish 2 is higher for case 2 corresponding to a grazing rate of 0.4 1/24 h for phosphorus

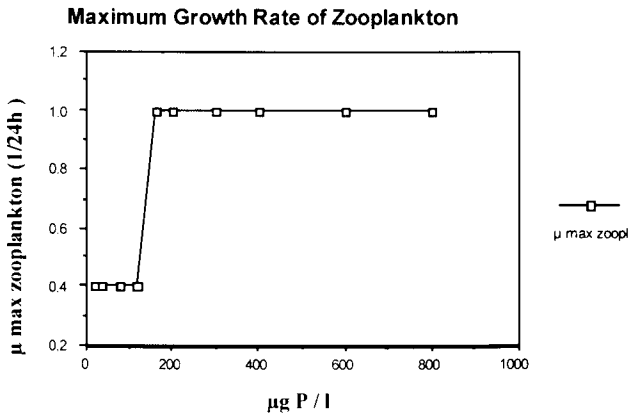

Fig. 9.8. The maximum *growth rate* of zooplankton obtained by the structural dynamic modelling approach is plotted versus zooplankton concentration.

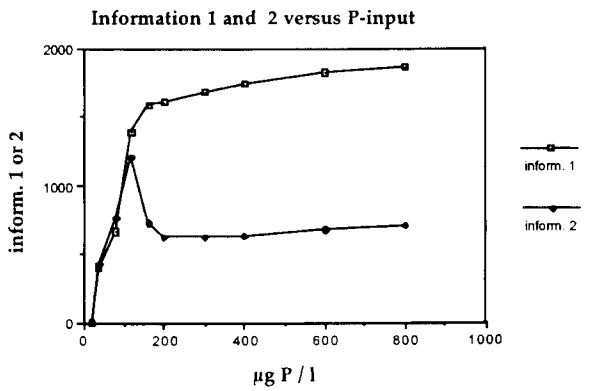

Fig. 9.9. The exergy is plotted versus phosphorus concentration. Information 1 corresponds to a maximum zooplankton *growth rate* of 1/24 h and information 2 corresponds to a maximum zooplankton growth rate of 0.4 1/24 h. The other parameters are the same for the two plots, including the maximum phytoplankton growth rate taken from Fig. 9.4 as function of the phosphorus concentration.

concentrations below 0.12 mg/l. Above this value the differences are minor, but at a phosphorus concentration of 0.12 mg/l the level is significantly higher for a grazing rate of 1.0 1/24 h, particularly for the lower exergy level, where the zooplankton level is also highest.

If it is presumed that exergy indices can be used as a goal function in ecological modelling, the results seem to be able to explain why we observe a shift in grazing rate of zooplankton at a phosphorus concentration in the range of 0.1–0.15 mg/l. The ecosystem selects the smaller species of zooplankton above this level of phosphorus

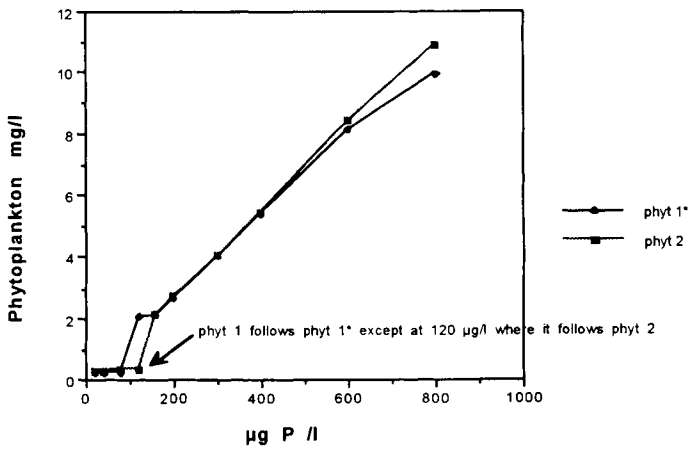

Fig. 9.10. The phytoplankton concentration as a function of phosphorus concentration for parameters corresponding to information 1 and information 2 (see Fig. 9.6). The plot called phyt 1* coincides with phyt 1, except for a phosphorus concentration of 0.12 mg/l, where the model shows limit cycles. At this concentration, information 1* represents the higher phytoplankton concentration, while information 1 represents the lower phytoplankton concentration. Notice that the structurally dynamic approach can explain the *hysteresis reactions*.

because it means a higher level of the exergy index, which can be translated to a higher rate of survival and growth. It is interesting that this shift in grazing rate only gives a little higher level of zooplankton, while the exergy index level gets significantly higher by this shift, which may be translated as survival and growth for the entire ecosystem. Simultaneously, a shift from a zooplankton, predatory fish dominated system to a system dominated by phytoplankton and particularly by planktivorous fish takes place.

It is interesting that the levels of exergy indices and the four biological components of the model for phosphorus concentrations at or below 0.12 mg/l parameter combinations are only slightly different for the two parameter combinations. It can explain why biomanipulation is more successful in this concentration range. Above 0.12 mg/l the differences are much more pronounced and the exergy index level is clearly higher for a grazing rate of 1.0 1/24 h. It should therefore be expected that after the use of biomanipulation the ecosystem easily reverts to the dominance of planktivorous fish and phytoplankton. These observations are consistent with the general experience of success and failure of biomanipulation (see above).

An interpretation of the results points towards a shift at 0.12 mg/l, where a grazing rate of 1.0 1/24 h yields limit cycles. It indicates an instability and a probably easy shift to a grazing rate of 0.4 1/24 h, although the exergy level is on average highest for the higher grazing rate. A preference for a grazing rate of 1.0 1/24 h at this phosphorus concentration should therefore be expected, but a lower or higher level of zooplankton is dependent on the initial conditions.

If the concentrations of zooplankton and fish 2 is low, and high for fish 1 and phytoplankton (i.e., the system is coming from higher phosphorus concentrations), there is a high probability that the simulation also gives a low concentration of zooplankton and fish 2. When the system is coming from high concentrations of zooplankton and of fish 2, there is also a high probability that the simulation gives a high concentration of zooplankton and fish 2, corresponding to an exergy index level slightly lower than that obtained by a grazing rate of 0.4 1/24 h. This grazing rate will therefore still prevail. As it also takes time to recover the population of zooplankton, and particularly of fish 2 and in the other direction of fish 1, these observations explain the presence of *hysteresis reactions*.

The model is considered to have general applicability and has been used to discuss the general relationship between nutrient level and vegetative biomass and the general experiences with application of *biomanipulation*. When the model is used in specific cases, it may however be necessary to include more details and change some of the process descriptions to account for the site-specific properties, which is according to general modelling strategy. It could be considered to include two state variables to cover zooplankton, one for the bigger and one for the smaller species. Both zooplankton state variables should of course have a current change of the grazing rate according to the maximum value of the goal function.

The model could probably also be improved by the introduction of size preference for the grazing and the two *predation* processes which is in accordance with numerous observations. In spite of these shortcomings of the applied model, it has been possible to give a correct qualitative description of the reaction to changed nutrient levels and biomanipulation, and even to indicate an approximately correct phosphorus concentration, where the structural changes may occur. This may be due to an increased robustness of the structurally dynamic modelling approach.

Ecosystems are very different from physical systems mainly due to their enormous *adaptability*. It is therefore crucial to develop models that are able to account for this property if we want to achieve reliable model results. The use of exergy as goal functions to cover the concept of fitness seems to offer a good possibility of developing a new generation of models that are able to consider the adaptability of ecosystems and describe shifts in species composition. The latter advantage is probably the most important, because a description of the dominant species in an ecosystem is often more essential than an assessment of the level of the focal state variables.

It is possible to model competition between a few species with quite different properties, but the structurally dynamic modelling approach makes it feasible to include more species even with only slightly different properties—something which is impossible with the usual modelling approach (see also the unsuccessful attempt to do so by Nielsen, 1992a,b). The rigid parameters of the various species make it difficult for the species to survive under changing circumstances. After some time only a few species will still be present in the model, opposite to what happens in reality where more species survive because they are able to adapt to the changing circumstances. It is therefore important to capture this feature in our models. The

structurally dynamic models seem promising to apply to lake management, as this type of model can be applied to explain our experience in the use of *biomanipulation*. It has the advantage over the use of catastrophe models, which can also be used to explain success and failure of *biomanipulation*, in that it is also able to describe the shifts in properties due to adaptation of shifts in species composition.

9.5 Application of Chaos Theory in Modelling

Chaos theory is concerned with unpredictable courses of events. The irregular and unpredictable time evolution of many non-linear systems has been called "chaos". Chaos theory has eliminated the Laplacian illusion of *deterministic predictability* and can therefore be conceived as a ticking bomb under reductionistic science.

Even very simple models can behave chaotically. The very simple model shown in Fig. 9.11 with equations in Table 9.9 behave chaotically at certain values of the parameter. This is shown in Figs. 9.12–9.14, where the parameter (p) for iny = p*x is varied. For p = 23.6 the model shows some fluctuations, which become smaller and smaller over time, and the state variables finally reach a steady state.

For p = 24, the model starts to behave strangely with a tendency to bifurcate and with more and more violent fluctuations If p = 25, the model behaves chaotically. When such a simple model behaves very differently with a minor change in one parameter, how can we develop models of very complex biological systems? This crucial question is the topic of this section.

Chaos theory is best illustrated by Lorenz's (1963, 1964) famous *Butterfly Effect*—the notion that a butterfly stirring the air in Hong Kong today can transform storm systems in New York next month. The effect was discovered accidentally by Lorenz in 1961. He was making a weather forecast and wanted to examine one sequence of

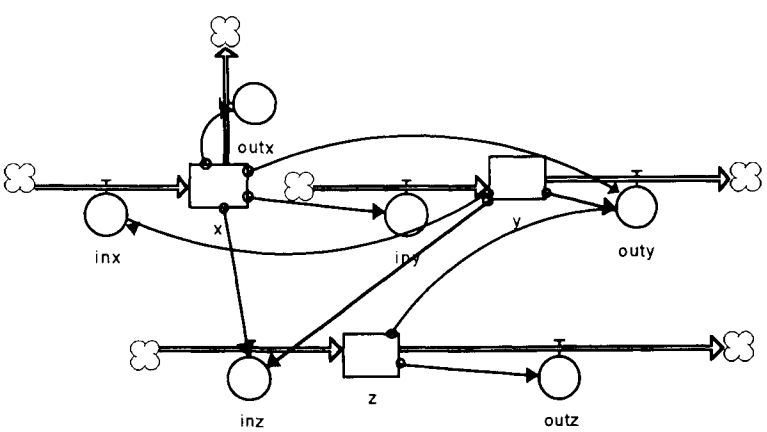

Fig. 9.11. A simple model showing *chaotic behaviour*.

Table 9.9. Equations of the model shown in Fig. 9.11

$x = x + dt * (inx - outx)$
INIT(x) = 1
$y = y + dt * (iny - outy)$
INIT(y) = 1
$z = z + dt * (inz - outz)$
INIT(z) = 1
$inx = 10*y$
$iny = 24*x$
$inz = x*y$
$outx = 10*x$
$outy = y+x**z$
$outz = 8*z/3$

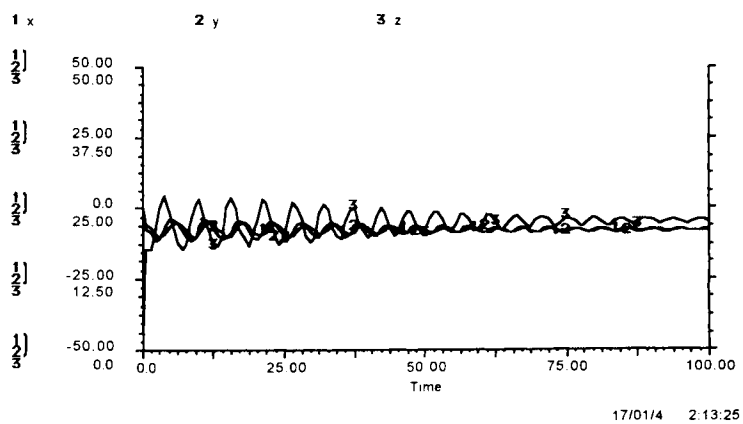

Fig. 9.12. Simulations of the model in Fig. 9.11 using $iny = 23.6 * x$ (see the equations in Table 9.9).

greater length. He tried to make what he thought was a shortcut. Instead of starting the whole run over again, he started half way through. To give the computer its initial values, he typed the numbers from the earlier printout. The new run should therefore duplicate the old one, but it did not. Lorentz saw that his new weather forecast was diverging so rapidly from the previous run that within a few months all resemblance has disappeared. There had been no malfunction of the computer or the program. The problem lay in the number he had entered. In the computer six decimal places were stored: 0.506127, but to save time—because he thought it was unessential—he used a rounded-off number with just three decimals: 0.506.

The explanation is simple: Lorenz's model is very sensitive to initial conditions and so is the weather itself. The effect is observed today in numerous relations and all ecological modellers know this problem. Therefore the initial values of the state variables are most often included in a modeller's sensitivity analysis and he uses

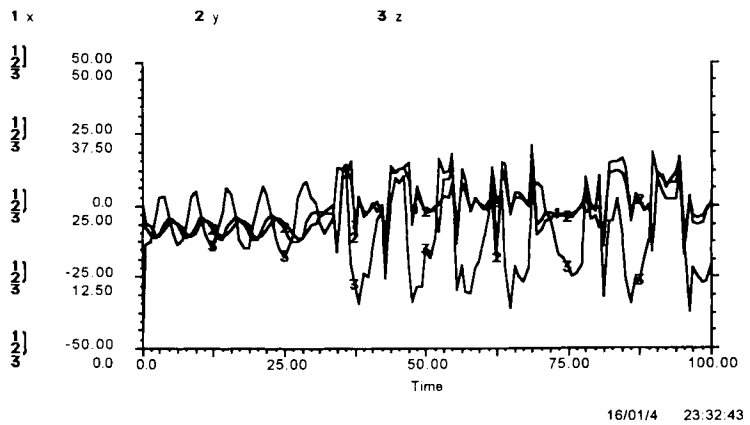

Fig. 9.13. Simulations of the model in Fig. 9.11, using $iny = 24 * x$ (see the equations in Table 9.9).

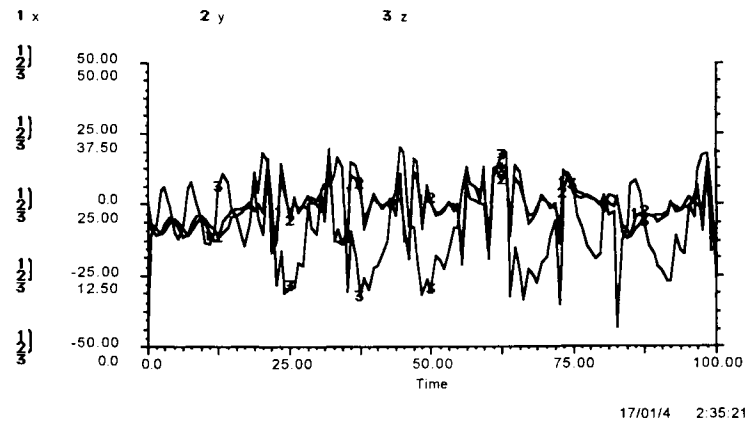

Fig. 9.14. Simulations of the model in Fig. 9.11, using $iny = 25 * x$ (see the equations in Table 9.9).

much effort to have the seasonal variations of the state variables repeated again and again, when the same forcing functions are imposed on the model (see also Section 2.6).

The definition of chaos implies that the distance between two curves with slightly different initial conditions grows exponentially:

$$d(t) = d(0)\ \varepsilon\ e^{l \cdot t} \tag{9.22}$$

where $d(t)$ is the distance at time $= t$, $d(0)$ is the distance at time $= 0$ and l is a positive number, called the *Lyapunov exponent*, which is a quantitative indicator for chaos. After the time $1/l$ the initial conditions are insignificant, i.e., "forgotten".

The Lyapunov exponent can be found by plotting the logarithm of the distance between the two curves neglecting the distance at time 0 (which is 0) versus the time.

Chaos is also known in relation to bifurcation and this form of chaos is nicely illustrated by examination of a simple model in population biology. May (1973, 1974, 1975, 1976, 1977) has examined the behaviour for non-linear differential and difference equations, for instance:

$$N_{t+1} = N_t(1 + r(1 - N_t/K)), \tag{9.23}$$

where N is the number of individuals in the population under consideration, r the growth rate per capita, t the time and K the carrying capacity of the environment. Notice that this equation expresses a time delay = 1 in the form the difference equation is given. As long as the non-linearity is not too severe, the time delay built into the structure of the difference equation (9.23) tends to compare with the natural response time of the system and there is simply a stable equilibrium point at $N\# = K$. However for $r = 2$ this point becomes unstable. It bifurcates to produce two new and locally stable fixed points of period 2, between which the population oscillates stably in a 2-point cycle. With increasing r, these two points also bifurcate to give four stable fixed points of period 4. In this way through successive *bifurcations* an infinite hierarchy of stable cycles of period $2n$ arises. Figure 9.15 illustrates the formation of bifurcations up to $r = 2.75$.

When we consider the many non-linear relationships are valid in ecology, we may wonder why chaos is not observed more frequently in nature or even in our models. An obvious answer could be that nature attempts to avoid chaos and, as opposed to the physical system, the ecosystem has many possible hierarchically organized regulation mechanisms to avoid chaotic situations (see Table 9.1). This does not

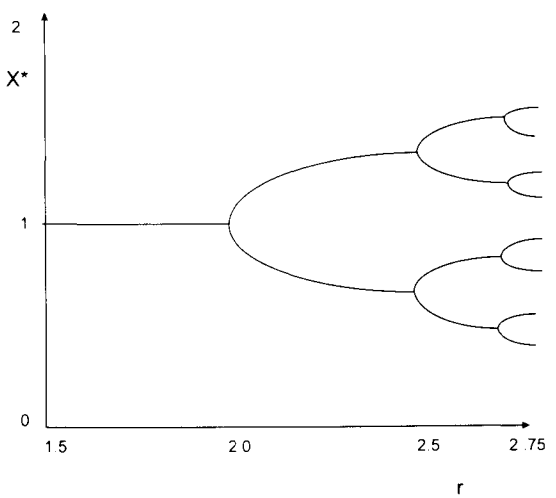

Fig. 9.15. The hierarchy of stable fixed points of periods 1, 2, 4, 8... $2n$, which are produced from Eq. (9.23) as the parameter r increases. The y-axis indicates relative values.

imply that chaotic or "almost chaotic" situations are not observed in ecosystems. They are only rarer than would be expected. The classical example is the almost legendary lemming (Shelford, 1943). According to this paper $r * T$ is 2.4, r being the growth rate per capita and T the time lag. Oscillation between two steady states should be expected as Shelford also found (Shelford, 1943). Hassel et al. (1976) have culled data on 28 different populations of seasonal breeding insects. They found that the growth may be described by a difference equation as follows:

$$N_{t+1} = q * N_t(1 - a * N_t)^{-\beta} \tag{9.24}$$

q is here related to r as follows: $r = \ln q$; a and β are constants.

Figure 9.16 shows the theoretical domains of stability behaviour for Eq. (9.24) applied to 28 populations by Hassel et al. By far the most of the populations are in the monotonic damping area and only one is in the chaos area (and, as indicated by Hassel et al., it is a laboratory population) and one in the stable limit cycles area.

Notice that there is a tendency for laboratory populations to exhibit cyclic and chaotic behaviour, whereas natural populations tend to have a stable equilibrium point. The laboratory populations are maintained in a homogeneous environment and are free from predators and many other natural mortality factors which, up to a certain level, may very well give a stabilizing effect.

The relationship between the parameters and the somewhat chaotic behaviour is discussed below. It may be concluded that natural populations are able to avoid chaotic situations to a large extent. Long experience gained during evolution has taught the natural population to omit those properties, i.e., the parameters, that may give chaotic situations because they threaten their survival, at least in some

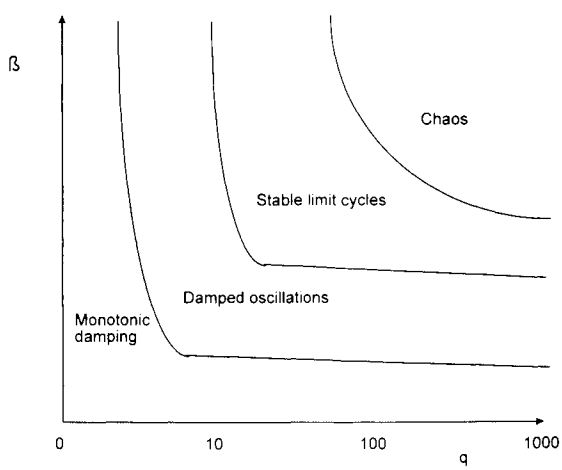

Fig. 9.16. The *dynamic behaviour* of Eq. (9.24). The curves separate the regions of monotonic and oscillatory damping to a stable point, stable *limit cycles* and *chaos*. The thin curve indicates where 2-point cycles give way to higher-order cycles. Redrawn after Hassel et al. (1976).

situations. Furthermore, natural populations have the flexibility mentioned in Section 9.2—a flexibility which gives the populations the ability, within certain limits, to select a combination of parameters which give a better chance for survival.

Figure 9.17 shows a model that has been applied in modelling experiments. However, here we have excluded fish as a state variable in the first place, we have given the phytoplankton and the bacteria the maximum growth rates found in the literature and now ask what the right maximum growth rate of the two zooplankton state variables would be to avoid chaotic situations. The answer, as seen in Fig. 9.18, is that a maximum growth rate of about 0.35–0.40 day^{-1} seems to give favourable conditions for the entire system, as the exergy is at maximum and stable conditions are obtained. A maximum growth rate of more than about 0.65–0.70 day^{-1} gives chaotic situations for the two zooplankton species.

Figure 9.19 shows a similar result when fish are included as a state variable (see the conceptual diagram in Fig. 9.17). The two zooplankton state variables have been given maximum growth rates of 0.35 and 0.40 day^{-1}. A maximum *growth rate* of about 0.08–0.1 day^{-1} seems favourable for the fish, but again too high a maximum growth rate (above 0.13–0.15 day^{-1}) for the state variable "fish" will give oscillations and chaotic situations with violent fluctuations.

The parameter estimation is often the weakest point in many of our ecological models (see Section 2.8), due to:

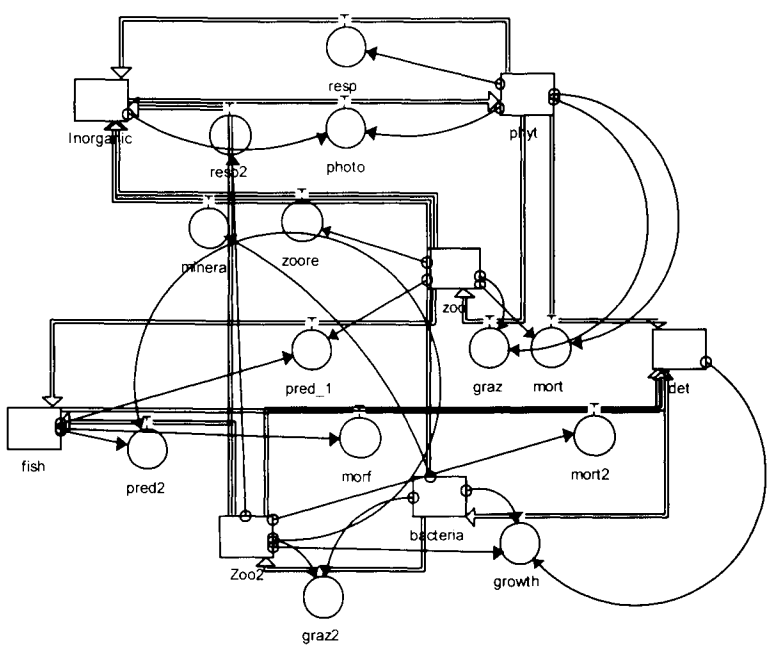

Fig. 9.17. Model used to examine the feasible parameters. The model consists of seven *state variables.*

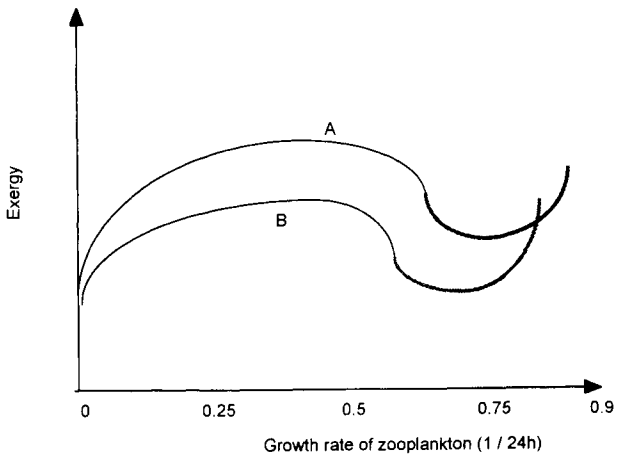

Fig. 9.18. *Exergy* is plotted versus maximum growth rate for the two zooplankton classes in Fig. 9.17. (A) corresponds to the state variable "zoo" and (B) the state variable "zoo2". The shaded lines correspond to chaotic behaviour of the model, i.e., violent fluctuations of the state variables and the exergy. The values shown for the exergy above a maximum growth rate of about 0.65-0.7 day^{-1} are therefore average values.

- an insufficient number of observations to enable the modelled to calibrate the number of more or less unknown parameters
- little or no literature information can be found
- ecological parameters are generally not known with sufficient accuracy
- the structure shows dynamical behaviour, i.e., the parameters are continuously changing to achieve a better adaptation to the ever-changing conditions (see also Jørgensen, 1988, 1992a,b).
- or a combination of two or more of these issues.

The results mentioned above seem to reduce these difficulties by imposing the ecological facts that all the species in an ecosystem have the properties (described by the parameter set) that are best fitted for survival under the prevailing conditions. The property of survival can currently be tested by the use of exergy, since it is survival translated into thermodynamics. *Co-evolution*, i.e., when the species have adjusted their properties to each other, is considered by application of exergy for the entire system. This method enables us to reduce the feasible parameter range, which can be utilized to facilitate our parameter estimation significantly.

It is interesting that the ranges of *growth rate* actually found in nature (see for instance Jørgensen et al., 1991) are those, which give stable, i.e., non-chaotic, conditions. All in all, it seems possible to conclude that the parameters that we can find in nature today are usually those that ensure a high probability of survival and growth in all situations; chaotic situations are thereby avoided. The parameters that could give possibilities for chaotic situations have simply been excluded by selection processes. They may give high exergy in some periods, but later the exergy becomes

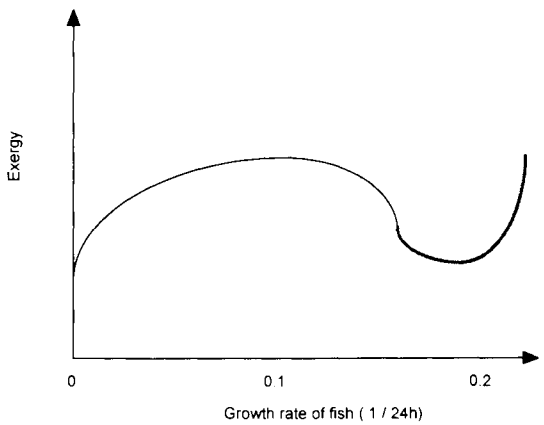

Fig. 9.19. The exergy is plotted versus the maximum growth rate of fish. The shaded line corresponds to chaotic behaviour of the model, i.e., violent fluctuations of the state variables and the exergy. The values shown for the exergy above a maximum growth rate of about 0.13–0.15 day^{-1} are therefore average values.

very low due to violent fluctuations and it is under such circumstances that the selection process excludes the *parameters* (properties) that cause chaotic behaviour.

Kauffman (1991, 1993) has studied a Boolean network and finds this network on the boundary between order and chaos may have the flexibility to adapt rapidly and successfully through the accumulation of useful variations. In such poised systems most mutations will have small consequences because of the system's homeostatic nature. Such poised systems will typically adapt to a changing environment gradually, but if necessary, they can change occasionally rapidly—a property that can be found in organisms and ecosystems. According to Kauffman, this explains why Boolean networks poised between order and chaos can generally adapt most readily and therefore have been the target of natural selection.

The hypothesis is bold and interesting in relation to the results obtained by the use of exergy as an indicator in the choice of parameters. The parameters that give maximum exergy are not much below the values that would create chaos (see Figs. 9.18 and 9.19): they are at "the edge of the chaos", to use the expression introduced by Kauffman. *Logistic* and even *exponential growth* (see Chapter 3) may also show chaotic behaviour if time lag is used on the number of individuals. The bigger the time lag, the smaller growth rate will cause chaotic behaviour of the model. Hannon and Ruth (1997) give some illustrative examples using *STELLA* as the modelling software. Some of the examples use difference equations, similar to Eq. (9.24) which is often a convenient method for introducing time lag.

Chaotic behaviour can occur by the use of too big integration steps and an inaccurate integration routine. If chaos is observed by model simulation, it is therefore always necessary to see if the chaotic behaviour still remains at smaller and smaller integration steps and by the use of more accurate (but usually also more time consuming) integration routines. Deterministic chaos requires that the chaotic behaviour is independent of the integration step or the choice of integration routine.

9.6 Application of Catastrophe Theory in Ecological Modelling

Applied *catastrophe theory* is, in a strict sense, a theory of equilibria. Thom's classification theorem (Thom, 1972, 1975) states that a dynamic system, governed by a scalar potential function and dependent on up to five external variables, changes in the equilibrium values of state variables for slow changes in the parameters (caused by the forcing functions). The system can be modelled by one out of seven canonical functions. These functions can be analytically deduced from the actual potential function through coordinate transformations and other mathematical techniques; for further details see Poston and Stewart (1978) in which a complete list of catastrophe functions can also be found. The theory has been applied in several fields including social sciences, medicine, ecology and economy (Zeeman, 1978; Poston and Stewart, 1978; Kempf, 1980; Loehle, 1989).

The usefulness of Thom's theorem lies in the graphical simplicity of catastrophe surfaces for displaying how the behaviour of equilibria is influenced by parameter changes. The simplicity is best exemplified by the catastrophe function with the widest application. The canonical potential function is:

$$Y = x^4/4 + a*x^2/2 + b*x \tag{9.25}$$

and the behaviour surface is given by the differential equation:

$$dY/dx = x^3 + x * a + b, \tag{9.26}$$

where a and b are the parameters that vary slowly compared with Y. x is a state variable. In a cusp-like system Eq. (9.26) will be the differential equation of the state variables in canonical coordinates at equilibrium. If b is varied for a in the region less than zero, different types of equilibria will appear, when a and b cross the bifurcation set:

$$4 * a^3 + 27 * b^2 = 0 \tag{9.27}$$

The standard cusp behaviour surface is shown in Fig. 9.20 which is derived from Eqs. (9.26) and (9.27).

The theory uses 11 elementary catastrophe shapes, of which four are considered in ecology: fold, cusp (most widely used in ecology up to now), swallowtail and butterfly. The fold is a *one-dimensional catastrophe*. A curve representing equilibria is S-shaped when plotted as response versus control. Dynamic movement along the X-axis results in *hysteresis*. It is, however, recommended to search for a second control variable, when hysteresis is observed. It may result in a cusp catastrophe.

In the region of two stable states, the cross section of the cusp manifold is S-shaped. As we move back in the plane in Fig. 9.20, the degree of folding decreases

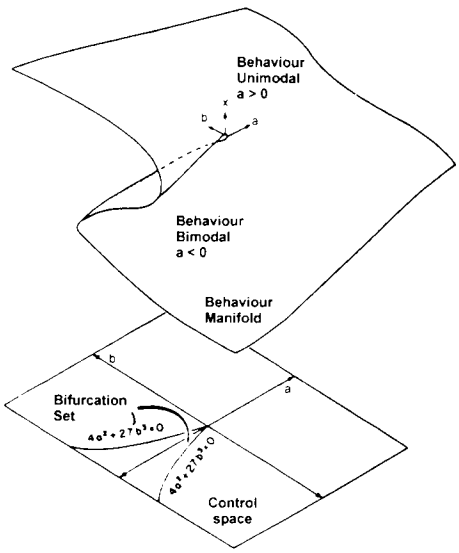

Fig. 9.20. The *standard cusp* behaviour surface.

until the surface becomes smooth. The response surface can consist of a series of cusp figures joined. Thus the cusp catastrophe model is not necessarily as simple to picture as in Fig. 9.20.

Two major factors are able to explain the relatively slow development of this theory in ecology, according to Loehle (1989):

1. The theory is based upon a highly specialized mathematical field: *topology*.
2. The procedure to follow is not explained in layman's terms outside the specialized mathematical literature. It is therefore difficult to use for most ecologists.

Catastrophe theory deals with shifts in equilibrium or attractor points on the system level, and there is much evidence that such shifts take place in the ecosystem. Phenomena that other methods would ignore or explain only partially can be described by catastrophe theory.

Typical living systems follow a catastrophic pattern in response to severe environmental stresses. They have developed mechanisms for dealing with stress due to environmental changes. One of these mechanisms is a sudden shift in properties, which may be called a catastrophe. Such catastrophes are therefore not necessarily negative events, but may be a rapid adaptation to a new situation. In addition, many systems take advantage of severe environmental conditions to test the survivability of the components of the system or eliminate weak ones.

Catastrophes typically occur in cases where two or more non-linear processes interact, which is the general case for ecosystems. Due to the non-linearity of ecological processes, catastrophic behaviour of ecosystems should be expected much

more often in an ecosystem than they are actually observed—a point that will be discussed further below. The emergence of catastrophic behaviour by the interaction of two or more non-linear ecological processes is clearly illustrated by Bendoricchio (1988) in his application of catastrophe theory to the *eutrophication* of the Venice Lagoon. Bendoricchio shows that the interaction between

1. *diffusion* described by the use of Rabinowitch's (1951) biochemical diffusive model,
2. the net phytoplankton growth obtained as the difference between the overall growth and the mortality, and
3. the overall growth related to the nutrient concentration by a *Michaelis–Menten equation*

leads to the canonic equation of a cusp catastrophe; see Eq. (9.26).

Illustration 9.1 gives a simple example of how catastrophes occur in a system of mathematical equations. Furthermore, because the example is supported by data it is a realistic ecological example.

Illustration 9.1

Catastrophic shifts in the oxygen concentration at spring and fall have been observed in Southern Belgian rivers and Dubois (1979) has explained these observations using the catastrophe theory.

The change in oxygen concentration can be expressed by the use of the following equation:

$$dC(t)/dt = \text{Exchange air/water} + \text{production by photosynthesis} - \text{consumption by respiration} \tag{9.28}$$

The consumption of oxygen, OC, can be given by a *Michaelis–Menten equation:*

$$OC = k2 * C(t)/(C(t) + k1) \tag{9.29}$$

where $C(t)$ is the oxygen concentration at time t, and $k1$ and $k2$ are known constants.

The production of oxygen by *photosynthesis*, PP, may be found by the use of a logistic equation:

$$PP = k3 * C(t)(1 - q * C(t)) \tag{9.30}$$

where $k3$ and q are constants.

The re-aeration, RA, is described using the following expression:

$$RA = Ka * (Cs - C(t)) \tag{9.31}$$

where Ka is the re-aeration constant (characteristic for the stream) and Cs is the oxygen concentration at saturation, that is a function of the temperature and barometric pressure.

We now have the following equation:

$$dC(t)/dt = Ka * (Cs - C(t)) + k3 * C(t)(1 - q * C(t)) - k2 * C(t)/(C(t) + k1) \quad (9.32)$$

A transformation of Eq. (9.32) is carried out by the use of the following symbols:

$$\begin{aligned} x &= C(t)/k1 \\ x\text{–}s &= Cs/k1 \\ a(T) &= Ka * Cs, \text{ where } T \text{ is the temperature} \\ b &= k3 - Ka \\ c &= q * k3\, k1/b \\ d &= k2/k1 \end{aligned} \quad (9.33)$$

Equation (9.32) is transformed to the following expression:

$$dx/dt = a(T) + b*x(1 - C*x) - d*x/(1 + x) \quad (9.34)$$

Figure 9.21 gives the relationship $-dx/dt + a(T)$ for particular values of the constants b, c and d ($b = 1$, $c = 0.1$ and $d = 4$) versus x. $a(T) = 0.5$ is also shown in the figure. $a(T)$ varies with the temperature and, as T, varies with the seasonal changes.

If we presume that the temperature varies according to a sine function, we can express $a(T)$ as a function of time, t, by using the following equation:

$$a(T) = B - G \sin(w*t) \quad (9.35)$$

where B, G and w are constants.

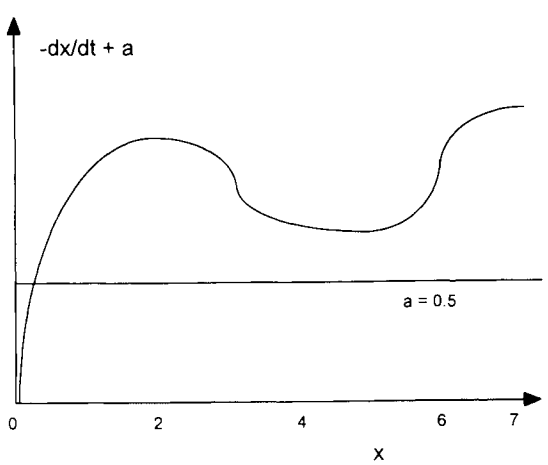

Fig. 9.21. $(-dx/dt + a)$ plotted versus x.

Figure 9.22 shows $-dx/dt$ for six different a values that occur at six different times of the year. For $a = 0.5$ there exists only one *attractor point* corresponding to $-dx/dt = 0$ and $x = S$. For $a = 1$, there are two attractor points, $x = S$ and $x = Q$, but x will still remain in S. For $a = 1.2$, x will jump to the second attractor point Q. For $a = 1.3$ or above the attractor point Q will be the only one. For $a = 1$, there are again two attractor points, but now x will remain in Q. At $a = 0.75$, x will jump back to attractor point S. So, the jump will take place by increasing $a(T)$ (i.e., during the spring months) at $a = 1.2$, while the jump back takes place at $a = 0.75$, i.e., by decreasing a. This explains the observed *hysteresis effect* (see Fig. 9.23) which illustrates the relationship between x and a.

The model (see the equations above) was constructed using the software STELLA. The results are shown in Figs. 9.24 and 9.25. The model was run for 1000 days. The oxygen is plotted versus the time in Fig. 9.24 and the temperature in Fig. 9.25. Comparing the two curves, it is possible to observe the hysteresis. By increasing temperature the oxygen will already jump from a high to a low level at about 6°C, while the jump from the high to low oxygen concentration takes place at 18°C, when the temperature is decreasing.

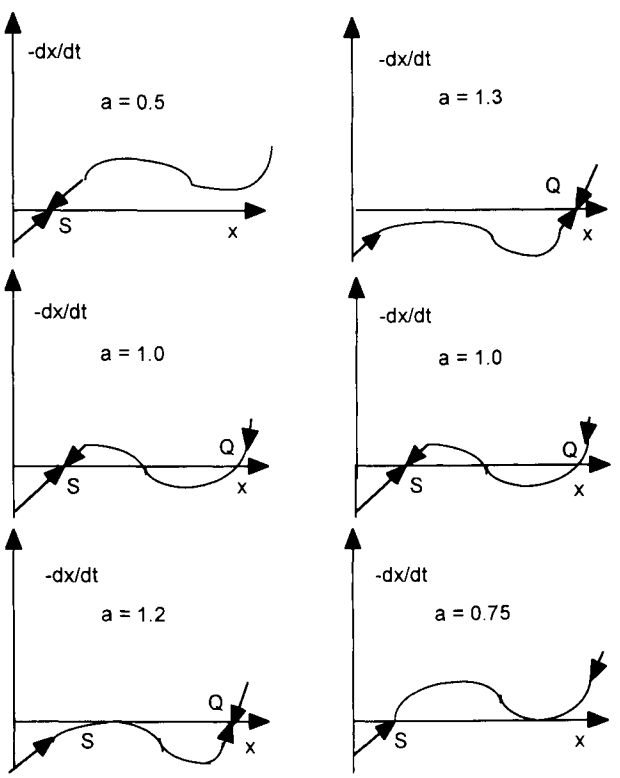

Fig. 9.22. dx/dt is plotted versus x for six different a-values. S and Q are *attractor points*. Arrows indicate how x will evolve. Notice that the six different a values correspond to six different time points.

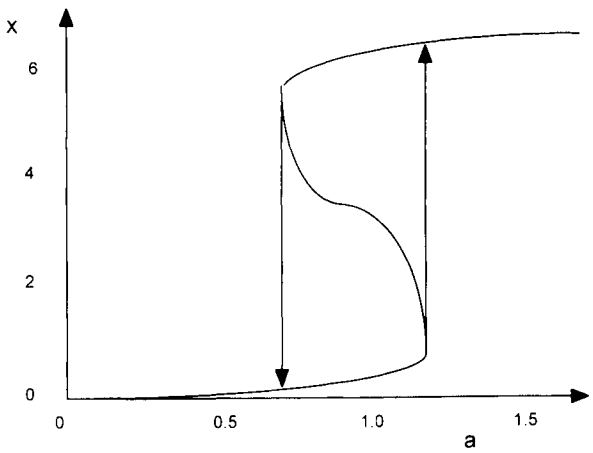

Fig. 9.23. Stable x-values are plotted versus a. Note the *hysteresis effect*.

This implies that, in this case, the hysteresis effect can be found by selecting temperature as a control variable, i.e., plotting x versus T, but Fig. 9.24 should already give the observer the idea to examine the possibility of using catastrophe theory to explain the observations, when two distinct levels of oxygen are seen.

The model used for the computations leading to Figs. 9.24 and 9.25 is shown in Fig. 9.26. As already mentioned, the results obtained are realistic in the light of measurements in very polluted Belgian rivers. If the loading of organic biodegradable matter is high, the water constantly has a high consumption of oxygen and becomes extremely susceptible to the input of new oxygen by the re-aeration process, which again is very much dependent on the oxygen saturation concentration and which, in turn, is very much dependent on the temperature.

If the water was less polluted, the consumption of oxygen would have been less and the susceptibility of the oxygen concentration to the re-aeration process would thereby be reduced.

What happens in the water can be further illustrated by the use of the concept buffer capacity. The most obvious buffer capacity to use would be the oxygen-temperature *buffer capacity* which is defined as:

$$\beta = \partial T / \partial x \tag{9.36}$$

Figure 9.27 shows the *buffer capacity* versus the time for the first 440 days. It is seen that the low buffer capacities coincide as expected with the jumps in oxygen concentration whenever the jump is towards higher or lower oxygen concentration. It is also seen that every second time the buffer capacity is low, the buffer capacity afterwards increases to extremely high values. This is the summer situation: the oxygen concentration is low and the high buffer capacity indicates that it is very difficult to increase the oxygen concentration. As can be seen, the buffer capacity/time graph reflects the *hysteresis effect* very nicely.

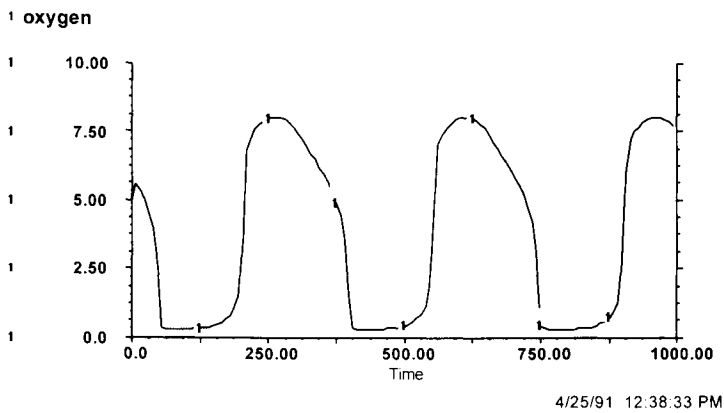

Fig. 9.24. Oxygen concentration (mg/l) x is plotted versus time (days). Results of the model in Fig. 9.26.

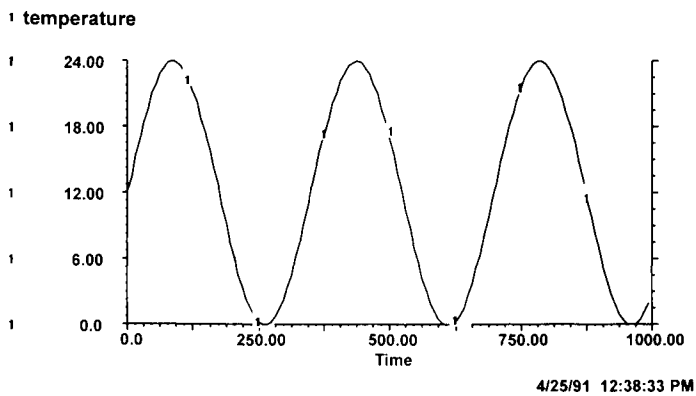

Fig 9.25. The temperature (T) in °C is plotted versus time (days). Results of the model in Fig. 9.26.

Catastrophe theory has not been widely accepted in ecology, because *reductionistic* ecology does not believe that it is possible to look through the "mist of complexity". It is clear, however, from the presentation in this chapter that ecosystems show discontinuous stability and that these observations can be modelled, and in some cases at least explained, by the use of catastrophe theory. Catastrophe modelling provides an extended insight which is valuable in our effort to transform our observations to a pattern of ecosystem theory.

It is not surprising that a complex non-linear system such as an ecosystem shows *discontinuous stability*. Many examples have been observed in physics and chemistry (see, e.g., Nicolis and Prigogine, 1989). It is quite surprising that it is not met more frequently in ecology but this can be explained by the *multilevel hierarchy* of

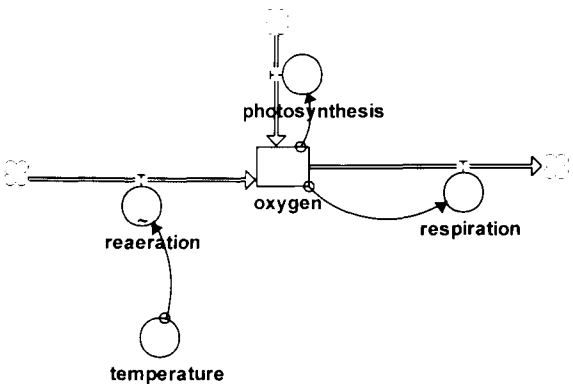

Fig. 9.26. Oxygen model used for the simulations presented above.

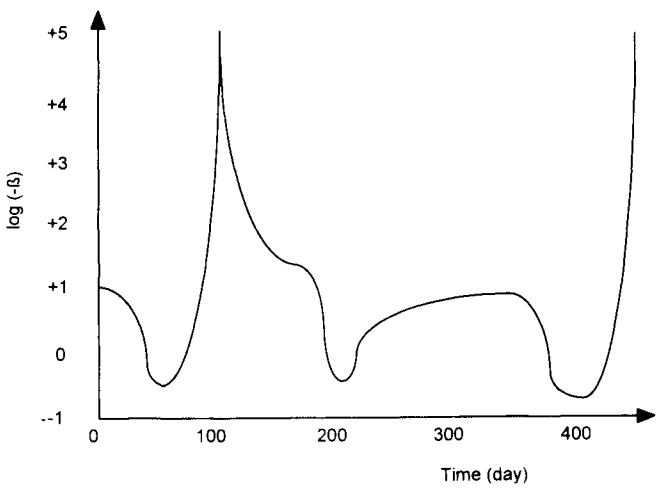

Fig. 9.27. β is plotted versus time. The results are taken from simulations using the model conceptualized in Fig. 9.26.

regulations (see Table 9.1). The flexibility of the system will to a certain extent attempt to prevent the occurrence of catastrophes.

A review of the models that show catastrophes indicates that *catastrophe behaviour* is most frequently associated with populations of *r*-strategists. Their strategy is basically opportunistic "boom and bust" and they simply show higher sensitivity to changes in the general conditions, particularly those determined by the external factors (Southwood, 1981). Therefore it is to be expected that sudden changes of forcing functions (external variables) will first challenge the *r*-strategists. They will be rapidly put on the spot and utilize the recently emerged conditions due

to their high potential of growth. On the other hand they will also violently react in a negative way, i.e., with high mortality, if the conditions were to deteriorate.

An ecosystem will be attracted to, but never reach, a steady state. Solar radiation is able to maintain the system far from thermodynamic equilibrium, and there exists a steady state that can be considered an attractor in a biogeochemical model. It can be found by setting all the derivates to zero. However, the external factors (forcing functions) and even the properties of the species will steadily change. This means that the system at time t will move toward its steady state, but at time $t+1$, when the steady state at time t still has not been reached, the steady state has meanwhile changed and the system moves towards this new steady state and before the new attractor point has been reached, a new steady state = attractor has emerged, etc. The ecosystem is moving towards a moving target and will therefore never reach it. This behaviour may also cause the appearance of limit cycles round the *attractor point,* dependent on the processes involved.

Catastrophe theory has been presented as a theory of equilibria, but in an ecological context it should rather be considered a theory describing a sudden change of the steady state to which the system is attracted.

The existence of *hysteresis* as a response of the state variables to changed external factors shows that the same or, in practice, "almost the same combination of external factors" may give different steady states. The choice between two or more possible steady states is dependent on the short-term history of the system.

Hysteresis could be explained by the ability of ecosystems to maintain as high a buffer capacity as possible. The jump back to the previous situation is prevented for as long as possible.

The present application of catastrophe theory in relation to ecosystems is primitive when the complexity of the ecosystems is considered. Having accepted the limitation in our description of the very complex systems (see also Chapter 2), we have to accept that we can only identify catastrophes and the related buffer capacities for the problem in focus, provided it is supported by a good model and good data.

This is still the general limitation in modelling and ecosystem research, i.e. that we cannot know all details with unlimited accuracy. In fact, it is a limitation placed on all sciences—one that the reductionists have not yet accepted. It may be reduced by the development of better instruments and tools, but it is impossible to eliminate completely because of the enormous complexity of nature, quantum theory (see Section 2.11) and chaos theory. All holistic approaches to ecosystem theory and management are, however, based on a full acceptance of these limitations.

As mentioned in the introduction to this section, there are many ecological models showing catastrophic behaviour which are in accordance with our observations in nature. One of the most interesting examples of catastrophic behaviour is a model of spruce *budworm dynamics*. The growth equations for budworms, the habitat size and foliage are all logistic. The three differential equations are:

$$dB/dt = \mu_b B(1 - B/KS) - CB^2/((K1*S)^2 + B^2) \tag{9.37}$$

$$dS/dt = \mu_s S(1 - S/K2\,E) \tag{9.38}$$

$$dE/dt = \mu_f E(1 - E)P * B * E2/S \tag{9.39}$$

where B is the budworm *population density*, S is the habitat size and E the percentage foliage on trees. μ denotes the growth rate (the indices b, s and f are used), K, C, $K1$, $K2$ and P are all constant. $K1$ is a proportional constant that captures the effectiveness of the predators to spot and prey on spruce budworms. The bigger size of the habitat, the more difficult it is to spot the budworms for the predators. If the transformation $B = K1 * S * X$ is applied, it can be shown that an increase of $R = \mu_b K1\ S/C$, i.e, the maturity of the forest increases, measured by S, leads to a sudden switch from stable to unstable, and an explosion in the budworm population occurs. The readers are encouraged to examine this interesting and illustrative model.

9.7 New Approaches in Modelling Techniques

This final section will give a brief overview of four recently developed modelling techniques: object-oriented models, individual-based models, model construction by using artificial intelligence and expert systems, and fuzzy knowledge-based models. They are developed as new methods of model construction as a recognition of the shortcoming in our data and in the rigidity of our present models.

Object-oriented models (OOM) are based on the idea that programs should represent the interactions between abstract representation of real objects rather than the linear sequence of calculations commonly associated with programming, referred to as procedural programming (Silvert, 1993). It may also be expressed as: "The structure of the model should reflect the structure of the system being modelled".

The central concept of *object-oriented programming* (OOP) is the concept of class which describes both the structure of an object and a set of procedures for initializing and using it in the model. One obvious example of a class is the definition of a population, which is the basic building block for many ecological models. Populations are characterized by variables such as mean size, age, number and exhibit processes such as reproduction, growth, mortality and so on. Each type of population is unique, although there are many similarities, such as the above-mentioned processes. We can therefore treat different classes of populations accordingly and need only add those particular features that need to be different in the model context.

The OOP defines different processes in different modules, which can be used in the various classes. It is possible to have several different versions of the process. The program can for instance have different growth routines. The growth routine is inherited from the class (see below for further explanation) but can also be redefined to cover all other growth expressions. It means that we can use the fact that every population is represented by a class that includes a growth procedure without knowing the precise details of how growth is calculated and it means that changes in

the growth procedure for certain classes do not require changes in the overall structure of the ecological model. This leads naturally to the concept of hierarchy. In ecological modelling it is often difficult to draw the line between processes relevant to the model and those that operate on a different level and should not be included. OOP offers a mechanism that lets us hide this more detailed information on the internal description of objects, so that we can use it without having to describe it explicitly in our model.

The *hierarchy* can be constructed by describing, for instance, first populations, then plants, then algae and finally *Scenedesmus* to cover species. This gives a hierarchy of four classes, each based on the one above it. At each stage we can add and modify information appropriate to the level of description by applying what is called inheritance. Plants may include two parameters beyond those shared by all populations, for instance, growth rate and carrying capacity. Algae then share these properties but also have nutrient limitation characterized by a half saturation constant, so growth has to be redefined in the algae class. The classes for species may finally give information on the settling rate, which in this case will be different for the various species, while all species of algae share the common properties of algae, of plants and of populations. This system has the advantage that changing an inherited method automatically changes all of the classes which inherit that method. Figure 9.28 illustrates class hierarchy for an object-oriented model of cotton plant and associated insect pests.

OOP has only recently received extensive notice even though it has evolved over several decades; see for instance Muetzelfeldt (1979) and Meyer and Pampagnin (1979). Today there are many languages that offer support for OOP. It is expected

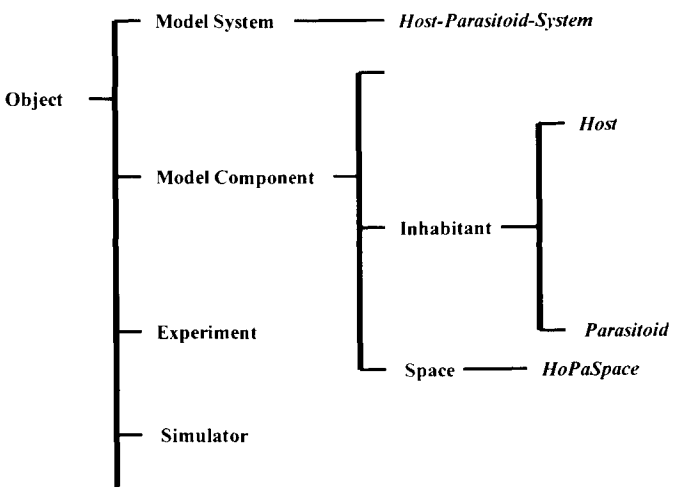

Fig. 9.28. Class *hierarchy* for an object-oriented simulation for cotton plant and associated insect pests. Reproduced from Baveco and Lingeman (1992) with permission.

that it will be increasingly used during the coming years as a more convenient method of programming ecological models.

OOP offers many advantages to developers of ecological models. First of all there is a close connection between object and natural groupings. The concept of inheritance is directly borrowed from biology. OOP makes it possible to develop models that are simpler to interpret for the modelled and which can easily be modified and refined very efficiently.

Examples of *object-oriented models* in ecology can be found in Sequeira et al. (1991), Baveco and Lingeman (1992) and Silvert (1993).

Individual-oriented or *individual-based models* (IBM) attempt to account for the enormous variability among individuals, usually represented in our models by one state variable. Individual-oriented modelling acknowledges two basic ecological principles which are violated in most ecological models, namely the individuality of individuals and the locality of their interactions. Without an inequality among population members, contest competition is not possible and individuals process local information!

The advantages of this modelling approach are obvious. Still, the defence for the approach is often made as a confrontation of *holism* versus *reductionism*, which is a misunderstanding. Ecosystems *have* the properties of individuality of individuals and the locality of their interactions. There is also no doubt that these properties are significant in a number of relations and they should therefore be accounted for in our models. This still does not change the fact that the ecosystem as a system has some properties that cannot be deducted from the sum of the components, and that the model (IBM or not) still cannot account for more than a tiny fraction of the details of the real ecosystems. We are therefore always forced to consider which simplification can be made and which cannot be made in each concrete modelling situation. There are indeed situations where we cannot exclude the individuality and the locality, but need these properties as a core of our model. An average state variable cannot be used in most cases to represent a population, as the core relationships are not linear.

The *individuality* of individuals can in principle be considered by three methods: (1) Leslie matrix models, (2) *i*-space configuration models and (3) by relating the properties of individuals to one or at the most a few core state variables such as, for instance, body size, length, weight or age. Leslie matrix models have been presented in Chapter 6. *i*-Space configuration models use continuous distribution functions. The change at one point along the size continuum is described by a mathematical equation (see, e.g., the example in DeAngelis and Rose, 1992). Benjamin (1999) gives a typical example where the crop growth is determined by the spatial planting pattern and the competition for light which is considered the limiting factor for growth. The application of the third method, i.e., to find a core variable that other variables can be related to, is completely according to the presentation of relations between parameters and body size shown in Section 2.9. Wyszomirski et al. (1999) use the size distribution in crowded and uncrowded monocultures to determine and explain the growth pattern. Hirvonen et al. (1999) have given another illustrative

example where the individual's memory in prey choice decision determined the selection of prey.

A very good overview of individual-based models in ecology is given in DeAngelis and Gross (1992) where many illustrative examples can be found. *Ecological Modelling* had a special issue in 1999 on "Individual-based Modelling in Ecology".

Ecological data bear a large inherent uncertainty due to inaccuracy of data and lack of sufficient knowledge about parameters and state variables. On the other hand, semi-quantitative model outputs might be sufficient in many management situations. ***Fuzzy knowledge-based models*** can be applied in such situations. Zadeh (1965) proposed a method to process imprecise knowledge by using a changed membership function. The membership function takes only two values: one when it belongs to the set and zero when it doesn't. The shape of the fuzzy set membership can be linear or trapezoidal, as shown in Fig. 9.29.

Ecologists often use natural language for describing their knowledge about ecosystems; for instance, "if vegetation is low and population of larks is very high and vegetation density is smaller than standard, then number of territories for the larks will be high." These linguistic rules can be defined in the form of *fuzzy sets* (Zimmermann, 1990). If A and B are fuzzy sets, where we know that if A is true B is also true, the problem is how do we account for A' that fulfils the premise only partially? To calculate the conclusion B' we have to set a relationship based upon approximated reasoning rules as follows

$$B' = A' \circ R \tag{9.40}$$

where $\circ$ is an operator called a composition operator and R is a fuzzy relation. Fuzzy set theory formulates many different forms of what are called composition operators and methods for the calculation of fuzzy relations.

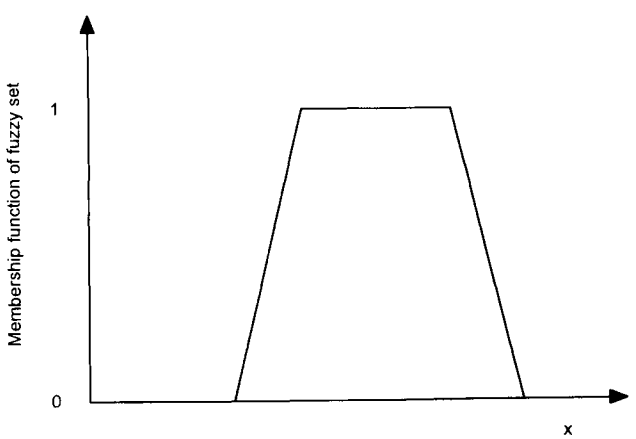

Fig. 9.29. A trapezodial fuzzy set F in x.

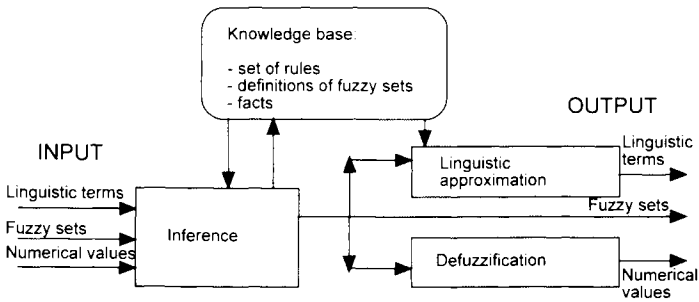

Fig. 9.30. Information flow in the fuzzy knowledge-based model.

The development of a fuzzy knowledge-based model first requires the determination of the model structure, i.e., input and output variables, the number of *submodels*, the connection between submodels, etc. Then the knowledge base is constructed by determining the linguistic rules. Fuzzy sets can then be defined to describe the linguistic rules. The major problem of "fuzzy" modelling is to find an appropriate set of rules to describe the modelled system. They must be taken directly from an *expert's experience*. The set of rules should be complete and provide correct answers for every possible input value. Therefore the sum of all input values (union of fuzzy sets) should cover the value space of all input variables.

The set of linguistic rules, definition of *fuzzy sets* and facts (data) comprise the main part of the fuzzy model: the fuzzy knowledge base (see Fig. 9.30). A fuzzy inference method is used to process this knowledge and compute output values corresponding to the input values. The input values can be numerical or fuzzy sets. Linguistic terms are also allowed as inputs. The output values have the form of fuzzy set that can be translated into a numerical value (by a so-called *defuzzification* process) or approximated to one of the linguistic terms that we have defined for the output variable (see Fig. 9.30).

Only a few examples of fuzzy knowledge based ecological models have been published, but it is probably a method that will have an increased use in the very near future because it is a very appropriate method for a number of ecological problems where our knowledge is only semi-quantitative. Salski (1992) has presented a very illustrative example giving details about this modelling technique.

The applications of ***machine learning*** **in the development of ecological models** are in their infancy. There are probably a number of possible applications in ecological modelling that would improve our models, particularly their ability to make more accurate predictions. Only fantasy sets the limits for the use of machine learning in ecological modelling. Let us mention a few possible applications to illustrate this model type:

- Use of a knowledge base to select more certainly and faster than today the most appropriate model structure from knowledge about the available data.

- a knowledge base that gives relations between forcing functions and some key state variables on the one side and the most crucial parameters on the other, is used to vary the parameters according to the variations of forcing functions and key state variables. With this method we can develop a structurally dynamic model (compare the properties of the structurally dynamic model presented in Section 9.4), where the structural changes are determined by previous experience, represented by the expert system.
- Basic physical, chemical and *ecological principles* are used to increase the robustness, explanation capability and verifiability of the model.
- *Artificial neural networks* have also been applied in ecological modelling. Usually, a three-layered neural network is applied with one input layer, one hidden layer and one output layer. The input layer contains the factors that are of importance for the modelling result included in the output layer. The hidden layer encompasses the equations that can be used to relate the inputs to the outputs. The equations may be based on statistics, causal relationships or any type of knowledge about the focal system or a combination of the three. A set of observations is used to "learn" the right parameters or test alternative equations etc., while an independent set is used test the validity of the model—in principle no different from other modelling approaches. The difference is that the model structure facilitates current improvement, when new observations are available to improve the relationships in the hidden layer

Much of the data collected by ecologists exhibit a variety of problems, including complex data interactions and non-independence of observations. Machine learning methods have shown a good ability to interpret complex ecological data sets and synthesize the interpretation in the form of a model. The resulting synthesis—the model—cannot replace our dynamic modelling approach which has a high extent of causality and therefore generates *general knowledge and understanding,* but the machine learning methods may be considered as supplementary modelling methods which are often able to utilize the data better than dynamic models.

Two machine learning methods will be presented in more detail here:

- *artificial neuron networks* (ANNs), and
- the application of *genetic algorithms*.

ANN is an excellent tool for analysing a complex data set and in most cases is superior to statistical methods that attempt to do the same job. The genetic algorithms can be used to generate rules which will increase our understanding of ecosystem behaviour and therefore facilitate modelling in general. This method has a very great potential for use in connection with dynamic models to improve *submodels* based on too weak knowledge or to introduce additional constraints on dynamic models (for instance the use of a *goal function*; see structurally dynamic modelling).

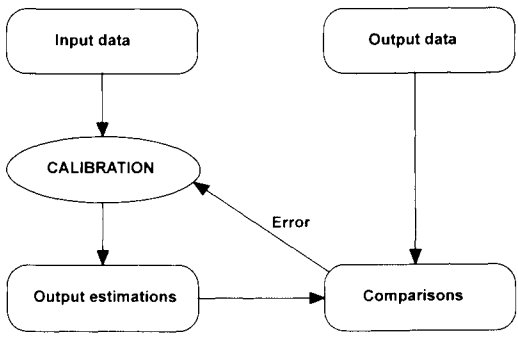

Fig. 9.31. The diagrams shows how data are used to establish the model *calibration*. The goal of the learning is to find a model that will associate the input with the outputs data as correctly as possible.

Artificial neuron networks (ANNs) are developed as models of biological neurons. They have found a wide application in science due to their power to interpret data. During the last decade they have been used increasingly in ecological modelling (see for instance the review by Lek and Guégan, 2000).

The two *ANNs* most applied in ecological modelling are *back propagation neuron network* (BPN) and *self-organizing mapping* (SOM).

BPN is a powerful system, often capable of modelling complex relationships between variables. It also allows the setting up of predictions of output variables for a given input object. The principles of BPN-ANNs are shown in Fig. 9.31. Data are used to establish the model calibration. The goal is to find a calibrated model that will correctly associate the input with the output. The loop calibrated system – output estimation – comparison – error used for corrections is continued until the comparison is satisfactory.

The BPN architecture is a layered feed *neuron network*. The information flows from the input layer to the output layer through the hidden layer (see Fig. 9.32). Nodes from one layer are connected to all the nodes in the next layer, but there are no connections between nodes within one layer.

Figure 9.33 shows a neuron with its connections. Each neutron is numbered. The inputs are indicated as $x_1, x_2, x_3, \ldots, x_n$ and are associated with a quantity called weight or connection strength, $w_{1j}, w_{2j}, w_{3j}, \ldots, w_{n,j}$ for the input to the j'th neutron. Both positive and negative weights may be applied. The net input, denoted activation, for each neutron is the sum of all its input multiplied by their weights $+z$, a bias term which may be considered the weights from supplementary input units:

$$a_j = \sum_i w_{ji} x_i + z \tag{9.41}$$

The output value, y_j, called the response, can be calculated from the activation of the neuron:

$$y_j = f(a_j) \tag{9.42}$$

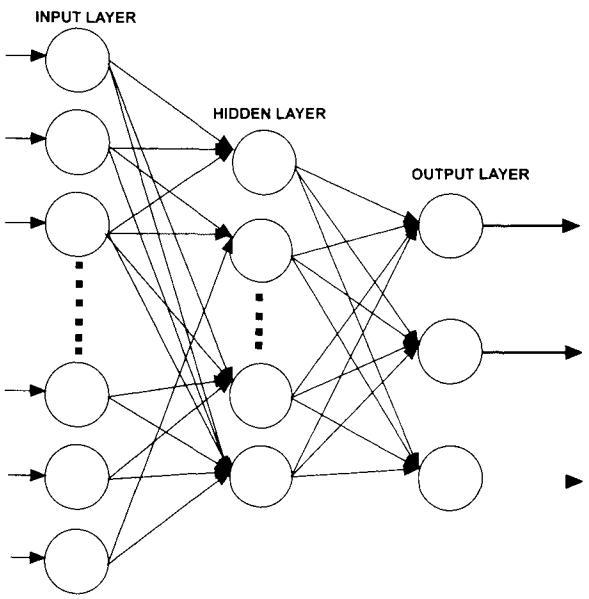

Fig. 9.32. Illustration of a three-layered neural network with one input layer, one hidden layer and one output layer.

Many functions may be used, e.g. a linear function, a threshold function and most often a *sigmoid function*:

$$y_j = 1/(1 + e^{-a}) \tag{9.43}$$

The weights establish a link between the input data and the associated output. They therefore contain the neuron network's knowledge about the problem/solution relationship. The forward-propagating step begins with the presentation of the input data to the input layer and continues as activation level calculations propagate forward to the output layer through the hidden layer using the equations presented above. The backward propagation step begins with the comparison of the network output pattern to the observations (the target values). The error values (the differences between outputs and target values), d, are determined and are used to change the weights, starting with the output layer and moving backwards through the hidden layer. If the output layer is designated by k, then its error signal, s_k, is:

$$s_k = d_k f'(a_k) \tag{9.44}$$

where $f'(a_k)$ is the derivate of the transfer function (most often the sigmoid function). For the hidden layer j, the error signal, s_j, is computed as:

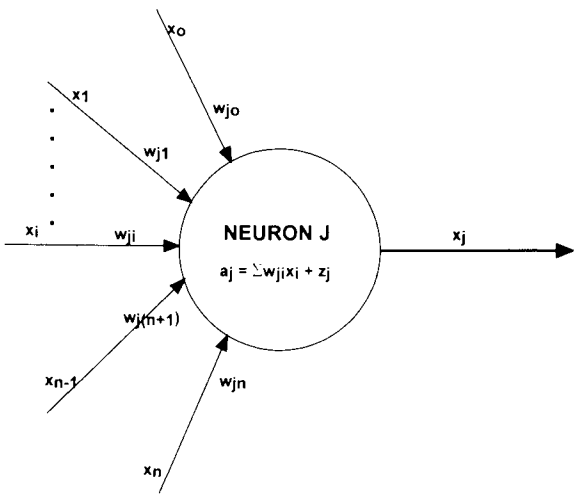

Fig. 9.33. The basic processing element (a neuron) in a network receives several input connection values associated with a weight. The resulting output value is computed according to the equations presented (see the text).

$$s_j = [\Sigma d_k w_{kj}] f'(a_j) \tag{9.45}$$

Each weight is adjusted by taking into account the d-value of the unit that receives input from that interconnection. The adjustment depends on three factors: d_k (error value of the target unit), y_j (output value for the source unit) and ñ:

$$\Delta w_{kj} = \tilde{n} d_k y_j \tag{9.46}$$

ñ is a *learning rate*, commonly between 0 and 1, chosen by the user. A very large value of ñ, close to 1, may lead to instability in the network and unsatisfactory learning. Too small value of ñ leads to excessively slow learning. Sometimes, ñ is varied to produce efficient learning of the network during the training procedure, for instance, high at the beginning and decreasing during the learning step.

Before the training begins, the connection weights are set to a small random value, e.g., between –0.3 and +0.3. The input data are applied to produce a set of output data. The error values are used to modify the weights. One complete calculation is called an epoch or iteration of training or learning procedure. The BPN algorithm performs gradient descent on this error surface by modifying the weights. The network can sometimes get stuck in a depression in the error surface. These are called local minima corresponding to a partial solution. Ideally, we seek a global minimum. Special techniques should be applied to get out of a local minimum, changing the learning parameter, ñ, the number of *hidden layer*, or by the use of a momentum term, m, in the algorithm. m is chosen generally between 0 and 1. The equation for weight modification of epoch $t + 1$ is thereby given as:

$$\Delta w_{kj}(t+1) = \tilde{n}d_k(t+1)y_j(t+1) + a\Delta w_{kj}(t) \tag{9.47}$$

A training set must have enough data to represent the pattern of the overall relationships. The training phase can be time-consuming depending on the structure, number of hidden layers, number of nodes and the number of data in the training set. A test phase is also usually required. The input data are fed into the network and the desired output patterns are compared with the results obtained by the *ANN* to assess the correlation coefficient between observed and estimated values.

Scardi and Harding (2000) have applied the presented method to develop an *ANN-model* of phytoplankton primary production for marine systems. They applied a global data set, consisting of 2218 sets of data of phytoplankton biomass, irradiance, temperature and primary production for testing and 825 sets of data from a single sampling station in the Gulf of Napoli for training. They showed that the ANN gave a $R^2 = 0.862$ compared with a $R^2 = 0.696$ obtained by a multiple linear regression model. Many other examples are given in Lek and Guégan (2000) and in Fielding (1999). From these examples, it can be concluded that ANN offers good possibilities to attain information from a heterogeneous, complex and comprehensive data set, but opposite a dynamic biogeochemical or population dynamic model ANN is not based on causality and will therefore always yield a model with less generality than the dynamic model types.

The relevant *multivariate algorithms* of *SOM* seek clusters in the data. The network consists of two types of unit: an input layer and an output layer. The array of input units operates simply as a flow-through layer for the input vectors and has no further significance. The output layer often consists of a two-dimensional network of neurons arranged on a square grid laid out in a lattice. Each neuron is connected to its nearest neighbours on the grid (see Fig. 9.34). The neurons store a set of weights, an n-dimensional vector if input data are n-dimensional.

Several *training strategies* have been proposed to find the clusters in the data. Originally, Kohonen (1984) proposed the following equation to find the activation level for a neuron (the procedure is described according to Lek and Guégan, 2000):

$$\|w' - x\| = \sqrt{\sum_{i=0}^{n} (w_i^j - x_i)^2} \tag{9.48}$$

which is simply the Euclidian distance between the points represented by the weight vector and the input in the n-dimensional space. A node whose weight vector closely matches the input vector will have a small activation level and a node whose weight vector is very different from the input vector will have a large activation level. The node in the network with the smallest activation level is deemed to be the winner for the current input vector. During the training process the network is presented with the input pattern and all the nodes calculate their activation levels by the use of Eq. (9.48). The winning node and some of the nodes around it are then allowed to adjust their weight vectors to match the current input vector more closely.

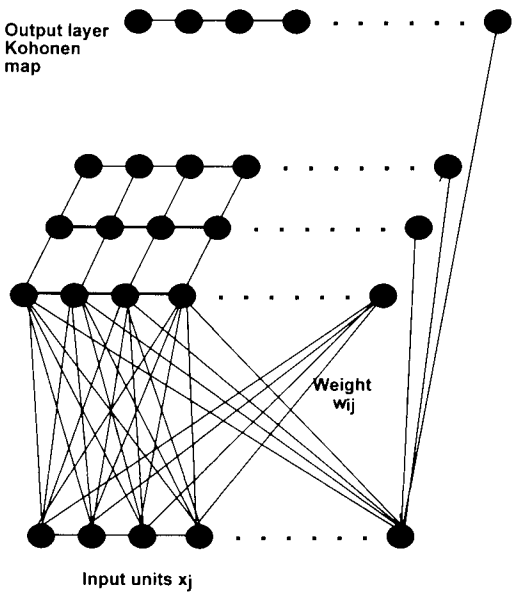

Fig. 9.34. A two-dimensional self-organizing feature map network.

The nodes included in the set are said to belong to the neighbourhood of the winner. The size of the winner's neighbourhood is decreased linearly after each presentation of the complete training set, until it includes only the winner itself. The amount by which the nodes in the neighbourhood are allowed to adjust their weights is also reduced linearly through the training period. The factor that governs the size of the weight variations is known as the learning rate. The adjustment to each item in the weight vector are made in accordance with:

$$\Delta w_i = -\tilde{n}(w_i - x_i) \tag{9.49}$$

where Δw_i is the change in weight and $-\tilde{n}$ is the learning rate. This is carried out from $i = 1$ to $i = n$, the dimension of the data. The learning is divided into two phases. In the first $\tilde{n}$ shrinks linearly from 1 to the final value 0 and the neighbourhood radius decreases in order to initially contain the whole map and finally only the nearest neighbours of the winner. During the second phase, tuning takes place. $\tilde{n}$ attains small values during a long period and the neighbourhood radius keeps the value 1. The effects of the weight updating algorithm is to distribute the neurons evenly throughout the regions of n-dimensional space populated by the training set. This effect is displayed and shows the distribution of a square network over an evenly populated two-dimensional square input space. By training with networks of increasing size, a map with several levels of groups and contours can be drawn. The construction of these maps allows close examination of the relationships between the items in the training set.

Several illustrations of the application of SOM in an ecological context have been presented in Lek and Guégan (2000) and in the journal *Ecological Modelling* during the last few years.

Genetic algorithms provide an alternative approach to model (*submodel*) selection. They develop iteratively a set of rules which help to explain the relationships between variables or attributes included in the data set. Several genetic algorithms are available but they all more or less have the same features. The algorithm called BEAGLE (Biological Evolutionary Algorithm Generating Logical Expressions) will be used to illustrate the basic ideas behind the application of genetic algorithms in ecological modelling.

BEAGLE consists of six main components:

1. SEED (Selectively Extracts Example Data) enables data files to be read in several simple formats, including ASCII files. It also performs one or both of the following optional functions: (1) it splits the data into two random subsets, and (2) it appends leading or lagging variables to time series.
2. ROOT (Root-Orientated Optimization Tester) enables the user to test one or more rules. If successful, these rules will then be used as a starting point for the subsequent components, but will usually quickly be replaced by better rules. If no preliminary rules are available ROOT will generate the required number of starting rules at random.
3. HERB (Heuristic Evolutionary Rule Breeder) generates new rules for the data file prepared by SEED. HERB evaluates all the existing rules against the training data set and then eliminates any rule that is unsuccessful. It finally makes a few random changes to some of the rules, cleans up any solecisms introduced by the mutation rules and performs appropriate syntactic manipulation to simplify the rules and make them more comprehensible. The whole set of modified rules is then tested again based on a chi-square statistic.
4. STEM (Signature Table Evaluation Module) uses the rules found by HERB to construct a signature table, reexamines the training data and counts the number of times each signature occurs. It also accumulates the average value of the target expression for each signature.
5. LEAF (Logical Evaluator And Forecaster) applies the induced rules to an additional data set which has the same structure as the training data. The success rate of the rules and combination of the rules is calculated.
6. PLUM (Procedural Language Utilization Module) translates the induced rules into a Pascal Procedure or a FORTRAN subroutine so that the rules can be exported into other software languages for practical use.

A typical illustration of the use of genetic algorithms in ecological modelling can be found in Recknagel and Wilson (2000). For instance, they are able to set up

predictive rules (threshold values for concentrations of nitrogen and phosphorus and temperature) for the presence and approximate concentration of *Mycrocystis* based upon data from Kasumigaura Lake. These rules are applied in a *eutrophication model* for *Kasumigaura Lake* to describe the succession of species or the change in species composition, resulting from changes in the variables included in the resulting rules.

The application of genetic algorithms in ecological modelling appears to be promising. They could probably be used much more widely to select *submodels* and to develop a more streamlined application of goal functions in structurally dynamic models. A combination of rules generated by genetic algorithms and the use of goal functions for the development of better structurally dynamic models will probably be seen in the very near future.

PROBLEMS

1. Examine the budworm population dynamic model presented in Section 9.6 by the use of STELLA.
2. Develop a logistic model with time lag for the population size determining the growth rate and the carrying capacity. Show that the model behaves chaotically at certain values of the time lag and the growth rate.
3. Develop a STELLA model of the competition model presented in Section 9.4. Find a parameter combination that gives stable behaviour. Change one of the parameters step-wise over a wide range of values and observe the behaviour of the model and of the total exergy of all the model components.
4. Follow the exergy of the model in Illustration 9.1 as the temperature is changed and explain the variation of exergy over time. Could exergy be used to explain the abrupt change of the state variables?
5. The use of artificial intelligence and machine learning has increased rapidly during the last ten years. List the advantages and disadvantages of these model types.
6. Structurally dynamic modelling has not been used in ecotoxicological modelling; why?
7. What advantages do you see in the application of the structurally dynamic approach in ecotoxicological models? Is the use of this model type of relevance or not of relevance in the development of ecotoxicological models?
8. Mention a few modelling cases where the use of individual based models would be beneficial.

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APPENDIX 1

Mathematical Tools

by **Poul Einer Hansen**

The purpose of the following pages is to offer a little help to those readers—biologists and others—who do not make frequent use of mathematics above the elementary level, and who find themselves unable to appreciate the extensive use of mathematics in the present volume. there is no shortcut to getting familiar with mathematics, and it should be stressed that reading the appendix will certainly not provide you with a full understanding of the methods and results involved, nor will it enable you to use them independently. However, it may give you some idea of what goes on and perhaps inspire a few to seek more thorough information elsewhere; there are numerous suitable textbooks in the field.

To start mathematically from scratch is not possible (and besides, if you were there you would hardly be reading this book in the first place). So let us assume that the reader is, or was once, familiar with subjects such as: arithmetics, elementary algebra, trigonometry, exponentials and logarithms, combinatorials, analytic geometry and some vector algebra in two and (less deeply) three dimensions, and introductory differential and integral calculus.

The two most important subjects to be dealt with in the appendix are *matrices* and *differential equations*; the question of *numerical methods* will also be touched upon. To get to the second floor of a house you have to pass through the first, meaning that we will have to treat some topics that are not directly relevant for the rest of the book, but are necessary to understand other topics that are.

A few *exercises* are interspersed in the text. It is strongly recommended that you try to solve these exercises along with reading. If you are stuck, ask a colleague or a friend for help. But remember: only just enough to get you going again!

A.1 Vectors

Recall that a plane *vector* is a directed line segment (or: an ordered pair of points) PQ; we say that $PQ = RS$ whenever PQ and RS are parallel, of equal length, and have the same direction.

If a coordinate system is drawn in the plane, then the vector from the origin (0,0) to the point (x, y) is said to have coordinates (x, y). Note that if the same vector is drawn with another point $R = (a, b)$ as origin, it will end in $S = (a+x, b+y)$. A vector can to a large extent be identified by its pair of coordinates, i.e., alternatively we could define a plane vector as an ordered pair of numbers, $\boldsymbol{v} = (x, y)$. Thus there are two ways of thinking of a vector: a geometrical one and an algebraical one. We shall focus mainly on the latter since most of the applications relevant for ecological modelling are algebraical/computational and do not offer any obvious geometrical interpretation. See Example A.1 below.

Plane *vector algebra* is based on the following definitions of (1) vector sum, (2) vector difference, (3) product of a number (a "scalar") and a vector, (4) scalar product of two vectors: let $\boldsymbol{u} = (x_1, y_1)$ and $\boldsymbol{v} = (x_2, y_2)$ be vectors and let k be a number, then

$$\begin{aligned} &(1)\ \boldsymbol{u}+\boldsymbol{v} = (x_1 + x_2, y_1 + y_2), \\ &(2)\ \boldsymbol{u}-\boldsymbol{v} = (x_1 - x_2, y_1 - y_2), \\ &(3)\quad k\boldsymbol{v} = (kx_2, ky_2), \\ &(4)\ \boldsymbol{u}\cdot\boldsymbol{v} = x_1x_2 + y_1y_2. \end{aligned} \tag{A.1}$$

The corresponding geometric definitions are: (1) if $\boldsymbol{u}$ and $\boldsymbol{v}$ are drawn as PQ and QR, respectively, then $\boldsymbol{u}+\boldsymbol{v} = PR$, (2) if $\boldsymbol{u}$ and $\boldsymbol{v}$ are drawn with a common point of origin, $\boldsymbol{u} = PQ$ and $\boldsymbol{v} = PS$, then $\boldsymbol{u}-\boldsymbol{v} = SQ$, (3) if $\boldsymbol{v} = PQ$ and R lies on the line through P and Q so that $|PR| = k|PQ|$ and in the same direction from P as Q when $k > 0$, opposite direction when $k < 0$, then $PR = k\boldsymbol{v}$, (4) $\boldsymbol{u}\cdot\boldsymbol{v} = |\boldsymbol{u}|\,|\boldsymbol{v}| \cos\varphi$ where $|\boldsymbol{u}|$ and $|\boldsymbol{v}|$ are the lengths of $\boldsymbol{u}$ and $\boldsymbol{v}$, respectively, and φ is the angle between them when they are drawn from a common point of origin.

It turns out that a large number of the algebraic rules knows from ordinary arithmetics hold in vector algebra as well, as we can carry out, without worrying, calculations like the following:

$$(3\boldsymbol{u} + 5\boldsymbol{v}) \cdot (2\boldsymbol{u} - \boldsymbol{v}) = 6\boldsymbol{u}^2 - 3\boldsymbol{u}\cdot\boldsymbol{v} + 10\boldsymbol{v}\cdot\boldsymbol{u} - 5\boldsymbol{v}^2 = 6\boldsymbol{u}^2 + 7\boldsymbol{u}\cdot\boldsymbol{v} - 5\boldsymbol{v}^2 \tag{A.2}$$

($\boldsymbol{u}^2$ is short for $\boldsymbol{u}\cdot\boldsymbol{u}$). The only thing to be cautious about is the scalar product. Firstly, it is a *number*, not a vector, i.e., an expression like $\boldsymbol{u} + \boldsymbol{v}\cdot\boldsymbol{w}$ is meaningless; secondly, a scalar product cannot have more than two factors; and thirdly, $\boldsymbol{u}\cdot\boldsymbol{v} = 0$ does not in general imply that either $\boldsymbol{u}$ or $\boldsymbol{v}$ is equal to the "zero vector" $\boldsymbol{o} = (0,0)$; in geometrical terms it only implies that they are perpendicular to each other, $\varphi = 90°$.

EXERCISE A.1

Repetition of plane vector algebra. Draw an XY-system; choose simple values of $\boldsymbol{u}$, $\boldsymbol{v}$, k and carry out the calculations involved in the definitions of the four vector-algebraic operations. Do the results correspond with the geometric definitions, when compared with the measurements made in the figure?

Example A.1

A fish population in a lake is divided into two age classes, juveniles and adults. The population may be described by the two-dimensional vector

$$\boldsymbol{x} = (x_1, x_2) \tag{A.3}$$

where x_1 is the number of juveniles and x_2 is the number of adults. (Both are in general functions of time, but we leave out this aspect here).

If two populations of the species in question, with population vectors $\boldsymbol{x}$ and $\boldsymbol{y}$, respectively, are brought together in a common environment, then the vector sum

$$\boldsymbol{x} + \boldsymbol{y} = (x_1 + y_1, x_2 + y_2) \tag{A.4}$$

can be interpreted as the vector for the resulting united population.

If $\boldsymbol{x}$ refers to densities, e.g., numbers of fish per m^3, and V denotes the volume of the lake, then the product

$$V\boldsymbol{x} = (Vx_1, Vx_2) \tag{A.5}$$

can be interpreted as the vector that describes the population in the lake in terms of absolute numbers.

If w_1 and w_2 denote the average weights of a juvenile fish and an adult fish, respectively, and we put $\boldsymbol{w} = (w_1, w_2)$, then the scalar product

$$\boldsymbol{x} \cdot \boldsymbol{w} = x_1 w_1 + x_2 w_2 \tag{A.6}$$

can be interpreted as the total weight of the population.

This example suggests that vector algebra may be useful also in ecology, but with emphasis on the algebraical and not the geometrical point-of-view.

Almost all of the above considerations on plane vectors can be carried over to three-dimensional space. We will think of a three-dimensional vector mostly as an ordered set of three numbers (a 'number triplet')

$$\boldsymbol{v} = (x, y, z) \tag{A.7}$$

and of the corresponding vector algebra as being based on the following "co-ordinate-oriented" definitions (where notation generalizes Eqs. (A.1) in an obvious manner):

$$\begin{aligned}
&(1)\ \boldsymbol{u}+\boldsymbol{v}=(x_1+x_2, y_1+y_2, z_1+z_2),\\
&(2)\ \boldsymbol{u}-\boldsymbol{v}=(x_1-x_2, y_1-y_2, z_1-z_2),\\
&(3)\quad k\boldsymbol{v}=(kx_2, ky_2, kz_2),\\
&(4)\ \boldsymbol{u}\cdot\boldsymbol{v}\ =x_1x_2+y_1y_2+z_1, z_2.
\end{aligned} \tag{A.8}$$

We note however that the geometric definitions hold as well, and that the algebra is just as nice in three as in two dimensions—it could be claimed that in some aspects it is even nicer. In three dimensions one usually introduces yet another composition, the so-called vector product which, even though it is algebraically somewhat less regular than the other four operations, has many important applications. But it is not particularly relevant to our purpose and therefore we leave it out.

When it comes to the various computation-oriented applications of vector algebra, there is no difficulty in passing from two to three dimensions. For instance, in Example A.1 we might as well have operated with three age classes instead of two; it would not have made the formulas more complicated to understand—just made them 50% longer!

We have seen that especially when the focus in on coordinate algebra rather than geometry/stereometry, there is a striking analogy between two- and three-dimensional vector algebra. Which leads to the question: why not go on to dimension 4, 5, etc.? This is indeed possible, and again it turns out that the simpler parts of the algebra is just as nice in higher dimensions as it was above. The figurative, i.e., the geometric or stereometric aspect of vector algebra in the proper sense must then largely be renounced. Yet it prevails, dialectically, as a source of inspiration for ideas, proofs and constructions of methods.

Let $\mathbf{R}^n$ be the n-dimensional number space, i.e., the set of all n-tuples of real numbers

$$\boldsymbol{x} = (x_1, x_2, \ldots, x_n). \tag{A.9}$$

The vector-algebraic operations in $\mathbf{R}^n$ are defined by

$$\begin{aligned}
&(1)\ \boldsymbol{x}+\boldsymbol{y}=(x_1+y_1, x_2+y_2, \ldots, x_n+y_n),\\
&(2)\ \boldsymbol{x}-\boldsymbol{y}=(x_1-y_1, x_2-y_2, \ldots, x_n-y_n),\\
&(3)\quad k\boldsymbol{x}=(kx_1, kx_2, \ldots, kx_n),\\
&(4)\ \boldsymbol{x}\cdot\boldsymbol{y}\ =x_1y_1+x_2y_2+\ldots+x_n, y_n.
\end{aligned} \tag{A.10}$$

(A change in notations was made: indices now follow coordinates instead of vectors; however this was already the case in Example A.1, so it should not give any trouble.) As already mentioned, virtually all the algebraic rules that hold for $n = 2$ and $n = 3$ hold for arbitrary n as well. And interpretations in various areas of application are straightforward; in some cases they even seem more natural when the limitation of the dimension n to 2 or 3 is abandoned.

In three dimensions the Nabla operator is often used

$$\nabla = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \right) = (\nabla_x, \nabla_y, \nabla_z)$$

With this definition we have:

$$\nabla a = \left(\frac{\partial a}{\partial x}, \frac{\partial a}{\partial y}, \frac{\partial a}{\partial z} \right) = \text{grad}\, a$$

$$\nabla \cdot \vec{v} = \frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z} = \text{div}\, \vec{v}$$

$$\nabla \times \vec{v} = \begin{vmatrix} (\nabla \times \vec{v})_x = \nabla_y v_z - \nabla_z v_y = \dfrac{\partial v_z}{\partial y} - \dfrac{\partial v_y}{\partial z} \\ (\nabla \times \vec{v})_y = \nabla_z v_x - \nabla_x v_z = \dfrac{\partial v_x}{\partial z} - \dfrac{\partial v_z}{\partial x} = \text{rot}\, \vec{v} \\ (\nabla \times \vec{v})_z = \nabla_x v_y - \nabla_y v_x = \dfrac{\partial v_y}{\partial x} - \dfrac{\partial v_x}{\partial y} \end{vmatrix}$$

As a consequence of these definitions we have the scalar field

$$\nabla \cdot (\nabla a) = \nabla^2 a = \left(\frac{\partial^2 a}{\partial x^2} + \frac{\partial^2 a}{\partial y^2} + \frac{\partial^2 a}{\partial z^2} \right)$$

where $\nabla^2 = \left(\dfrac{\partial^2}{\partial x^2}, \dfrac{\partial^2}{\partial y^2}, \dfrac{\partial^2}{\partial z^2} \right)$ is called the Laplacian operator, and as a consequence of the fundamental rules of vector algebra

$$\nabla \times (\nabla a) = 0$$
$$\nabla (\nabla \cdot \vec{v}) = \text{a vector field}$$
$$\nabla \cdot (\nabla \times \vec{v}) = 0$$
$$\nabla \times (\nabla \times \vec{v}) = \nabla (\nabla \cdot \vec{v}) - \nabla^2 \vec{v}$$

EXERCISE A.2

A chemical plant is organized in four divisions, D1–D4. When working, D1 emits 800 m^3 of CO_2 per hour, D2 uses 500 m^3 atmospheric CO_2 per hour, D3 used 600 m^3, and D4 emits 1000 m^3. Suppose that the four divisions work 8, 10, 5, and 7 hours per day, respectively.

(1) Find the daily net outlet of CO_2 from the plant, by use of vector algebra in $\mathbf{R}^4$. (Hint: The "outlet vector" has both positive and negative coordinates.)

(2) How many hours instead of 5 should D3 run per day if the plant wants to be CO_2 neutral, provided the three other divisions keep up their schedule?

A.2 Matrices

Matrices

An $m \times n$ *matrix* is a rectangular array of numbers, termed the *elements* of the matrix, arranged in m rows and n columns. For example,

$$\boldsymbol{A} = \begin{pmatrix} 200 & 750 & 350 \\ 150 & 400 & 250 \end{pmatrix} \tag{A.11}$$

is a 2×3 matrix. The general form of an $m \times n$ matrix is:

$$\boldsymbol{A} = \begin{pmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ & \dots & & \\ a_{m1} & a_{m2} & \dots & a_{mn} \end{pmatrix} \tag{A.12}$$

Matrices are usually referred to by capital letters in boldface, but the matrix $\boldsymbol{A}$ in (A.12) is also sometimes referred to as $\{a_{ij}\}$. In self-explanatory terms, we speak of the i'th *row vector* ($i = 1,...,m$) and of the j'th *column vector* ($j = 1,...,n$), respectively

$$(a_{i1}\, a_{i2} \dots a_{in}) \quad \text{and} \quad \begin{pmatrix} a_{1j} \\ a_{2j} \\ \dots \\ a_{mj} \end{pmatrix} \tag{A.13}$$

which can be considered as matrices, respectively an $m \times 1$ *row matrix* and a $1 \times n$ *column matrix*. In ordinary vector algebra (see Section A.1), it is not important whether vectors are written row-wise or column-wise (though for aesthetic reasons one should stick to one *or* the other), but as soon as the matrix point-of-view is taken we must be sure to distinguish between them, as will later become clear.

Example A.2

The result of a division of a set, e.g., a population, according to two criteria can be given in the form of a matrix. For instance, suppose that the fish population in Example A.1 besides being subject to the age distribution is also divided into, say, genotypes *aa*, *aA*, and *AA* with respect to a particular gene; and that the following estimates have been made of the numbers of fish that have the various combinations of age and genotype:

	Genotype *aa*	Genotype *aA*	Genotype *AA*
Juveniles	200	750	350
Adults	150	400	250

The information in the table is set out in a slightly more concentrated form by matrix A in Eq. (A.11), if it has been agreed what the various rows/columns are labelled. The first row vector of A gives the distribution of juveniles on genotypes. The second column vector gives the age distribution of the heterozygotes. The age distribution of the entire population can be found by taking the sum of the three column vectors, i.e., summing the elements in each row, which yields 1400 juveniles and 700 adults.

A function from $\mathbf{R}^n$ to $\mathbf{R}^m$ is of the general form

$$y = f(x) \tag{A.14}$$

where $x \in \mathbf{R}^n$, $y \in \mathbf{R}^m$. This means that the function depends on n variables and takes values that have m coordinates; written out more thoroughly it is of the form

$$f(x) = \begin{pmatrix} f_1(x_1, x_2, \ldots, x_n \\ f_2(x_1, x_2, \ldots, x_n \\ \cdots \\ f_m(x_1, x_2, \ldots, x_n \end{pmatrix}. \tag{A.15}$$

For example, a function from $\mathbf{R}^3$ to $\mathbf{R}^2$ could be defined by

$$f(x) = \begin{pmatrix} 5x_1^2 + x_2 x_3 \\ x_2 \sin(x_1 - 4x_3) \end{pmatrix}. \tag{A.16}$$

A function from $\mathbf{R}^n$ to $\mathbf{R}^m$ is said to be linear if each of the m coordinate functions is linear and homogeneous in the independent variables x_j, i.e., there are constants a_{ij} ($i = 1,\ldots,m; j = 1,\ldots,n$) so that

$$f(x)=\begin{pmatrix} a_{11}x_1+a_{12}x_2+\ldots+a_{1n}x_n \\ a_{21}x_1+a_{22}x_2+\ldots+a_{2n}x_n \\ \cdots \\ a_{m1}x_1+a_{m2}x_2+\ldots+a_{mn}x_n \end{pmatrix}. \tag{A.17}$$

The pattern formed by the coefficients is identical to matrix A in Eq. (A.12), and we shall say that A is the matrix of (or belonging to) the function f. Note that the i'th coordinate of $f(x)$ is equal to the scalar product of the i'th row vector of A and the vector x; they are both $\mathbf{R}^n$-vectors, so it is meaningful to talk about their scalar product.

Example A.3

Suppose that the fish in the previous example is a herbivore and feeds on four different types of algae, Alga 1–4. It has been established that the approximate daily intake of the four algae is as follows:

	Per juvenile	Per adult
g of Alga 1	10	30
g of Alga 2	10	50
g of Alga 3	0	40
g of Alga 4	15	10

(A.18)

If x_1, x_2 are the numbers of juveniles and adults, respectively, and if y_i is the total daily consumption of Alga i in the lake (i = 1,2,3,4), it follows readily from Table (A.18) that

$$\begin{aligned} y_1 &= 10x_1 + 30x_2 \\ y_2 &= 10x_1 + 50x_2 \\ y_3 &= 0x_1 + 40x_2 \\ y_4 &= 15x_1 + 10x_2. \end{aligned} \tag{A.19}$$

This is a linear function from $\mathbf{R}^2$ to $\mathbf{R}^4$, with matrix

$$A=\begin{pmatrix} 10 & 30 \\ 10 & 50 \\ 0 & 40 \\ 15 & 10 \end{pmatrix}. \tag{A.20}$$

The *transpose* of an $m\times n$ matrix A is the $n\times m$ matrix which has the rows of A as its columns and *vice versa*. It is denoted A^T; some authors prefer A'. For example, the matrix in the preceding example, see Eq. (A.20), has the transpose

$$A^T = \begin{pmatrix} 10 & 10 & 0 & 15 \\ 30 & 50 & 40 & 10 \end{pmatrix}. \tag{A.21}$$

Note that the transpose of a row matrix is a column matrix, and the transpose of a column matrix is a row matrix.

EXERCISE A.3

(*Continuation of Example A.3*). One gram of Alga i contains u_i units of a certain trace element ($i = 1,2,3,4$). Let v_1 be the number of units of the trace element taken up per day by a juvenile fish, and let v_2 be the number of units taken up by an adult. Show that $\boldsymbol{v} = \boldsymbol{g}(\boldsymbol{u})$ where $\boldsymbol{g}$ is a linear function from $\mathbf{R}^4$ to $\mathbf{R}^2$, with the matrix A^T from Eq. (A.21).

It is possible to define algebraic operations for matrices in such a way that the resulting matrix algebra has two qualities: (1) it obeys most of the algebraic rules known from arithmetics and vector algebra (in fact, for some matrices the algebra is even nicer than vector algebra), (2) matrix calculations have meaning and are useful in the context of applications. We shall proceed directly to the definitions.

(1) Let $\boldsymbol{A} = \{a_{ij}\}$ and $\boldsymbol{B} = \{b_{ij}\}$ be $m \times n$ matrices. The *sum* $\boldsymbol{A}+\boldsymbol{B}$ is the mxn matrix $\boldsymbol{C}$ whose ij'th element is

$$c_{ij} = a_{ij} + b_{ij}. \tag{A.22}$$

i.e., $\boldsymbol{A}+\boldsymbol{B}$ is formed by adding the elements of A and B at each position. Note that the sum of two matrices can be formed if, and only if, they have the same number of rows and the same number of columns.

(2) Similarly, the *difference* $\boldsymbol{C} = \boldsymbol{A}-\boldsymbol{B}$ of two $m \times n$ matrices is defined by

$$c_{ij} = a_{ij} - b_{ij}. \tag{A.23}$$

(3) Let $\boldsymbol{A} = \{a_{ij}\}$ be an $m \times n$ matrix and let k be a real number. The product $k\boldsymbol{A}$ is the $m \times n$ matrix C whose ij'th element is

$$c_{ij} = ka_{ij}. \tag{A.24}$$

i.e., the elements of $\boldsymbol{A}$ are multiplied uniformly by k.

The definitions of matrix sum, matrix difference and scalar-matrix product are straightforward, and so are their interpretations in many applied situations. For

example, consider two fish populations like the one in Example A.2, both divided by two criteria and described by a 2×3 matrix, $\boldsymbol{A}$ and $\boldsymbol{B}$, respectively; if the two populations are united then it is clear that the total population is described by $\boldsymbol{A}+\boldsymbol{B}$. Similarly, if some incident in the lake causes an immediate uniform mortality factor of 30%, then the matrix describing the population is changed from $\boldsymbol{A}$ to $k\boldsymbol{A}$, with k = 0.7. It is left for the reader to contemplate these examples and to supplement them with others. At any rate it seems fair to state that the introduction of operations (1)–(3) is not problematic. The fourth matrix operation, multiplication, is a bit more complicated.

(4) Let $\boldsymbol{A} = \{a_{ij}\}$ be an $m \times n$ matrix and let $\boldsymbol{B} = \{b_{ij}\}$ be an $n \times p$ matrix. The product $\boldsymbol{AB}$ is the $m \times p$ matrix $\boldsymbol{C}$ whose ik'th element is

$$c_{ik} = \sum_{j=1}^{n} a_{ij} b_{jk} = a_{i1} b_{1k} + a_{i2} b_{2k} + \ldots + a_{in} b_{nk}, \tag{A.25}$$

i.e., c_{ik} is the scalar product of the i'th row in $\boldsymbol{A}$ and the k'th column in $\boldsymbol{B}$. Note that the product of two matrices can be formed if, and only if, the number of columns of the first factor is equal to the number of rows of the second factor; this condition ensures that a row of the first actor and a column of the second factor have the same dimension so that their scalar product exists.

For example, if

$$\boldsymbol{A} = \begin{pmatrix} 3 & 0 & 2 & 2 \\ 0 & 1 & 3 & 0 \\ 1 & 0 & 2 & 1 \end{pmatrix}, \quad \boldsymbol{B} = \begin{pmatrix} 10 & 30 \\ 10 & 50 \\ 0 & 40 \\ 15 & 10 \end{pmatrix}. \tag{A.26}$$

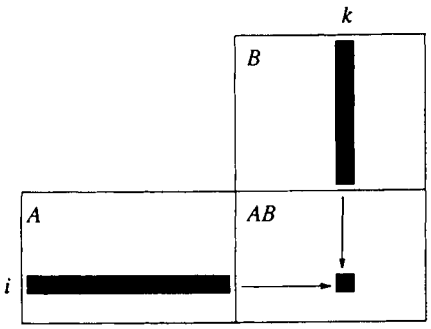
their product is found to be

$$\boldsymbol{C} = \boldsymbol{AB} = \begin{pmatrix} 60 & 190 \\ 10 & 170 \\ 25 & 120 \end{pmatrix}. \tag{A.27}$$

where each element in $\boldsymbol{C}$ is calculated by (A.25); for instance, c_{31} is the scalar product of the third row of $\boldsymbol{A}$ and the first column of $\boldsymbol{B}$:

$$c_{31} = 1\times10 + 0\times10 + 2\times0 + 1\times15 = 10 + 0 + 0 + 15 = 25. \tag{A.28}$$

Calculation "by hand" of $\boldsymbol{C} = \boldsymbol{AB}$ is made easier by the triple-rectangular layout shown below; it suggests how the ik'th element of $\boldsymbol{C}$ is found by scalar multiplication of the row of $\boldsymbol{A}$ on the level with that position in $\boldsymbol{C}$ and the column of $\boldsymbol{B}$ directly above it.



Why do we define a matrix product in the above, rather peculiar way? Why not choose a simpler definition, e.g., by $c_{ij} = a_{ij}b_{ij}$? The question is both natural and logical, and it is true that we may define algebraic operations in which ever way we want. However, if simplicity is a merit, so is fruitfulness, and it turns out that definition (4), strenuous as it may appear, is the one that together with (1)–(3) leads to the best combination of nice algebraic properties and a powerful potential in applications.

What lies behind (4) has to do with the concept of 'composite function'. More precisely: if $\boldsymbol{g}$ and $\boldsymbol{f}$ are linear functions, respectively from $\mathbf{R}^p$ to $\mathbf{R}^n$ with matrix $\boldsymbol{B}$ and from $\mathbf{R}^n$ to $\mathbf{R}^m$ with matrix $\boldsymbol{A}$, then the composite function

$$h(x) = (f \circ g)(x) = f(g(x)) \tag{A.29}$$

exists and is a linear function from $\mathbf{R}^p$ to $\mathbf{R}^m$ with matrix $\boldsymbol{AB}$. We shall not give a formal proof for this fact but merely illustrate it by an example.

Example A.4

(*Continuation of the fish and algae examples*). Suppose that the four algae contain three trace elements T_1, T_2, T_3 in the following quantities:

	1 g of A1	1 g of A2	1 g of A3	1 g of A4
Units of T1	3	0	2	2
Units of T2	0	1	3	0
Units of T3	1	0	2	1

(A.30)

Let z_1 denote the total number of units of T_i (i = 1,2,3) in an amount of algae consisting of y_1 g of A1, y_2 g of A2, y_3 g of A3 and y_4 g of A4. From Table (A.30) follows

$$\begin{aligned} z_1 &= 3y_1 + 2y_3 + 2y_4 \\ z_2 &= y_2 + 3y_3 \\ z_3 &= y_1 + 2y_3 + y_4. \end{aligned} \tag{A.31}$$

showing that $z = f(y)$ is linear and has the matrix A in Eq. (A.26).

What is the total daily uptake of the three trace elements by the fish population? To answer this question we must combine the function $y = g(x)$ from Eq. (A.19) with the function $z = f(y)$ in Eq. (A.31) which leads to

$$z_1 = 3\times(10x_1 + 30x_2) + 2\times40x_2 + 2\times(15x_1 + 10x_2) = 60x_1 + 190x_2$$

$$z_2 = 1\times(10x_1 + 50x_2) + 3\times40x_2 = 10x_1 + 170x_2$$

$$z_3 = 1\times(10x_1 + 30x_2) = 2\times40x_2 + 1\times(15x_1 + 10x_2) = 25x_1 + 120x_2$$

The composite function $z = (f \circ g)(x)$ is linear and has the matrix $C = AB$ in Eq. (A.27) where A is the matrix of f and B is the matrix of g (termed A in Eq. (A.20) but we must rename it here). This illustrates the above-mentioned connection between matrix multiplication and composition of linear functions.

EXERCISE A.4

Let

$$A = \begin{pmatrix} 2 & 1 & 0 \\ -3 & 2 & -1 \end{pmatrix}, \quad B = \begin{pmatrix} 1 & 1 \\ 2 & -1 \\ -1 & 0 \end{pmatrix} \tag{A.32}$$

Calculate those of the following expressions that have a meaning:

(1) $A + B$, (2) $A + B^T$, (3) $A^T - 4B$, (4) AB, (5) BA, (6) A^TB, (7) $A + 5$.

The algebra resulting from the definitions made above is nice in the sense that most of the algebraic rules known from arithmetics and vector algebra hold also in the case of matrices. Thus, matrix addition is commutative and associative: $A + B = B + A$ and $A + (B + C) = (A + B) + C$, and it is distributive with respect o both scalar-matrix multiplication and matrix–matrix multiplication: $k(A + B) = kA + kB$, $A(B + C) = AB + AC$ and $(A + B)C = AC + BC$. But there is one important exception: *matrix multiplication is*

not generally commutative, i.e., in most cases $AB = BA$ *does not hold.* That AB exists does not imply that BA exists; if both exist they may be of different dimension (see Exercise A.4, nos. 4 and 5); and when both products exist and have the same dimension they will usually not bear any resemblance to each other. For example,

$$A = \begin{pmatrix} 1 & 2 \\ 3 & -1 \end{pmatrix}, B = \begin{pmatrix} 3 & 0 \\ 5 & -2 \end{pmatrix} \text{ implies } AB = \begin{pmatrix} 13 & -4 \\ 4 & 2 \end{pmatrix}, BA = \begin{pmatrix} 3 & 6 \\ -1 & 12 \end{pmatrix} \tag{A.33}$$

(verify this!). That matrix multiplication is generally not commutative has to do with the fact that the same is true for composition of functions, and it implies that one must be cautious when working out a matrix algebraic expression and not by force of habit reduce members like, say, $5AB - 3BA$ to $2AB$.

Note that any linear function from $\mathbf{R}^n$ to $\mathbf{R}^m$, see Eq (A.17), can be written in the form of a matrix product:

$$y = Ax \tag{A.34}$$

where A is the matrix of f and x and y are column matrices. Since A is an $m \times n$ matrix and x is an $n \times 1$ matrix, their product exists and is an $m \times 1$ column matrix whose i'th coordinate is the scalar product of the i'th row of A and the vector x, which is identical to the i'th coordinate on the right hand side of Eq. (A.17)

EXERCISE A.5

In an XY-system in the plane, consider the linear transformations (functions) g and f given by

$$\begin{aligned} g\begin{pmatrix} x \\ y \end{pmatrix} &= \begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} -y \\ x \end{pmatrix} = \begin{pmatrix} 0 \cdot x - 1 \cdot y \\ 1 \cdot x + 0 \cdot y \end{pmatrix} \\ f\begin{pmatrix} x' \\ y' \end{pmatrix} &= \begin{pmatrix} x'' \\ y'' \end{pmatrix} = \begin{pmatrix} x' \\ 2y' \end{pmatrix} = \begin{pmatrix} 1 \cdot x' + 0 \cdot y' \\ 0 \cdot x' + 2 \cdot y' \end{pmatrix} \end{aligned} \tag{A.35}$$

(1) Explain that g is a rotation by $+90°$ of the plane around the origin, and that f is a vertical stretching by a factor 2 of the plane away from the horizontal axis.

(2) Write down the matrix A for f and the matrix B for g.

(3) Combine the formulas in (A.35) to express x'' and y'' in terms of x and y, i.e., the composed function $f \circ g$. Verify that it has the matrix AB.

(4) Rewrite the two functions with interchanged coordinate symbols so that combination of the formulas yields the composed function $\boldsymbol{g} \circ \boldsymbol{f}$. Verify that it has the matrix $\boldsymbol{BA}$. Are the two composed functions identical to each other?

(5) Draw the unit circle $x^2 + y^2 = 1$ and equip it with eyes, nose and mouth so as to look like a smiling face lying down with its top to the right. Imagine the figure is subjected first to $\boldsymbol{g}$, then to $\boldsymbol{f}$. What does it turn into? Imagine instead that the figure is subjected first to $\boldsymbol{f}$, then to $\boldsymbol{g}$. What does it look like now? What is the connection to (3) and (4)? [The two resulting faces are different, but they do have some traits in common. For instance, they have the same area. And they are both still smiling].

A.3 Square Matrices. Eigenvalues and Eigenvectors

The matrix algebra of $n \times n$ matrices, so-called *square matrices of order n*, is particularly nice. All four operations can be carried out without restrictions and they result invariably in a matrix of the same type. Moreover, as we shall see, 'matrix division' is widely possible for such matrices.

The elements a_{ii} $(i = 1,...,n)$ in an $n \times n$ matrix form the *diagonal*. A *diagonal matrix* is an $n \times n$ matrix where all elements outside the diagonal are zero. Diagonal matrices have an especially simple algebra: if $\boldsymbol{A}$ and $\boldsymbol{B}$ are $n \times n$ diagonal matrices, so are both $\boldsymbol{A} + \boldsymbol{B}$ and $\boldsymbol{AB}$ since we get from the definitions of matrix sum and product:

$$\boldsymbol{A}+\boldsymbol{B} = \begin{pmatrix} a_{11}+b_{11} & 0 & \dots & 0 \\ 0 & a_{22}+b_{22} & \dots & 0 \\ & \dots & & \\ 0 & 0 & \dots & a_{nn}+b_{nn} \end{pmatrix}, \quad \boldsymbol{AB} = \begin{pmatrix} a_{11}b_{11} & 0 & \dots & 0 \\ 0 & a_{22}b_{22} & \dots & 0 \\ & \dots & & \\ 0 & 0 & \dots & a_{nn}b_{nn} \end{pmatrix} \tag{A.36}$$

implying in particular that $\boldsymbol{AB} = \boldsymbol{BA}$ holds for any two $n \times n$ diagonal matrices.

The $n \times n$ diagonal matrix

$$\boldsymbol{I} = \begin{pmatrix} 1 & 0 & \dots & 0 \\ 0 & 1 & \dots & 0 \\ & \dots & & \\ 0 & 0 & \dots & 1 \end{pmatrix} \tag{A.37}$$

is called the *unit matrix* of order n; it plays the same role in matrix algebra as does 1 in ordinary mathematics in the sense that $\boldsymbol{AI} = \boldsymbol{IA} = \boldsymbol{A}$ for any $n \times n$ matrix $\boldsymbol{A}$.

A *discrete dynamical model* for a system described by n time-dependent state variables, x_{it} $(i = 1,...,n,\ t = 0,1,2,...)$ has the general form $\boldsymbol{x}_{t+1} = \boldsymbol{f}(\boldsymbol{x}_t)$ (cf. (A.16))

where the state variables x_{it} have been arranged in the column vector $\boldsymbol{x}_t = (x_{1t}, ..., x_{nt})^T$. If $\boldsymbol{f}$ is linear and homogeneous in each coordinate, the model becomes

$$\mathbf{x}_{t+1} = \boldsymbol{A}\boldsymbol{x}_t \tag{A.38}$$

where $\boldsymbol{A}$ is the $n \times n$ square coefficient matrix, cf. (A.17). Such a model is called a *matrix projection*. Iteration from $t = 0$ yields $\boldsymbol{x}_1 = \boldsymbol{A}\boldsymbol{x}_0$, $\boldsymbol{x}_2 = \boldsymbol{A}(\boldsymbol{A}\boldsymbol{x}_0) = \boldsymbol{A}^2\boldsymbol{x}_0$, ... ,

$$\boldsymbol{x}_t = \boldsymbol{A}^t \boldsymbol{x}_0 \quad (t = 0,1,2,...) \tag{A.39}$$

Thus, to predict the behaviour of the model in the long term one must have an idea of how the matrix power $\boldsymbol{A}^t$ varies for increasing t, a problem to which we shall return.

Two examples of situations where model (A.38) has been used are:

(1) Rotation of a fixed set of objects between n classes ("compartments"), with fixed probabilities/frequencies of transition between the various classes. See Example A.5 below. The situation is closely related to what statisticians term a *discrete-time stationary Markov process*.

(2) Discrete, age-distributed population dynamics. See Example A.6 below; see also the blue whale model discussed in Example 6.2 in Chapter 6.

Example A.5

A large group of citizens, always the same persons, are asked regularly whether or not they support a certain political issue. It is recorded how many YES and how many NO there are; these numbers are denoted x_{t1} and x_{t2}, respectively at poll number $t = 0,1,2,...$. The persons asked cannot refuse to answer, nor can they answer DON'T KNOW. Furthermore it has been established from previous experience that a person who says YES has probability 70% of giving the same answer next time (and 30% of saying NO), and a NO has probability 20% of saying YES next time (and 80 of saying NO again). From this information we conclude that

$$\begin{aligned} x_{1,t+1} &= 0.7x_{1t} + 0.2x_{2t} \\ x_{2,t+1} &= 0.3x_{1t} + 0.8x_{2t} \end{aligned}, \tag{A.40}$$

or in vector-matrix formulation

$$\boldsymbol{x}_{t+1} = \boldsymbol{A}\boldsymbol{x}_t, \quad \boldsymbol{A} = \begin{pmatrix} 0.7 & 0.2 \\ 0.3 & 0.8 \end{pmatrix}. \tag{A.41}$$

Suppose the polls involve 1000 persons of which 800 said YES and 200 said NO at the first poll. Iteration of (A.40)/(A.41) yields

t	0	1	2	3	4	5	...	
x_{1t}	800	600	500	450	425	413	...	(A.42)
y_{1t}	200	400	500	550	575	587	...	

There seems to be a tendency to stabilize near $\boldsymbol{x} = (400, 600)^{\mathrm{T}}$. This distribution is in fact stationary in the sense that $\boldsymbol{x}_t = (400, 600)^{\mathrm{T}}$ implies $\boldsymbol{x}_{t+1} = \boldsymbol{x}_{t+2} = \ldots = (400, 600)^{\mathrm{T}}$.

Example A.6

Consider a population of mice that do not live beyond the age of 3 years. Every year it is recorded how many females there are in each of the age groups 0–1, 1–2 and 2–3 years; the numbers are denoted x_{1t}, x_{2t}, x_{3t}, respectively, in year t. On average females in age group 1 give birth to 0.5 female offspring surviving to the next census, age group 2 females have 1.1 such daughters, and age group 3 females have 0.8 daughters. Females in age group 1 have a chance of 60% of surviving to next census, and in age group 2 a change of 80%. These assumptions imply that the following expressions must hold for the number of newborn females at next census, respectively for survival to next census:

$$x_{1,t+1} = 0.5x_{1t} + 1.1x_{2t} + 0.8x_{3t} \tag{A.43}$$

$$x_{2,t+1} = 0.6x_{1t}, \quad x_{3,t+1} = 0.8x_{2t} \tag{A.44}$$

Equations (A.43) and (A.44) can be combined in vector-matrix form as

$$\boldsymbol{x}_{t+1} = \boldsymbol{A}\boldsymbol{x}_t, \quad \text{where} \quad \boldsymbol{A} = \begin{pmatrix} 0.5 & 1.1 & 0.8 \\ 0.6 & 0 & 0 \\ 0 & 0.8 & 0 \end{pmatrix}, \quad \boldsymbol{x}_t \begin{pmatrix} x_{1t} \\ x_{2t} \\ x_{3t} \end{pmatrix} \tag{A.45}$$

Suppose that a population of 1000 newborn females is left to itself at time $t = 0$, i.e., we have $\boldsymbol{x}_0 = (1000, 0, 0)^{\mathrm{T}}$. Iteration of (A.45) yields

t	0	1	2	3	4	5	...	
x_{1t}	1000	500	910	1169	1377	1810	...	
x_{2t}	0	600	300	546	701	826	...	(A.46)
x_{3t}	0	0	480	240	437	561	...	

(Figures are rounded to whole numbers). There is a tendency of growth of the population; it is irregular at first but becomes more uniform after a few iterations.

EXERCISE A.6

Modify the population model in Example A.6 by taking into account that the mice may live beyond the age of 3 years: let the third age group consist of all females of age 2 or more, and suppose that such a mouse has 60% probability of surviving one more year, regardless of its actual age; on the average a female in the third group still has 0.8 surviving daughters per year. (The blue whale model presented in Example 6.2 in Chapter 6 has such an age group with 'internal survival').

As above, start with a population of 1000 newborn females; iterate the model equations to predict population figures for some years. Do you find any apparent differences between the figures and those listed in (A.46)?

For the population in Example A.6, convert the Table (A.46) to give the figures of *percentage* of the entire population in each age group each year, not the absolute population figures. Do you observe a tendency in the percentages for increasing t? Repeat the percentage calculation for the model in this exercise.

A *linear equation system* has the form $\boldsymbol{Ax} = \boldsymbol{b}$, where $\boldsymbol{A}$ is a given $m \times n$ matrix, $\boldsymbol{b}$ is a given $\mathbf{R}^m$-vector and $\boldsymbol{x}$ is an unknown $\mathbf{R}^n$-vector. It is intuitively clear that in most cases such a system of "m linear equations with n unknowns" will, largely, have a unique solution only when $m = n$; when $m < n$ there are usually infinitely many solutions, and when $m > n$ there are usually no solutions at all. [The reader is invited to explore this point by writing down at random two equations with three unknown, and then three equations with two unknown, and see what happens when one tries to solve the system].

On the other hand, in the case of n linear equations with n unknowns there is usually (though *not* always; see below) exactly one solution which can be found by successive elimination of the unknowns, e.g., by "the substitution method", as is well known at least in the cases $n = 2$ and $n = 3$.

The concept of inverse matrix is closely connected with that of inverse linear function. Let us look once again at the general linear function $\boldsymbol{y} = \boldsymbol{Ax}$, cf. (A.17), and imagine we want to deduce a reverse correspondence, i.e., to solve the equations with respect to the x_i's. It follows from the above remarks on linear equation systems that this problem makes sense only for $m = n$; on the other hand, when $m = n$ it is usually possible to solve $\boldsymbol{y} = \boldsymbol{Ax}$ into a reverse correspondence which is again linear, $\boldsymbol{x} = \boldsymbol{By}$; the $n \times n$ matrix $\boldsymbol{B}$ is termed the *inverse* of $\boldsymbol{A}$ and denoted $\boldsymbol{A}^{-1}$; it satisfies $\boldsymbol{AA}^{-1} = \boldsymbol{A}^{-1}\boldsymbol{A} = \boldsymbol{I}$, the $n \times n$ unit matrix which is the matrix for the *identical function* $\boldsymbol{i}$ in $\mathbf{R}^n$ defined by $\boldsymbol{i}(\boldsymbol{x}) = \boldsymbol{x}$.

EXERCISE A.7

Solve the equations

$$\begin{aligned} y_1 &= x_1 - x_2 + x_3 \\ y_2 &= x_1 + x_2 + 4x_3 \\ y_3 &= -3x_1 + 3x_2 + 2x_3 \end{aligned} \tag{A.47}$$

with respect to x_1, x_2 and x_3. [Hint: start by simultaneously eliminating x_1 and x_2 from the first and the third equation]. Write down the 3×3 matrix $\boldsymbol{A}$ that you have thereby inverted; write down also $\boldsymbol{A}^{-1}$. Verify directly by matrix multiplication that $\boldsymbol{A}\boldsymbol{A}^{-1} = \boldsymbol{I}$; if you have the energy, verify also that $\boldsymbol{A}^{-1}\boldsymbol{A} = \boldsymbol{I}$.

Solve whenever possible the following equations with respect to x_1 and x_2:

$$\begin{array}{lll} (1)\ 3x_1 + x_2 = y_1 & (2)\ 3x_1 + x_2 = y_1 & (3)\ ax_1 + bx_2 = y_1 \\ \quad -x_1 + 4x_2 = y_2 & \quad 12x_1 + 4x_2 = y_2 & \quad bx_1 + dx_2 = y_2. \end{array} \tag{A.48}$$

In each case, write down the corresponding 2×2 matrix inversion result.

As suggested above, and as illustrated by one of the questions in Exercise A.7, it happens sometimes that a given $n\times n$ matrix $\boldsymbol{A}$ does *not* have an inverse. How can we determine whether or not this is the case?

There exists an indicator, a number attached to $\boldsymbol{A}$ and denoted $\det\boldsymbol{A}$, the *determinant* of $\boldsymbol{A}$, which gives us the answer in a rather simple way:

$$\text{when } \det\boldsymbol{A} \neq 0,\ \boldsymbol{A}^{-1} \text{ exists,}$$

$$\text{when } \det\boldsymbol{A} = 0,\ \boldsymbol{A}^{-1} \text{ does not exist.}$$

A thorough introduction to the determinant is beyond the scope of this appendix; however we shall present a few pieces of information:

(1) For the 2×2 and the 3×3 cases we have (note the alternative $|\,|$-notation):

$$\det\boldsymbol{A} = \begin{vmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{vmatrix} = a_{11}a_{22} - a_{12}a_{21}, \tag{A.49}$$

$$\det\boldsymbol{A} = \begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{vmatrix} = \begin{aligned} &a_{11}a_{22}a_{33} + a_{12}a_{23} + a_{31} + a_{13}a_{21}a_{32} \\ &\quad - a_{13}a_{22}a_{31} - a_{11}a_{23}a_{32} - a_{12}a_{21}a_{33} \end{aligned} \tag{A.50}$$

A similar, but more complicated formula can be set up for the general $n\times n$ case.

(2) For a 2×2 matrix $\boldsymbol{A}$, $\det\boldsymbol{A}$ is equal to the area of the parallelogram spanned in $\mathbf{R}^2$ by the column vectors of $\boldsymbol{A}$; the sign is '+' when the shortest rotation from the first to the second column vector is counterclockwise, '–' when it is clockwise. For a 3×3 matrix $\boldsymbol{A}$, $\det\boldsymbol{A}$ is equal to the volume (supplied with a sign) of the

parallelepiped spanned in $\mathbf{R}^3$ by the column vectors of $\boldsymbol{A}$. A similar "signed n-dimensional volume" interpretation can be established even in the $n \times n$ case.

(3) In general $\det \boldsymbol{A}^{\mathrm{T}} = \det \boldsymbol{A}$. As a consequence, the word 'columns' in [2] may be replaced by 'rows'. This rule is of an algebraic nature and cannot be perceived geometrically.

(4) When $\boldsymbol{A}$ is a *diagonal* matrix, its determinant is equal to the product of the diagonal elements: $\det \boldsymbol{A} = a_{11}a_{22}...a_{nn}$; the same holds even for a *triangular* matrix, i.e., a square matrix where all elements below the diagonal (or all elements above the diagonal) are zero. Note that the rule is in accordance with (A.49) and (A.50).

(5) If a row in $\boldsymbol{A}$ is multiplied by a scalar and added to another row, $\det \boldsymbol{A}$ is unchanged. If two rows are interchanged, $\det \boldsymbol{A}$ changes sign. Similar rules apply to columns.

Let us mention without going into detail that [4]–[5] enable us to compute the value of any given square matrix. By [5] we can produce zeroes at every position below the diagonal whereupon [4] can be applied.

A square matrix is said to be *regular* when its determinant is non-zero, *singular* when it is zero. From the above it follows that when $\boldsymbol{A}$ is regular, then the system $\boldsymbol{Ax} = \boldsymbol{b}$ has the unique solution $\boldsymbol{x} = \boldsymbol{A}^{-1}\boldsymbol{b}$. In particular, when $\boldsymbol{A}$ is regular, then the so-called *homogeneous* system $\boldsymbol{Ax} = \boldsymbol{o}$ only has the trivial solution $\boldsymbol{x} = \boldsymbol{A}^{-1}\boldsymbol{o} = \boldsymbol{o}$. this again impplies that when $\boldsymbol{A}$ is square and the system $\boldsymbol{Ax} = \boldsymbol{o}$ is known to have a non-zero solution, then $\boldsymbol{A}$ must be singular, i.e., $\det \boldsymbol{A} = 0$. It can be proved that if on the other hand $\det \boldsymbol{A} = 0$, then $\boldsymbol{Ax} = \boldsymbol{o}$ does have non-zero solutions.

A linear function $\boldsymbol{f}(\boldsymbol{x}) = \boldsymbol{Ax}$ from $\mathbf{R}^n$ to $\mathbf{R}^n$ "changes the direction" of most vectors, meaning that $\boldsymbol{Ax}$ is usually not proportional to $\boldsymbol{x}$. However it is of interest, not the least in many applications, to find the possible exceptions to this rule. If a non-zero vector $\boldsymbol{v}$ and a scalar (a number) λ satisfy the equation

$$\boldsymbol{f}(\boldsymbol{v}) = \lambda \boldsymbol{v}. \tag{A.51}$$

then λ is said to be an *eigenvalue* (a latent root) for $\boldsymbol{A}$ and $\boldsymbol{v}$ and *eigenvector* belonging to the eigenvalue λ. For example, if

$$\boldsymbol{A} = \begin{pmatrix} 4 & -2 \\ -1 & 5 \end{pmatrix}, \quad \boldsymbol{v} = \begin{pmatrix} 2 \\ 1 \end{pmatrix} \tag{A.52}$$

then 3 is an eigenvalue and $\boldsymbol{v}$ an eigenvector for $\boldsymbol{A}$ because $\boldsymbol{Av} = 3\boldsymbol{v}$ (verify this!).

In the 2×2 case the equation $\boldsymbol{Av} = \lambda \boldsymbol{v}$ written out in coordinates becomes

$$\begin{aligned} a_{11}v_1 + a_{12}v_2 &= \lambda v_1 \\ a_{21}v_1 + a_{22}v_2 &= \lambda v_2 \end{aligned} \quad \text{or} \quad \begin{aligned} (a_{11} - \lambda)v_1 + a_{12}v_2 &= 0 \\ a_{21}v_1 + (a_{22} - \lambda)v_2 &= 0 \end{aligned}. \tag{A.53}$$

The system to the right is quadratic and homogeneous, and therefore it has non-zero solutions in v_1 and v_2 if and only if its determinant is zero:

$$\begin{vmatrix} a_{11}-\lambda & a_{12} \\ a_{21} & a_{22}-\lambda \end{vmatrix} = 0. \tag{A.54}$$

To be an eigenvalue λ must satisfy this quadratic equation; depending on the elements of A it may have two roots, one (double) root, or no roots; for each root λ the corresponding eigenvectors are found by inserting λ in (A.53) and solving with respect to v_1 and v_2.

The general $n \times n$ case is dealt with in a quite similar manner. The system $\boldsymbol{Av} = \lambda \boldsymbol{v}$ is rewritten as the homogeneous system $(\boldsymbol{A} - \lambda \boldsymbol{I})\boldsymbol{v} = \boldsymbol{o}$ whose determinant, if the system should have non-zero solutions in $\boldsymbol{v}$, must be equal to zero:

$$\det(\boldsymbol{A} - \lambda \boldsymbol{I}) = 0. \tag{A.55}$$

This so-called *characteristic equation* for A is polynomial in λ of degree n and has at most n roots; for each root the corresponding eigenvectors are found by inserting in $\boldsymbol{Av} = \lambda \boldsymbol{v}$ and solving with respect to $\boldsymbol{v}$. In most (but not all) cases the solution is a "one-dimensional infinity" of eigenvectors because $\boldsymbol{v}$ is determined up to a scalar factor only.

Example A.7

The eigenvalues of the matrix A in (A.52) and their corresponding eigenvectors are found int he following way:

$$\begin{vmatrix} 4-\lambda & -2 \\ -1 & 5-\lambda \end{vmatrix} = 0 \Leftrightarrow \lambda^2 - 9\lambda + 18 = 0 \Leftrightarrow \lambda = \begin{cases} 3 \\ 6 \end{cases}$$

$$\underline{\lambda = 3}: \quad \begin{matrix} (4-3)v_1 - 2v_2 = 0 \\ -v_1 + (5-3)v_2 = 0 \end{matrix} \Leftrightarrow \begin{matrix} v_1 - 2v_2 = 0 \\ (-v_1 + 2v_2 = 0) \end{matrix} \Leftrightarrow \boldsymbol{v} = t\begin{pmatrix} 2 \\ 1 \end{pmatrix} (t \in \mathbf{R})$$

$$\underline{\lambda = 6}: \quad \begin{matrix} (4-6)v_1 - 2v_2 = 0 \\ -v_1 + (5-6)v_2 = 0 \end{matrix} \Leftrightarrow \begin{matrix} (-2v_1 - 2v_2 = 0) \\ -v_1 - v_2 = 0) \end{matrix} \Leftrightarrow \boldsymbol{v} = t\begin{pmatrix} 1 \\ -1 \end{pmatrix} (t \in \mathbf{R})$$

Note that among the eigenvalues and eigenvectors found are those mentioned above in connection with (A.52).

To find the eigenvalues of the matrix

$$A=\begin{pmatrix} 0 & -2 & 4 \\ -1 & 1 & 2 \\ -1 & 2 & 1 \end{pmatrix} \tag{A.56}$$

start by working out the characteristic equation. After some calculations one arrives at the polynomial equation

$$-\lambda^3 + 2\lambda^2 + \lambda - 2 = 0, \tag{A.57}$$

which can be solved, e.g., by guessing integer roots (they must divide the constant member which is 2), to have the three solutions $\lambda = 1$, $\lambda = -1$, $\lambda = 2$ which are the three eigenvalues of A. To determine the eigenvectors for, say, $\lambda = 1$ we subtract 1 in the diagonal of A and write down the homogeneous system with these coefficients:

$$\begin{aligned} -v_1 - 2v_2 + 4v_3 &= 0 \\ -v_1 \qquad + 2v_3 &= 0 \\ -v_1 + 2v_2 \qquad &= 0 \end{aligned} \tag{A.58}$$

One of the equations can be cancelled, e.g., the first one because it results from multiplying the second equation by 2 and subtracting the third equation. By choosing $v_3 = t$ we get from the second equation $v_1 = 2t$ which again, when inserted in the third equation, leads to $x_2 = t$. We have thus found the eigenvectors for $\lambda = 1$ to be

$$\boldsymbol{v} = t(2, 1, 1) \quad (t \in \mathbf{R}). \tag{A.59}$$

EXERCISE A.8

Find the eigenvalues, and for each eigenvalue the corresponding eigenvectors, for the matrices

$$(1)\ A=\begin{pmatrix} 5 & 4 \\ 4 & 11 \end{pmatrix}, \quad (2)\ A=\begin{pmatrix} 1 & 3 \\ 0 & 1 \end{pmatrix}, \quad (3)\ A=\begin{pmatrix} 2 & 5 \\ -8 & 9 \end{pmatrix} \tag{A.60}$$

For the 3×3 matrix A in Example A.7, find the eigenvectors corresponding to each of the eigenvalues $\lambda = 1$ and $\lambda = 2$.

The *spectral properties* of a square matrix A, i.e., its eigenvalues and eigenvectors, are of particular interest when A is the projection matrix in a model to be investigated. Suppose that the model is given by (A.38), and that λ is an eigenvalue and $\boldsymbol{v}$ a corresponding eigenvector: if $\boldsymbol{x}_t = \boldsymbol{v}$, then $\boldsymbol{x}_{t+1} = A\boldsymbol{v} = \lambda\boldsymbol{v}$, $\boldsymbol{x}_{t+2} = A(\lambda\boldsymbol{v}) = \lambda^2\boldsymbol{v}$, etc., and in general

$$\boldsymbol{x}_{T+t} = \lambda^t \boldsymbol{v} \quad (t = 0,1,2,...), \tag{A.61}$$

so that the model predicts uniform 'growth' by the factor λ per time unit in each variable.

The claim that some $\boldsymbol{x}_T$ should be equal to $\boldsymbol{v}$ is restrictive. However an *approximative* growth rule similar to (A.61) holds under much weaker conditions. Let us consider a special but relevant case, viz. that on *non-negative matrices* $\boldsymbol{A}$, i.e., $a_{ij} \geq 0$ for all i,j; this property holds in many applications, the elements a_{ij} representing quantities, rates etc. We further assume that the zero elements in $\boldsymbol{A}$ are not too numerous or too unfortunately placed, or to put it precisely: the powers $\boldsymbol{A}^t$ (t = 1,2,3,...) eventually become positive in *all* positions. (For example, $\boldsymbol{A}$ is not triangular.) For such "well-behaved, non-negative" matrices the following result holds: $\boldsymbol{A}$ has a positive, so-called dominating eigenvalue λ, numerically larger than all other eigenvalues, and a corresponding eigenvector $\boldsymbol{v}$ with positive coordinates; furthermore the iterated model equation (A.39) implies that for any non-negative (and non-zero) initial vector $\boldsymbol{x}_0$ and for some constant k,

$$\boldsymbol{x}_t \approx k\lambda^t \boldsymbol{v} \quad (t >> 1) \tag{A.62}$$

The precise meaning of this equation is that $\lambda^{-t}\boldsymbol{x}_t$ tends to a limit vector proportional to $\boldsymbol{v}$ for $t \to \infty$. But to get the picture of (A.62) it is enough to think of it as stating that regardless of the initial values of the state variables they tend to stabilize with *relative* sizes given by the coordinates of $\boldsymbol{v}$, and to grow uniformly by the factor λ per time unit.

The models in Example A.5 and Example A.6 illustrate the implications of (A.62). See also the following exercise and the discussion in Chapter 6 of the blue whale model.

EXERCISE A.9

Opinion polls. Find the eigenvalues and the corresponding eigenvectors of the matrix $\boldsymbol{A}$ in Equation (A.41). Which eigenvalue is the dominating one? Interpret Table (A.42) in the light of (A.62); verify that the vector $(400, 600)^T$ found by guessing in Example A.5 is in fact the limit of $\boldsymbol{x}_t$ for $t \to \infty$.

Mouse population. When the characteristic equation of $\boldsymbol{A}$ in Eq. (A.45) is worked out it becomes

$$-\lambda^3 + 0.5\lambda^2 + 0.66\lambda + 0.384 = 0, \tag{A.63}$$

having one positive root, the dominating one, which can be found to be approximately $\lambda = 1.263$. Verify this. (Incidentally there are no other real roots.) Find a corresponding 'percentage eigenvector', i.e., the eigenvector which is uniquely determined by the extra claim $v_1 + v_2 + v_3 = 100$.

Equation (A.62) implies that regardless of the initial population the mouse population tends to a 'stable age distribution' given by v and to eventually grow by 26.3% per time unit in each of the three age classes. Is this in accordance with figures in Table (A.46)?

Repeat the calculations for the modified mouse population model int he last part of Exercise A.6, and compare the results for the two models.

A.4 Differential Equations

Example A.8

A culture of bacteria grows in a chemostat under constant conditions. Let $N(t)$ denote the number of bacteria at time t hours after the experiment started. The chance that a bacteria divides into two during a small time interval Δt must be proportional to Δt; suppose it has been found that the proportionality factor is 0.13, thus from time t to $t+\Delta t$ the $N(t)$ bacteria give rise to $0.13 \times N(t)\,\Delta t$ new bacteria and

$$N(t+\Delta t) = N(t) + 0.13N(t)\Delta t. \tag{A.64}$$

If the member $N(t)$ is moved to the left hand side this becomes $N(t+\Delta t) - N(t)$, also denoted $\Delta N(t)$ or just ΔN; after division with Δt we get

$$\frac{\Delta N(t)}{\Delta t} = 0.13N(t). \tag{A.65}$$

or by taking the limit for $\Delta t \to 0$:

$$\frac{\mathrm{d}N(t)}{\mathrm{d}t} = N'(t) = 0.13N(t). \tag{A.66}$$

This is a simple and frequent example of the type of problem we shall deal with in this section, the *differential equations*. As we shall see shortly, the 'solutions' of (A.66) are *exponential growth* functions of the type

$$N(t) = N_0\, \mathrm{e}^{0.13t}. \tag{A.67}$$

where $N_0 = N(0)$ can have any value, though of course only positive (and integer) values are biologically meaningful.

A fundamental equation in dynamic modelling is

$$x(t+\Delta t) = x(t) + r(*)\Delta t. \tag{A.68}$$

It projects the value of a state variable x a small time step Δt ahead by giving it an increment which is assumed to be proportional to Δt, the coefficient of proportionality, r, being the *rate of charge* (or: rate of increase) or x. If we rewrite (A.68) as

$$\frac{x(t+\Delta t)-x(t)}{\Delta t} = r(*). \tag{A.69}$$

it becomes clear that since Δt is small, r is largely identical to the differential quotient of the state variable x. To define the 'rate of change' as $r = dx/dt = x'(t)$ would in fact be mathematically more correct, while (A.68)/(A.69) are slightly imprecise, approximate equations. But we shall not linger on this.

The symbol $r(*)$ suggests that r may depend on various quantities. In the simplest case where r is a constant it follows immediately that x is a linear function of time:

$$\frac{dx}{dt} = r = \text{constant} \quad \Rightarrow x(t) = x(0) + rt \tag{A.70}$$

A more general situation is that instead of being constant r is a function of t only. This case, too, is solved by a simple integration:

$$\frac{dx}{dt} = r(t) \Rightarrow x(t) = x(0) + \int_0^t r(\tau)d\tau, \tag{A.71}$$

or $x(t) = R(t) + c$ where R is a primitive function of r (and the integration constant c is left to be determined).

However we must usually expect that r depends on time not only directly, through external 'forcing functions', but also indirectly, through feedback from x and interference with other state variables $y(t), z(t), \ldots$. The mechanism is then rather of the form

$$\frac{dx}{dt} = r(t, x, y, z, \ldots), \tag{A.72}$$

and must be seen in the context of similar equations for y, z, etc.

As long as we take a practical, computational point of view only and use (A.68) together with similar equations for y, z, etc. to project the model numerically, there is no serious problem in passing from (A.70) or (A.71) to (A.72). But we may also think of the model in a more theoretical manner, asking: given the various rate functions of type (A.72), which functions $x(t), y(t), z(t), \ldots$ will satisfy the model equations? Then things become rather more complicated.

It is possible to carry out numerical 'solutions' of a model based on equations of type (A.68)/(A.72) knowing next to nothing abut the underlying mathematical theory. However some theoretical basis is a valuable support for understanding what

goes on during computer simulations and for interpreting what comes out of them. To supply the reader with such a basis is the goal in the rest of the appendix. It will be necessary to start modestly and take some time with the case where there is only one state variable (or where the change in x is not affected by other state variables), i.e., (A.72) becomes

$$\frac{dx}{dt} = r(t,x). \tag{A.73}$$

This is the general form of an *ordinary differential equation* (ODE) of first order; if d^2x/dt^2 had occurred too the equation would have been of second order, etc. A *solution* is a function $x = x(t)$ that satisfies the equation, which means that $x'(t)$ is identically the same function of t as is $r(t,x(t))$. The *complete solution* is the set of all solutions. As suggested by the special case where r depends on t only, cf. (A.71):

$$\frac{dx}{dt} = r(t) \quad \Leftrightarrow \quad x(t) = R(t) + c \quad (c \in \mathbf{R}), \tag{A.74}$$

it is in general true that when the complete solution can be deduced at all, it is typically of the form $x = x(t,c)$ where each value of the constant c yields a specific solution.

An *initial condition* is a claim that the solution should pass through a specific point in the tx-plane, i.e., for $t = t_0$ we should have $x = x(t_0) = x_0$. It can be proved that for a reasonably well-behaved rate function r and initial condition determines a unique solution of (A.73): "there is one and only one solution that satisfies $x(t_0) = x_0$". The proof is complicated and we shall not go beyond the following intuitive, quasi-geometric argument:

If a function $x = x(t)$ initiates at (t_0,x_0) and satisfies (A.73), it must start with slope $r_0 = r(t_0,x_0)$. After a short time, Δt, it reaches a value of approximately $x_0 + r_0\Delta t = x_1$ and the slope therefore changes slightly, into $r_1 = r(t_0 + \Delta t, x_1)$; after another time increment of Δt the function becomes $x_1 + r_1\Delta t = x_2$, etc. It seems reasonable to imagine that when Δt tends to zero this process, though involving broken lines with an increasing number of 'edges', gets closer and closer to a smooth curve that satisfies (A.73) at every point.

To solve (A.73) mathematically is not generally possible; even when the expression for r is fairly simple it may happen that we are incapable of finding the explicit solution. Why is it so? One could argue that already the problem of integration understood as writing down explicitly the primitives of a given function, see (A.74), is often impossible. Another argument is that compared to other 'equations in one unknown' (A.73) is substantially more intricate; in equations like $3x + 7 = 19$ or $x^2 - 3x + 2 = 0$ or $\cos x = 0.629$ the unknown is a number; in a pair of equations like $2x_1 + 3x_2 = 7$ and $-4x_1 + 9x_2 = 1$ the unknown is a pair of numbers (or: a vector, cf. Section A.2-3), but in (A.73) the unknown is a function, and there are extremely many more functions than numbers or vectors.

After these introductory remarks we shall proceed to the more tangible task of dealing with a few special types of ODE's which we can solve and which are met in applications like ecological modelling.

Some ODEs are of the form

$$\frac{dx}{dt} = f(x)g(t). \tag{A.75}$$

We say that *the variables in* (A.75) *can be separated.* Rewrite the equation as

$$\frac{1}{f(x)}\frac{dx}{dt} = g(t). \tag{A.76}$$

and assume that $H(x)$ is a primitive function of $1/f(x)$. According to the chain rule the left hand side of (A.76) is equal to the derivative with respect to t of the composite function $H(x(t))$, so if G is a primitive function of g we get from (A.76)

$$H(x) = G(t) + c \quad (c \in \mathbf{R}). \tag{A.77}$$

The same result cam be written in the suggestive formulation

$$\int \frac{1}{f(x)}dx = \int g(t)dt, \tag{A.78}$$

where a constant of integration is understood on the right hand side. Finally, one may hope to solve (A.77) with respect to x, to get the solutions in explicit form.

Example A.9

The solution of a differential equation of the simple type $dx/dt = \alpha x$, cf. Example A.8, is carried out by (A.75)/(A.78) in the following way:

$$\begin{aligned} \frac{dx}{dt} = \alpha x \quad &\Leftrightarrow \quad \int \frac{1}{x}dx = \int \alpha dt \quad \Leftrightarrow \quad \ln|x| = \alpha t + c_1 \\ &\Leftrightarrow \quad x = \pm e^{\alpha t + c_1} \qquad \text{or} \quad x = c\,e^{\alpha t}\ (c \in \mathbf{R}). \end{aligned} \tag{A.79}$$

Note the difference in behaviour for $t \to \infty$ of the solutions according to the *sign* of α: When $\alpha > 0$ (e.g., unlimited growth of a population, or of a capital investment $|x(t)|$ tends to ∞ for increasing t; when $\alpha < 0$ (e.g., decay of an amount of radioactive material, or of a polluter in an environment, or of a population under stress) $x(t)$ tends to 0.

Example A.10

A variation of (A.79) is

$$\frac{dx}{dt} = \alpha x + \beta, \tag{A.80}$$

where a constant member β has been added to the right hand side. To solve (A.80) we define a new constant x^* by $x^* = -\beta/\alpha$, so that $\alpha t + \beta = \alpha(x^* - x^*)$, and proceed

$$\begin{aligned} \frac{dx}{dt} = \frac{d}{dt}(x - x^*) = \alpha(x - x^*) \quad &\Leftrightarrow \quad x - x^* = ce^{\alpha t} \\ &\Leftrightarrow \quad x = x^* + ce^{\alpha t} \\ &\Leftrightarrow \quad x - \frac{\beta}{\alpha} + ce^{\alpha t} \ (c \in \mathbf{R}). \end{aligned} \tag{A.81}$$

The behaviour for $t \to \infty$ depends on α in a similar way as in Example A.9. Equation (3.13) (waste decay) is an instance of (A.80).

EXERCISE A.10

Consider the bacteria population in Example A.8, with a relative growth rate of 0.13 per hour. Suppose we remove bacteria continuously, at a constant rate of 520 bacteria per hour. Set up a differential equation for the population size $N(t)$, and solve it under the initial condition $N(0) = N_0$. Depending on N_0, what happens for $t \to \infty$?

Consider the concentration $c = c(t)$ of a certain chemical compounds S in a lake with volume $V = 30\,000$ m^3. A watercourse passing through the lake has a water flux of 1500 m^3 per hour. The water flowing into the lake has a concentration of 2.5 g/l of the compound S, while the outflow of course has the concentration $c(t)$. Set up a differential equation for $c(t)$, and solve it under the initial condition $c(0) = c_0$. Depending on c_0, what happens for $t \to \infty$?

Example A.11

Another variation of (A.79) is

$$\frac{dx}{dt} = \alpha(t)x, \tag{A.82}$$

where the quantity α depends on t. It is solved in the same way as (A.79), but instead of just $\int \alpha dt = \alpha t + c_1$ we now get $\int \alpha(t)dt = A(t) + c_1$, where $A(t)$ is a primitive function of $\alpha(t)$, and end up with the solution

$$x = ce^{A(t)} \quad (c \in \mathbf{R}). \tag{A.83}$$

Numerous exponential growth/decay equations of the form (A.82) are approximations of (A.83), the constant α being in fact time dependent.

Example A.12

According to *von Bertalanffy*, cf. Section 3C.6, the growth of an individual fish is approximately governed by a differential equation of the form

$$\frac{dw}{dt} = Hw^{2/3} - kw, \tag{A.84}$$

where $w(t)$ is the weight of the fish and H and k are constants. The equation can be solved by the substitution $w = x^3$, by which (A.84) becomes a differential equation in x, and application of results in Example A.10:

$$\begin{aligned} & 3x^2 \frac{dx}{dt} = Hx^2 - kx^3 \\ \Leftrightarrow\ & \frac{dx}{dt} = \frac{H}{3} - \frac{k}{3}x = -\frac{k}{3}\left(x - \frac{H}{k}\right) \\ \Leftrightarrow\ & x = \frac{H}{k} + ce^{-(k/3)t} \\ \Leftrightarrow\ & w = \left(\frac{H}{k} + ce^{-(k/3)t}\right)^3 \quad (c \in \mathbf{R}) \end{aligned} \tag{A.85}$$

The constant c is negative because $w(t)$ increases. If we define w_∞ = final weight = $(H/k)^3$ and denote by t_0 the time when the fish originates ($w(t_0) = 0$), (A.85) becomes

$$w(t) = w_\infty \left(1 - \exp\left(-\frac{k}{3}(t - t_0)\right)\right)^3. \tag{A.86}$$

as mentioned in Section 3C.6. (The length growth measure, l, is connected with x).

The *linear first order differential equation* generalizes the equations in Example A.10–A.11:

$$\frac{dx}{dt} = \alpha(t)x + \beta(t). \tag{A.87}$$

In Example A.11 the solution in the so-called *homogeneous* case, i.e., for $\beta(t) \equiv 0$, was found to be $x = c\, e^{A(t)}$ where $dA(t)/dt = \alpha(t)$. In the hope that the solution of the general *inhomogeneous* equation (A.87) bears some resemblance to the homogeneous solution we write, tentatively, $x = y\, e^{A(t)}$ where the arbitrary constant has been replaced by a variable $y = y(t)$, and insert this in (A.87), remembering that $y\, e^{A(t)}$ must now be differentiated as a *product*. The trick turns out to work: the problem in x is transformed into simpler problem in y and we get the complete inhomogeneous solution:

$$\begin{aligned} \frac{d}{dt}\left\langle y e^{-A(t)} \right\rangle &= \frac{dy}{dt} e^{-A(t)} + y e^{-A(t)} \alpha(t) = \alpha(t) y e^{-A(t)} + \beta(t) \\ &\Leftrightarrow \frac{dy}{dt} = \beta(t) e^{A(t)} \\ &\Leftrightarrow y = \int \beta(t) e^{-A(t)} dt \\ &\Leftrightarrow x = e^{A(t)} \int \beta(t) e^{-A(t)} dt \,, \end{aligned} \tag{A.88a}$$

where an integration constant is understood in the integral on the right hand side. If $B(t)$ denotes a primitive function of $\beta(t) e^{-A(t)}$ the solution becomes $x = e^{A(t)}(B(t) + c)$ where c is an arbitrary constant. We can now write the solution in another way:

$$\frac{dx}{dt} = \alpha(t) x + \beta(t) \quad \Leftrightarrow \quad x(t) = x_0(t) + c e^{A(t)}, \tag{A.88b}$$

where $x_0(t) = e^{A(t)} B(t)$. Equation (A.88) can be expressed verbally in the following way: *the complete inhomogeneous solution is found by adding the complete homogeneous solution to a particular inhomogeneous solution.*

Example A.13

As an example of the use of (A.86–88) we have shown the details of the solution of the Streeter-Phelps' BOD/DO model in Section 3C.1. The equation is

$$\frac{dD}{dt} = -K_a D + K_1 L_0 e^{-K_1 t}. \tag{A.89}$$

From this expression one finally arrives at the particular solution (3.44) by using the initial condition $D(0) = D_0$.

EXERCISE A.11

Solve the differential equation

$$\frac{dx}{dt} = -\frac{1}{t}x + t^2 \quad (t > 0). \tag{A.90}$$

Find the particular solution determined by $x(1) = \frac{1}{2}$.

EXERCISE A.12

Include nitrification in Streeter-Phelps' BOD/DO model in Example A.13, see Section 3C.1. Verify the solution given in Section 3C.1.

Solve the Mass Balance Equation (3.14) for a completely mixed system with a periodic forcing function. [Hint: the use of an integral table may facilitate the integration].

Example A.14

The logistic equation. The differential equation of exponential growth/decay (A.79) expresses that the relative growth rate of x, i.e., the quantity

$$\frac{1}{x}\frac{dx}{dt} \tag{A.91}$$

is constant. Quite often, when x is some biological quantity (e.g., the size of an organ, of an organism, or of a population) this model is approximately true, the constant being the (positive) growth rate r of the quantity; the model then predicts exponential growth of x by $x(t) = c\,e^{rt}$, cf. (A.79). But this is only true as long as x is relatively small; when x becomes larger x will almost always tend to 'limit its own growth'. This can be modeled by modifying (A.79) so that the relative growth rate instead of being just a constant is assumed to *decrease with* x. The simplest way it can do this is by decreasing linearly, and this is achieved if we write

$$\frac{1}{x}\frac{dx}{dt} = r \cdot \left(1 - \frac{x}{K}\right), \tag{A.92}$$

where K is a positive constant, the value of x for which dx/dt becomes zero. We can solve (A.92), the *logistic differential equation*, by the technique sketched above in Eqs. (A.75–79). After division by the term in parentheses on the right hand side we get

$$\frac{1}{x(1-x/K)}\frac{dx}{dt}=r, \tag{A.93}$$

or by (A.78):

$$\int \frac{1}{x(1-x/K)}\,dx=\int r\,dt. \tag{A.94}$$

An ingenious rewriting of the integrand on the left hand side takes us on:

$$\int\left(\frac{1}{x}+\frac{1}{K-x}\right)dx=\int r\,dt$$

$$\begin{aligned}
&\Leftrightarrow \ln|x|-\ln|K-x|=rt+c_1\\
&\Leftrightarrow \quad \ln\left|\frac{x}{K-x}\right|=rt+c_1\\
&\Leftrightarrow \quad \frac{K-x}{x}=\frac{K}{x}-1=\pm e^{-rt-c_1}=\pm e^{-c_1}e^{-rt}=ce^{-rt}\\
&\Leftrightarrow \quad x=\frac{K}{1+ce^{-rt}} \quad (c\in\mathbf{R})
\end{aligned} \tag{A.95}$$

The function given by (A.95) is termed a *logistic function*. Usually we can assume $c > 0$ in which case the function shows an S-shaped graph, increasing from small positive values to values near K. The logistic equation plays a part in the text proper in Section 3C.6.

EXERCISE A.13

Draw the graph of the logistic function (A.95)

(1) for $K = 1, r = 1, c = 1$

(2) for $K = 10, r = 0.4, c = 2$.

What is the significance of each of the parameters K, r, c for the variation of the function and the look of its graph?

A population grows logistically in an environment which can sustain 1000 individuals, i.e., its *carrying capacity* is $K = 1000$. It has been observed that at time $t = 0$ the population size is 100, and at time $t = 5$ it is 500. Find the expression for the population size $N(t)$. At what time has the population reached a size of 95% of its carrying capacity?

A differential equation $dx/dt = r(t,x)$ is *autonomous* if the right hand side does not depend on time, i.e., the equation is of the form $dx/dt = r(x)$. Since the variables can be separated the solution is in principle directly as hand:

$$\frac{dx}{dt} = r(x) \quad \Leftrightarrow \quad \int \frac{dx}{r(x)} = \int dt \quad \Leftrightarrow \quad F(x) = t + c \quad \Leftrightarrow \quad x = \Phi(t+c) \quad (c \in \mathbf{R}), \tag{A.96}$$

where $F(x)$ is a primitive function of $1/r(x)$ and Φ is the inverse function of F. (It can easily happen that these two functions cannot be found explicitly).

The autonomous one-variable case is in itself of little interest, mathematically because the solution is readily found by (A.96), modelwise because such an equation can be expected to give no more than a crude approximation to reality, leaving out the effects of all non-constant forcing functions caused by diurnal and seasonal rhythms, external environmental changes, management, etc. As a preparation for matters in the next section we shall, however, close this one by commenting briefly on a phenomenon connected with the autonomous case: that 'of equilibrium'.

An *equilibrium* (or *steady state*) for a system modelled by the equation $dx/dt = r(x)$ is a zero x^* for the function r, i.e., $r(x^*) = 0$. The constant function $x(t) = x^*$ satisfies the differential equation so that the system, once it has reached state x^*, will according to the model stay there indefinitely. However, in the real world small perturbations will inevitably occur and will slightly change the value of x, and the question thus arises whether the system, following such a perturbation, will seek back towards x^* or rather tend to move further away from it. In the first case we speak of a (locally) *stable* equilibrium, in the second case of an *unstable* equilibrium. [We do not go into the subtler shades of the terminology]. In a more precise formulation: the equilibrium x^* is locally stable if there is an interval $\mathbf{I}$ around x^* such that for any $x_0 \in \mathbf{I}$ the solution of $dx/dt = r(x)$ determined by the initial condition $x(0) = x_0$ will satisfy

$$x(t) \to x^* \quad \text{for} \quad t \to \infty. \tag{A.97}$$

Linear approximation near $x = x^*$ yields

$$r(x) \approx r(x^*) + r'(x^*) \cdot (x - x_0) = \alpha \cdot (x - x^*), \tag{A.98}$$

where $\alpha = r'(x^*)$. It can be shown that in this case we may, so to speak, treat '$\approx$' as if it was '$=$' and insert (A.98) into the differential equation which leads to

$$\frac{dx}{dt} = r(t) \approx \alpha \cdot (x - x^*) \quad \Rightarrow \quad x = x^* + ce^{\alpha t} \tag{A.99}$$

This means that provided $x(0)$ is not too far from the equilibrium x^*, the behaviour of the solution for increasing t is completely governed by the sign of $\alpha = r'(x^*)$, apparently so that *the equilibrium is stable if* $r'(x^*) < 0$, *unstable if* $r'(x^*) > 0$.

Example A.15

The logistic equation (A.92) (we rename r as r_0) is autonomous, with $r(x) = r_0x(1 - x/K) = r_0x - (r_0/K)x^2$. There are two equilibria, $x^* = 0$ and $x^{**} = K$. From

$$r'(x) = r_0 - (r_0 / K) \cdot 2x \tag{A.100}$$

we get $r'(0) = r_0 > 0$, and $r'(K) = r_0 - 2r_0 = -r_0 < 0$, i.e., 0 is an unstable and K is a stable equilibrium. the results are in accordance with the general behaviour of the solutions for increasing t. In fact *any* solution with $x(0) > 0$ will tend to K for $t \to \infty$.

EXERCISE A.14

Harvesting. A population that would otherwise grow logistically according to (A.92), with $K = 1000$ and $r = 0.25$, is subjected to continuous exploitation at a constant rate of $\beta = 200$ individuals being removed per time unit. Write down the modified logistic differential equation that holds for the population size $N(t)$. Show that there are two equilibria. Are they stable or unstable? Give a biological interpretation. If β increases, what is the highest value it can have for the population still to be sustainable? Generalize to arbitrary values of all parameters, or if you know of any realistic values in a specific situation, try them out.

Apply the equilibrium/stability theory to the two simple models in Exercise A.10.

A.5 Systems of Differential Equations

We shall now leave the one-variable systems and turn to the more complicated, but also more realistic case of a system described by several interacting state variables and modelled by equations of type (A.72), one for each state variable. Though the number of variables in a real situation may be large, perhaps counted in hundreds, we shall limit most of the considerations below to systems with just two state variables which helps us to keep the overview and still allows for illustrating most of the points of interest.

Let us thus consider a system described by the state variables $x(t)$ and $y(t)$ and governed by the following *system of simultaneous differential equations*:

$$\frac{dx}{dt} = r(t, x, y), \quad \frac{dy}{dt} = s(t, x, y), \tag{A.101}$$

where r and s are arbitrary (but reasonably nice) functions of three variables. A *solution* of (A.101) is a specific pair of functions $x = x(t)$, $y = y(t)$ which, when

inserted, satisfy both equations. An argument similar to the one put forward in connection with the one-variable equation (A.74), $dx/dt = r(t,x)$, supports the result that an initial condition of the type (t_0, x_0, y_0) (which means that for $t = t_0$ we must have $x = x_0, y = y_0$) will in general determine a unique solution: "there is one and only one solution that satisfies $x(t_0) = x_0$ and $y(t_0) = y_0$". The theorem actually holds; we omit the proof.

In the fairly rare cases where we can write it down explicitly, the *complete solution* of (A.101) will typically express both x and y in terms of t and *two* independent, arbitrary constants, say, c_1 and c_2. A choice of both c_1 and c_2 corresponds to a particular solution; and when an initial condition is inserted into the expression for the complete solution, two equations in the unknown c_1 and c_2 emerge which we can solve and thereby find the solution determined by the initial condition.

The system (A.101) is *autonomous* when neither of the right hand sides depend on the variable t. An important type of autonomous system is

$$\frac{dx}{dt} = ax + cy, \quad \frac{dy}{dt} = bx + dy, \tag{A.102}$$

where a, b, c, d are constants. We shall illustrate (A.102) by some examples.

Example A.16

Consider the system

$$\frac{dx}{dt} = 0.5x + y, \quad \frac{dy}{dt} = -0.75x + 2.5y. \tag{A.103}$$

The equations resemble the one-variable equation $dx/dt = a\,x$, so why not look for a solution of the form $x = x0e^{\,t}, y = y_0e^{\,t}$? Insertion and a little rewriting yields

$$(0.5 - \lambda)x_0 + y_0 = 0, \quad -0.75x_0 + (2.5 - \lambda)y_0 = 0. \tag{A.104}$$

If this homogeneous linear system must have non-trivial, i.e., non-zero solutions (see Section A.3, Equations (A.53–55)) its determinant must be equal to zero. In other words, we arrive at an eigenvalue–eigenvector problem for the 'coefficient matrix'

$$A = \begin{pmatrix} a & c \\ b & d \end{pmatrix} = \begin{pmatrix} 0.5 & 1 \\ -0.75 & 2.5 \end{pmatrix}$$

which turns out to have the following eigenvalues and corresponding eigenvectors:

$$\underline{\lambda = 1}: \quad v = c_1 \begin{pmatrix} 2 \\ 1 \end{pmatrix}, \quad \underline{\lambda = 2}: \quad v = c_2 \begin{pmatrix} 2 \\ 3 \end{pmatrix} \tag{A.105}$$

(the reader is invited to verify (A.105): note that the symbols c_1 and c_2 replace the "t" used in Section A.3). From Eq. (A.105) and the preceding remarks it follows that we have the solutions $x = 2c_1e^t, y = c_1e^t$ ($c_1 \in \mathbf{R}$) *and* the solutions $x = 2c_2e^{2t}, y = 3c_2e^{2t}$ ($c \in \mathbf{R}$); using the 'linearity' in x and y of the system it follows readily that we may even add these two rays of solutions, to arrive at the 'double infinity' of solutions given by

$$\begin{aligned} x &= 2c_1e^t + 2c_2e^{2t} \\ y &= c_1e^t + 3c_2e^{2t} \end{aligned} \tag{A.106}$$

Finally it can be verified that, as suggested by the presence of the two independent arbitrary constants, a solution of type (A.106) passes through any (t_0, x_0, y_0), and we can conclude that (A.106) is the *complete* solution of (A.102).

Example A.17

Consider the system

$$\frac{dx}{dt} = -y, \qquad \frac{dy}{dt} = x. \tag{A.107}$$

Proceeding as in Example A.16 leads to the question $\lambda^2 + 1 = 0$ which has no roots, i.e., (A.107) has no solutions of the form (A.106). However, looking for some time at (A.107) may bring the basic trigonometric functions cosine and sine to the mind. After a few trials we find that $x = \cos t, y = \sin t$ is a solution, and similarly that $x = -\sin t, y = \cos t$ is also a solution. As a consequence of the linearity of the system, both solutions may be multiplied by arbitrary constants, say, c_1 and c_2. And, like in Example A.16 when two solutions are added we get another solution, i.e., all pairs of functions of the form

$$\begin{aligned} x &= c_1 \cos t - c_2 \sin t \\ y &= c_1 \sin t + c_2 \cos t \end{aligned} \tag{A.108}$$

are solutions. Finally it can be verified, just as in Example A.16, that (A.108) is the complete solution of (A.107).

EXERCISE A.15

Consider the system

$$\frac{dx}{dt} 3x - 2y, \qquad \frac{dy}{dt} = 5x + y. \tag{A.109}$$

Try to find solutions along the same lines as in the two preceding examples. What goes wrong? Now we have a problem. Linear combinations of functions of the type $e^{\lambda t}$ cannot be solutions, and linear combinations of $\cos \mu t$ and $\sin \mu t$ cannot either. But experience may have taught you that linear combinations of *products* of the two types just mentioned, i.e., of $e^{\lambda t} \cos \mu t$ and $e^{\lambda t} \mu t$ yield functions of the same kind when they are differentiated, so we will look for solutions of this type. Trying not to have too many coefficients to determine we write tentatively

$$x = e^{\lambda t} \cos \mu t, \quad y = A\, e^{\lambda t} \cos \mu t + B\, e^{\lambda t} \sin \mu t. \tag{A.110}$$

Insert (A.110) in (A.109), and find λ, μ, A and B so that (A.109) is satisfied. Repeat the process with sine in the place of cosine in the x expression, and deduce another solution. Finally, write down the complete solution as an arbitrary linear combination of the two 'standard solutions' you have found. [There are many other ways the solution can be written, yet they all lead to the same set of pairs of functions.]

Example A.18

Consider the system

$$\frac{dx}{dt} = 4x - y, \qquad \frac{dy}{dt} = 4x\,. \tag{A.111}$$

Proceeding once again as in Example A.16 leads to a characteristic equation with $\lambda = 2$ as double root for which the eigenvectors $c_1(1, 2)$ ($c_1 \in \mathbf{R}$) are found, implying that a 'single infinity' of solutions is given by $x = c_1 e^{2t}, y = 2c_1 e^{2t}$. *But this cannot be the complete solution.* As a counter-example at random: there is no solution of the above type that satisfies $x(0) = 0, y(0) = 1$. And if we try to repair the method by means of sine and cosine factors, which worked well in Example A.17 and Exercise A.15, it turns out that we will get nowhere.

It can be proved however that the complete solution is given by

$$\begin{aligned} x &= c_1 e^{2t} + c_2 t e^{2t} \\ y &= 2c_1 e^{2t} + c_2 (2t+1) e^{2t}. \end{aligned} \tag{A.112}$$

That t occurs as a factor of e^{2t} in the 'second part' of the solution is typical for systems with a double root in the characteristic equations for the coefficient matrix.

Together, the preceding three examples and Exercise A.15 cover quite well the various possibilities for the solution of the system (A.102). when the coefficient matrix on the right hand side has two eigenvalues λ_1 and λ_2, the solutions are built of

linear combinations of $e^{\lambda_1 t}$ and $e^{\lambda_2 t}$; when there is one eigenvalue λ_1, the solutions are built of linear combinations of $e^{\lambda_1 t}$ and $te^{\lambda_1 t}$; when there are no eigenvalues, the solutions are built of linear combinations of $e^{\lambda t}\cos \mu t$ and $e^{\lambda t}\sin \mu t$ where the constants λ and μ are determined by the four coefficients in the equations. (In a few cases, see Example A.17, it may happen that $\lambda = 0$ so that the solutions are linear combinations of $\cos \mu t$ and $\sin \mu t$ alone).

Let us take a look at one particular property, of interest a.o. in applications, which the solutions of (A.102) may have or may not have: that every particular solution 'disappears' (i.e., tends to 0 in both coordinates) for $t \to \infty$. From the overview of the three possible cases it appears that all the various members in a solution of (A.102) contain a factor of the type $e^{\lambda t}$, and the solutions thus all disappear for $t \to \infty$ if and only if all occurring factors of that type have a *negative* (not positive and not zero) λ value. A closer look at the three cases reveals that the condition can be simplified into the following: *all solutions of* (A.102) *disappear for* $t \to \infty$ *if and only if* $a+d < 0$ *and* $ad - bc > 0$.

EXERCISE A.16

Show that all solutions of the system

$$\frac{dx}{dt} = -5x - y, \quad \frac{dy}{dt} = 4x - y \tag{A.113}$$

disappear for $t \to \infty$, (1) by determining the type of functions of t that occur in the complete solution, (2) by using simplified criterion mentioned above.

Try out the criterion with some of the systems in the above examples and exercises.

Consider now an arbitrary autonomous system

$$\frac{dx}{dt} = r(x, y), \qquad \frac{dy}{dt} = s(x, y). \tag{A.114}$$

An *equilibrium or steady state* for (A.114) is a point (a state) (x^*, y^*) such that $r(x^*, y^*) = s(x^* y^*) = 0$. Given such an equilibrium, the constant functions $x(t) = x^*, y(t) = y^*$ satisfy the equations (A.114) so that if the system gets into this state it will, according to the model, stay there indefinitely. But like in the one-variable case the question arises: is the equilibrium stable or unstable? And the answer is found in a similar way. By first-order approximation near the equilibrium, the system (A.114) is replaced by the following linear system in the small perturbations of the state variables, $u = x - x^*$ and $v = y - y^*$:

$$\frac{du}{dt} + au + cv, \qquad \frac{dv}{dt} = bu + dv, \tag{A.115}$$

where the constants a, b, c, d are found as partial derivatives of the rate functions on the right hand sides in (A.114), evaluated at (x^*, y^*):

$$\begin{aligned} a &= r'_x(x^*, y^*), \quad c = r'_y(x^*, y^*), \\ b &= s'_x(x^*, y^*), \quad d = s'_y(x^*, y^*). \end{aligned} \tag{A.116}$$

[Readers who are familiar with differentiable vector functions will recognize (A.116) as expressing that the coefficient matrix $\boldsymbol{A}$ in (A.115) is equal to the *Jacobian* (the functional matrix) of the right hand side of (A.114) worked out at the equilibrium point.] With (A.115–116) at hand, we can use the linear condition for 'disappearance' to deduce the following condition for local stability: *the equilibrium is stable if* $a + d < 0$ *and* $\det \boldsymbol{A} = ad - bc > 0$, *where a, b, c, d are the partial derivatives given by* (A.116).

Example A.19

Consider the system

$$\begin{aligned} \frac{dx}{dt} &= r(x, y) = -x^2 + y + 3, \\ \frac{dy}{dt} &= s(x, y) = x + y^2 + 1. \end{aligned} \tag{A.117}$$

Suppose we have found the equilibrium $(x^*, y^*) = (2,1)$ (it is easily verified that $r(2,1) = s(2,1) = 0$). Is the equilibrium stable or unstable?

By partial differentiation and insertion of (2,1) we get:

$$\begin{aligned} & r'_x(x, y) = -2x, r'_y(x, y) = 1, s'_x(x, y) = 1, s'_y(x, y) = -2y \\ \Rightarrow \quad & a = -4, \quad b = 1, \quad c = 1, \quad d = -2 \\ \Rightarrow \quad & a + d = -6 < 0, \quad ad + bc = 7 > 0. \end{aligned}$$

We conclude that (2,1) is a locally *stable* equilibrium for the system (A.117).

EXERCISE A.17

Consider the system

$$\begin{aligned} \frac{dx}{dt} &= x \cdot (5 - 2x - y) = 5x - 2x^2 - xy, \\ \frac{dy}{dt} &= y \cdot (5 - x - 3y) = 5y - xy - 3y^2. \end{aligned} \tag{A.118}$$

Find all equilibria of the system. Are they stable or unstable?

Example A.20

Two-species composition. Consider the Lotka–Volterra model for two competing populations given in Section 6.4, Eqs. (6.9–10). By renaming K_1/α_{12} as L_2 and K_2/α_{21} as L_1, we can write down the model as

$$\begin{aligned} \frac{dN_1}{dt} &= r(N_1, N_2) = r_1 N_1 \left(1 - \frac{N_1}{K_1} - \frac{N_2}{L_2}\right) \\ \frac{dN_2}{dt} &= s(N_1, N_2) = r_2 N_2 \left(1 - \frac{N_1}{L_1} - \frac{N_2}{K_2}\right) \end{aligned} \tag{A.119}$$

The quantity K_1 is the carrying capacity of the environment for the N_1 population in the absence of the N_2 population; and *vice versa* for K_2. The quantity L_2 might be termed 'interaction capacity' because it can be interpreted as the N_2 population size which will cause the growth of the N_1 population to drop to zero when there are very few N_1 individuals, i.e., when $N_1/K_1 << 1$; and *vice versa* for L_1. Note that a high degree of competition from species i towards the other corresponds to a *small* value of L_i.

To find the possible *equilibria* of (A.119) we must set both right hand sides equal to zero and solve the two resulting equations with respect to N_1 and N_2. It turns out that there are four solutions: (1) the trivial equilibrium $N_1 = N_2 = 0$ where both species are absent; (2) $N_1 = K_1$ and $N_2 = 0$, i.e., the N_2 population is absent and the N_1 population is in logistic equilibrium with itself; (3) the reverse situation: $N_1 = 0$ and $N_2 = K_2$; and finally (4) the real two-species equilibrium found by assuming $N_1 > 0$, $N_2 > 0$ and solving the two linear equations that correspond to the parentheses on the right hand sides of the equations both set equal to zero. This equilibrium is found to be

$$N_1^* = \frac{L_1 K_1 (L_2 - K_2)}{L_1 L_2 - K_1 K_2}, \qquad N_2^* = \frac{L_2 K_2 (L_1 - K_1)}{L_1 L_2 - K_1 K_2}. \tag{A.120}$$

It is however meaningful only when both these expressions have positive values. The four possible sign combinations correspond to the four entries in Table 6.2, and to the four graphs in Fig. 6.3. When $K_1 < L_1$ and $K_2 < L_2$, meaning that for each of the two species intraspecific competition is heavier than interspecific competition, then we have the situation termed Case 4 in Chapter 6. A *stability* analysis leads to somewhat lengthy calculations and is omitted here; it shows that in Case 3 the equilibrium is unstable and in Case 4 it is stable. The latter corresponds to a situation where the two species have a sufficiently small niche overlap for coexistence to prevail.

Example A.21

Predator–prey model. Consider Lotka–Volterra's simple predator–prey model, given in Section 6.3, Eqs. (6.14–6.15). By renaming r_1/p_1 as N_2^* and d_2/p_2 as N_1^*, cf. Eqs. (6.16–6.17), we can write down the model as

$$\frac{dN_1}{dt} = r_1 N_1\left(1 - \frac{N_2}{N_2^*}\right) \qquad \frac{dN_2}{dt} = d_2 N_2\left(\frac{N_1}{N_1^*} - 1\right). \tag{A.121}$$

Apart from the trivial equilibrium $N_1 = N_2 = 0$ there is a unique non-zero equilibrium, namely $N_1 = N_1^*, N_2 = N_2^*$. A stability analysis shows that the equilibrium is not stable in the above sense, but "something in between stable and unstable": it can be verified that, regardless of the initial conditions, the model predicts *periodic* oscillations around (N_1^*, N_2^*), the so-called 'phase plot' in the N_1N_2 plane being a convex, softly triangular closed curve encircling the equilibrium point. Such a periodicity is of course rather unrealistic and several modifications of (A.121) have been suggested to make up for this. One of them is given in Eqs. (6.18–6.19); for suitable values of the parameters it has a stable equilibrium.

EXERCISE A.18

Explain that the model (A.118) in Exercise A.17 is an instance of the Lotka–Volterra competition model (A.119), and identify the parameter values. Are the results in Exercise A.17 in accordance with the theory in Section 6.3 and Example A.20? Which of the four cases do we have?

Consider the *modified predator–prey model* in Eqs. (6.18–19), and let $r_1 = 2, z_1 = \beta_{12} = \gamma_{21} = \beta_2 = 1$. Find the unique equilibrium in the region $N_1 > 0, N_2 > 0$ and assess whether or not it is stable.

Same question for the *host–parasite model* in Eqs. (6.20–21), with parameter values r_1 and $r_2 = 1, K_1 = K_2 = 10$.

Same question for the *symbiosis model* in Eqs. (6.22–23), with parameter values $r_1 = r_2 = 1, K_1 = 30, K_2 = 20, \alpha_{12} = 1/2, \alpha_{21} = 1/3$.

To conclude this section, let us give a brief review of the generalization of the above to *systems of n simultaneous differential equations*. Such a system has the general form

$$\frac{d\boldsymbol{x}}{dt} = \boldsymbol{r}(t, \boldsymbol{x}), \tag{A.122}$$

where $\boldsymbol{x}$ is an n-dimensional vector (we may think of $\boldsymbol{x}$ as composed of n state variables) and $\boldsymbol{r}$ is a vector function with n coordinates, each of them being a function of the $n+1$ variables $t, x_1, x_2, \ldots, x_n$. The system is *autonomous* if t does not occur in any of the right hand side expressions. An important autonomous system is

$$\frac{d\mathbf{x}}{dt} = A\mathbf{x}\,, \tag{A.123}$$

where A is an $n \times n$ matrix with constant elements. The solution of (A.123) is closely connected with the eigenvalues and eigenvectors of A. In the simple case where A has n different real eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$, the solutions of (A.123) are built of linear combinations of exponential functions of type $e^{\lambda_i t}$. Normally there are however less than n real eigenvalues, and in that case the solutions of (A.123) are built of exponential functions and functions of type $e^{\lambda_i t}\cos \mu t$ and $e^{\lambda_i t}\sin \mu t$, sometimes supplemented by functions of the types $te^{\lambda_i t}$, $t^2 e^{\lambda_i t}$, etc.

Also in the n-dimensional case we may ask about conditions for the system to have the property that all solutions disappear for $t \to \infty$. In the light of the description of the solutions just given we can conclude that the disappearance property is present if and only if all the quantities terms "λ" are negative. If just one is positive, the solutions will in general numerically tend to ∞ for increasing t.

For an arbitrary autonomous system $d\mathbf{x}/dt = \mathbf{r}(\mathbf{x})$ and *equilibrium* is defined as a state $\mathbf{x}^*$ such that $\mathbf{r}(\mathbf{x}^*) = 0$. *Stability* of the equilibrium is determined by the Jacobian of $\mathbf{r}(\mathbf{x})$ worked out as $\mathbf{x}^*$, in a similar way as in the two-dimensional case.

EXERCISE A.19

Consider the system

$$\frac{dx}{dt} = -2x + y - 2z, \quad \frac{dy}{dt} = 2x - 3y + 4z, \quad \frac{dz}{dt} = 2x - 5y + 6z\,. \tag{A.124}$$

Do all solutions of (A.124) disappear for $t \to \infty$? Replace the diagonal coefficients –2, –3, 6 in the system by –5, –6, 3, respectively. Do all solutions for the new system disappear for $t \to \infty$?

Example A.22

Yeast culture model. The model treated in Illustration 6.1 and written out as a CSMP program in Table 6.3 is, with the simplifications implicit in the computer program, identical to the following system of three simultaneous differential equations:

$$\begin{aligned} \frac{dY_1}{dt} &= r_1 Y_1\left(1 - \frac{A}{A_m}\right) \\ \frac{dY_2}{dt} &= r_2 Y_2\left(1 - \frac{A}{A_m}\right) \\ \frac{dA}{dt} &= a_1\frac{dY_1}{dt} + a_2\frac{dY_2}{dt}. \end{aligned} \tag{A.125}$$

where Y_1 and y_2 are the concentrations of type 1 and 2, respectively, and A is the alcohol concentration; the other symbols are the parameters of the model among which is A_m, the alcohol concentration at which yeast production stops completely. The actual values of the parameters as well as the initial conditions can be found in Table 6.3.

The equilibrium properties of (A.125) are a little special since *all* states with $A = A_m$ are equilibria. As a consequence, none of them can be stable in the sense defined above. It is clear, though that from any initial point (Y_{10}, Y_{20}, A_0) with $A_0 < A_m$, the system will converge to some final equilibrium (Y_{1m}, Y_{2m}, A_m) where Y_{1m} and Y_{2m} depend on the initial point. Anyway, as commented upon in Illustration 6.1, the ability of the model to explain the results of such mixed growth experiments seems to be unsatisfactory.

In the above treatment of systems of differential equations we made an issue out of 'equilibrium' and 'stability'. It should be added that in practical modelling they are somewhat less important, a.o. because most systems are not autonomous, for the same reasons as already mentioned at the end of Section A.4. Besides, the systems are often so large that a purely mathematical treatment must be abandoned. Still, the concept of *steady state* is a central one, and at any rate it is of value that the modeller has some theoretical background—preferably more than conveyed in this appendix—to be able to understand what lies behind equilibrium and stability, also in a more complicated context.

The standard model example in Chapter 2 (phosphorus cycle in an aquatic ecosystem), treated at length in Illustration 2.1, has only two state variables, phosphorus in solution and phosphorus in algae. But because of the time-dependent forcing function $S(t)$, solar radiation, the model is not autonomous, and the equilibrium and stability concepts in their simple form are not relevant to the study of it.

The Larsen eutrophication model presented in Section 3C.1 is another example of a non-autonomous system of differential equations that we have met in the text proper.

Finally it should be emphasized that an important class of problems is not touched upon at all in this appendix. We refer to ecological models involving functions of two or more variables (typically functions of both time and spatial position) and leading into a *partial differential equation* as exemplified by the diffusion equation, see Section 3A.2, and the hydronamical mass balance equations, see Section 3A.3. The mathematical theory of partial differential equations (PDEs) is considerably more complicated than that of ordinary differential equations, and we have to refrain from it.

A.6 Numerical Methods

Numerical analysis, also termed 'numerical methods', is a branch of mathematics that deals with approximate methods of solving problems which cannot, or can only with trouble, be exactly solved. Already the everyday routine of replacing numbers in a calculation by decimal approximations, e.g., find the area A of a circle with radius $r = 11/3$ like this:

$$A = \pi r^2 = \pi\left(\frac{11}{3}\right)^2 \approx 3.14 \cdot 3.67^2 = 42.292346 = 42.3, \tag{A.126}$$

can be considered a numerical method. (The calculation just shown is not too elegant but that is not the point.) Another one consists of using *Taylor polynomials* to approximate values of functions. For example, the exponential function $f(t) = e^t$ has at $t = 0$ the third order Taylor polynomial $f_3(t) = 1 + t + t^2/2 + t^3/6$, and we can write

$$e^{0.3} = f(0.3) \approx f_3(0.3) = 1 + 0.3 + 0.3^2/2 + 0.3^3/6 = 1.3495. \tag{A.127}$$

By including an expression for the *remainder* in Taylor's formula we might have evaluated the deviation of 1.3495 from $e^{0.3}$; it turns out that the deviation is negative and of the order of size –0.0004. This exemplifies an important part of numerical analysis: to investigate the *error* introduced by replacing an exact solution by an approximate one.

Yet another simple example of a numerical method is *Newton–Raphson iteration*, also known as Newton's method for solving an equation in one unknown. By taking all members to the left hand side the equation takes the form $f(x) = 0$ so that the problem is to find a zero ξ for a given function f. It is assumed that f is differentiable and that we have as a starting point one approximation x_0 of ξ, possibly rather crude but not too wild. Newton's idea was to replace the function of f in the neighbourhood of $x = x_0$ by the linear approximation $f_1(x) = f(x_0) + f'(x_0)(x - x_0)$ and solve the linear equation $f_1(x) = 0$; it is readily verified that the unique solution is

$$x_1 = x_0 - \frac{f(x_0)}{f'(x_0)}. \tag{A.128}$$

For example, if $f(x) = x^2 - 2$ and if we have found out that there is a root not too far from $x_0 = 1$, then (A.128) yields: $f(1) = -1, f'(1) = [2x]_{x=1} = 2, x_1 = 1 - (-1)/2 = 1.5$; the root in question is of course $\xi = \sqrt{2} \cong 1.414$, and it is true that x_1 is a better approximation of this root than x_0. Newton's method has a useful feature shared by many other numerical methods: it can be *iterated*, thus leading to better and better approximations of the root we are looking for. Continuing the above example we can use (A.128) again but with $x_0 = 1.5$ which yields: $f(1.5) = 0.25, f'(1) = [2x]_{x=1.5} = 3, x_1 = 1.5 - 0.25/3 = 17/12 \cong 1.417$, a considerable improvement as an approximation to the true root.

Newton's method has been generalized in various ways, e.g., to solve a system of n equations in n unknowns. Such a system may be written $f(x) = o$ where f is a function from $\mathbf{R}^n$ to $\mathbf{R}^n$; by such methods similar to those suggested in the discussion of Eqs. (A.114–116) it can be shown that if the n-tuple x_0 is a first approximation of the solution, then we may get a better one from the vector-matrix equation

$$x_1 = x_0 - f'(x_0)^{-1} f(x_0), \tag{A.129}$$

where $f'(x_0)$ is the Jacobian of f worked out at x_0.

EXERCISE A.20

The equations

$$\begin{aligned} r(x,y) &= x^2 + xy + y^2 - 18 = 0, \\ s(x,y) &= \quad -x^3 + y^3 - 20 = 0 \end{aligned} \tag{A.130}$$

have the solution in the neighbourhood of $x_0 = 2, y_0 = 3$. Use (A.129) to find a two-decimal approximation, better than the one given by x_0 and y_0, for the solution.

We shall deal briefly with two numerical problems, both of interest for ecological modelling: (1) that of computing the value of a definite integral $\int_a^b f(t)\mathrm{d}t$ when it is impossible, or just very troublesome, to find the expression of a primitive function $F(t)$ for the integrand $f(t)$; (2) that of computing values of a particular solution of a given differential equation when it is likewise little tempting to solve the equation directly.

Numerical integration. Suppose we want to find a good approximation of $\int_a^b f(t)\mathrm{d}t$ where values of the integrand f in the interval $a \le t \le b$ can be computed as accurately as we wish, by an expression or otherwise. For simplicity we assume that f is positive in the interval, but the formulas below are valid also when this assumption does not hold. It is well known that if the graph of f has been drawn in the TX-system, then $\int_a^b f(t)\mathrm{d}t$ is equal to the area of the region bounded by the graph, the T-axis, and the vertical lines $t = a$ and $t = b$. Now let $t_0 = a, t_1, t_2, \ldots, t_n = b$ be *equidistant* points in the interval, i.e., $t_i - t_{i-1} = (b-a)/n = \Delta t$ for $i = 1, 2, \ldots, n$, and let $x_i = f(t_i)$ for all i. Since the broken line connecting the points $(x_i, f(x_i))$ approximates the graph of f, the area A of the region under the broken line approximates the integral. The region is a polygon built of n trapezoids, all with base Δt while the parallel sides of the i'th trapezoid are x_{i-1} and x_i. Thus we get the following expression for A:

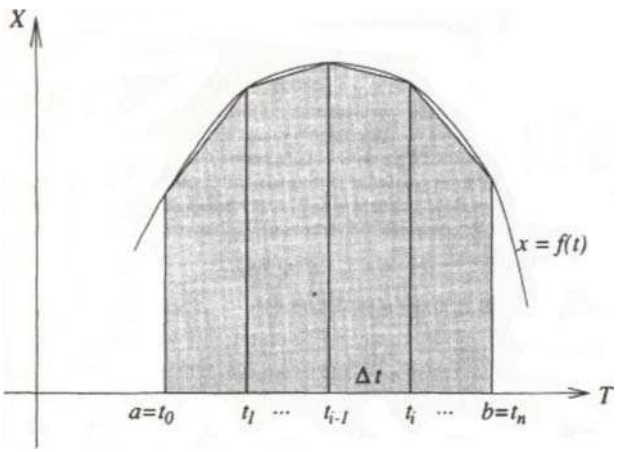
$$\begin{aligned} A &= \frac{x_0 + x_1}{2}\Delta t + \frac{x_1 + x_2}{2}\Delta t + \ldots + \frac{x_{n-1} + x_n}{2}\Delta t \\ &= \left[\frac{x_0 + x_n}{2} + x_1 + x_2 + \ldots + x_{n-1}\right] \cdot \Delta t. \end{aligned} \tag{A.131}$$

Inserting the values of x_i and Δt and using the summation symbol Σ we arrive at the so-called *Trapezoid formula* of numerical integration:

$$\int_a^b f(t)\mathrm{d}t \approx \left[\frac{f(a)+f(b)}{2} + \sum_{i=1}^{n-1} f(t_i)\right] \cdot \frac{b-a}{n}, \tag{A.132}$$

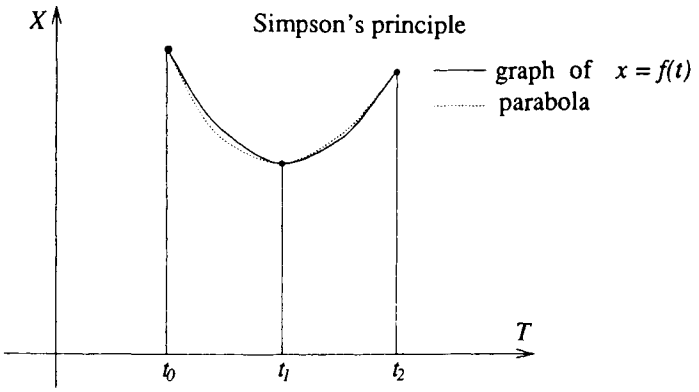
where we might also have inserted $t_i = a + i \cdot \Delta t = a + i \cdot (b-a)/n$ ($i = 0, 1, 2, ..., n$).

The Trapezoid formula is seldom used because it is possible, by calculations only slightly longer, to approximate the integral much more accurately. Geometrically speaking the problem with the Trapezoid formula is that it does not take into account the curvature of the graph. When for instance the function is concave in the interval the trapezoid region ignores all the curved segments above the polygon (see figure), and consequently (A.132) underestimates the integral.



We shall present one simple but efficient improvement of the Trapezoid formula, resting on the following principle: assume that n is even, $n = 2m$. By taking *two* Δt intervals at a time and approximating the graph of f by *parabola segments* instead of by line segments we will in general keep much closer to the graph, as the reader will intuitively recognize when trying to draw the parabola through three neighbouring points of a smooth curve. We need the following auxiliary result (which the reader is encouraged to verify): let $P(t)$ be an arbitrary polynomial of second degree, let t_0, t_1, t_2 be three equidistant points so that $t_1 - t_0 = t_2 - t_1 = \Delta t$, and let $x_i = P(t_i)$ for $i = 0, 1, 2$; then

$$\int_{t_0}^{t_2} P(t)\mathrm{d}t = (x_0 + 4x_1 + x_2) \cdot \frac{\Delta t}{3}. \tag{A.133}$$



By repeated use of (A.133) we get the following formula for the area B of the region under the approximating curve pieced together of m parabola segments:

$$B = (x_0 + 4x_1 + x_2)\cdot\frac{\Delta t}{3} + (x_2 + 4x_3 + x_4)\cdot\frac{\Delta t}{3} + \ldots + (x_{2m-2} + 4x_{2m-1} + x_{2m})\cdot\frac{\Delta t}{3}$$
$$= [x_0 + x_{2m} + 4(x_1 + x_3 + \ldots + x_{2m-1}) + 2(x_2 + \ldots + x_{2m-2})]\cdot\frac{\Delta t}{3}, \qquad \text{(A.134)}$$

leading to *Simpson's* formula

$$\int_a^b f(t)\mathrm{d}t \approx \left[f(a) + f(b) + 4\sum_{i=1}^{m} f(t_{2i-1}) + 2\sum_{i=1}^{m-1} f(t_{2i})\right]\cdot\frac{b-a}{3n}. \qquad \text{(A.135)}$$

A more thorough examination points to Simpson's formula being markedly superior to the Trapezoid formula, and practice confirms the result.

Example A.23

We will evaluate the integral $\int_0^1 f(t)\mathrm{d}t$ where $f(t) = 1/(1+t^2)$. Taking $\Delta t = 0.1$ and using a pocket calculator we can construct the following table of f values:

$f(0 = 1$	$f(0.2) = 0.961538$	$f(0.1) = 0.990099$
$f(1) = 0.5$	$f(0.4) = 0.862069$	$f(0.3) = 0.917431$
1.5	$f(0.6) = 0.735294$	$f(0.5) = 0.800000$
	$f(0.8) = 0.609756$	$f(0.7) = 0.671141$
	3.168657	$f(0.9) = 0.552486$
		3.931157

The Trapezoid formula with $n = 5$ yields

$$\int_0^1 \frac{dt}{1+t^2} \approx 0.2 \cdot (0.75 + 3.168657) \qquad = 0.783731.$$

The Trapezoid formula with $n = 10$ yields

$$\int_0^1 \frac{dt}{1+t^2} \approx 0.1 \cdot (0.75 + 3.168657 + 3.931157) \qquad = 0.784981.$$

Simpson's formula with $n = 2$ (i.e., $m = 1$) yields

$$\int_0^1 \frac{dt}{1+t^2} \approx \frac{0.5}{3} \cdot (1 + 0.5 + 4 \cdot 0.8) = \frac{4.7}{6} \qquad = 0.783333.$$

Simpson's formula with $n = 10$ (i.e., $m = 5$) yields

$$\int_0^1 \frac{dt}{1+t^2} \approx \frac{0.1}{3} \cdot (1 + 0.5 + 4 \cdot 3.931157 + 2 \cdot 3.168657) \qquad = 0.785398.$$

The function chosen can be integrated directly so that we can verify the approximations:

$$\int_0^1 f(t)dt = [\text{Arc tan } t]_0^1 = \frac{\pi}{4} - 0 \qquad = 0.785398.$$

We note that when we pass from $n = 5$ to $n = 10$ in the Trapezoid formula we get a somewhat better approximation of the integral, but when we pass from the Trapezoid formula to Simpson's formula the improvement is dramatic.

EXERCISE A.21

Calculate $\int_0^1 \sqrt{t}dt$ to four decimal places by use of

(1) the Trapezoid formula with $n = 6$,
(2) Simpson's formula with $n = 6$,
(3) direct integration.

Numerical solution of differential equations. This topic will be treated mainly with reference to an ordinary equation of the standard form $dx/dt = r(t,x)$, but the ideas and methods below have their natural counterparts in the theory of systems of differential equations and, for that matter, in the theory of partial differential equations.

In Section A.4 we introduced the fundamental dynamical-modelling equation

$$x(t + \Delta t) = x(t) + r(*)\Delta t \tag{A.68}$$

and showed that it can be viewed as an alternative formulation of the differential equation $dx/dt = r(*)$, perhaps less precise but also more appealing in the way it tells us how to pass from any point (t,x) of a solution to the neighbouring point $(t + \Delta t, x + r(*)\Delta t)$. This point of view was further utilized as an argument for the 'Existence and Uniqueness Theorem' which states that given a (reasonably nice) function $r = r(t,x)$ and an initial condition (t_0, x_0), there is one and only one solution $x = x(t)$ satisfying $x(t_0) = x_0$. The argument was, in brief, that repeated use ('iteration') of (A.68) starting from (t_0,x_0) with a given value of the time step Δt leads to a broken-line function with a quasi-solution character, and it seems reasonable to believe that if this process is repeated with still smaller values of Δt at the broken-line function will converge to 'the true solution' through (t_0,x_0).

In fact, (A.68) shows a simple and direct way of solving the differential equation numerically. Viewed from that angle the process is termed *Euler's method*. It is easy to carry out, yet practical use of the method is not frequent because there are methods which, by computations of the same order of magnitude, lead to much better results.

The problem with Euler's method is similar to that of the Trapezoid formula of numerical integration: it has a one-sided way of taking into account the curvature of the solution function, and this often leads to an accumulation of the error. We shall illustrate this point by a simple but characteristic example.

Example A.24

Suppose we want to find $x(1)$ where $x = x(t)$ denotes the solution of the differential equation $dx/dt = x$ determined by $x(0) = 1$. We can solve the equation directly into $x = ce^t$, and the $x(0) = c = 1$ we get $x(t) = e^t$ and thus $x(1) = e = 2.718$.

Now, what happens if we try to compute the same function value numerically? According to Euler's method we have, for any starting point and any time step:

$$x(t+\Delta t) \approx x(t)+x(t)\Delta t = (1+\Delta t)x(t), \tag{A.136}$$

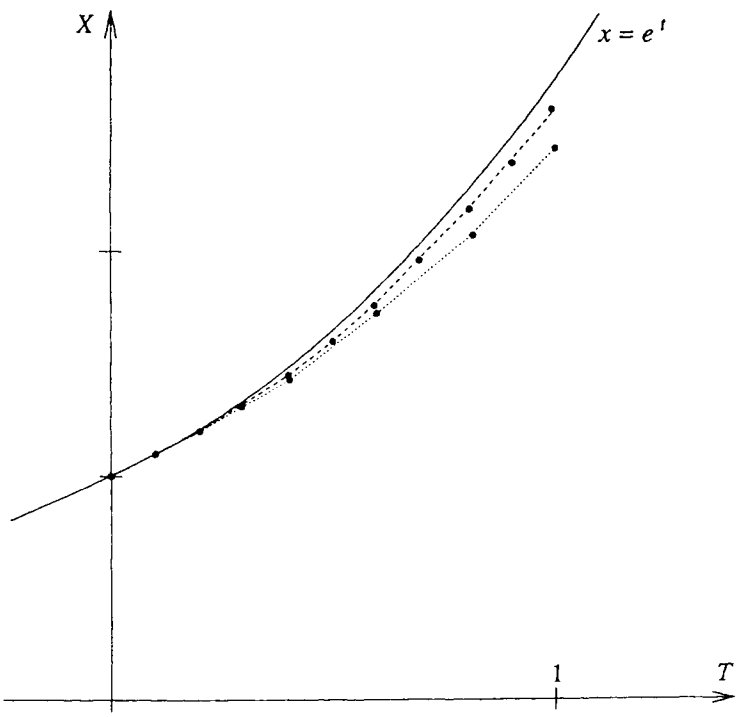
which by iteration n times yields

$$x(t+n\Delta t) \approx (1+\Delta t)^n x(t). \tag{A.137}$$

If we take $t = 0$, $\Delta t = 1/n$ (and recall that $x(0) = 1$), (A.137) becomes

$$x(1) \approx (1 + 1/n)^n. \tag{A.138}$$

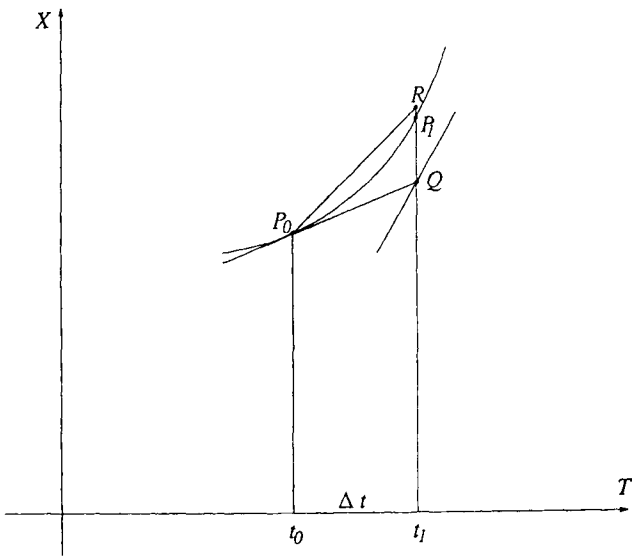
It is well-known that the quantity on the right hand side converges to e for $n \to \infty$. But the convergence is rather slow; for example we have $(1 + 1/5)^5 = 1.2^5 \approx 2.488$ and, still far from the limit, $(1 + 1/10)^{10} = 1.1^{10} \approx 2.594$.



The above figure shows the graph of the true solution together with the graphs of two broken-line quasi-solutions corresponding the Euler's method and $\Delta t = 0.2$ and $\Delta t = 0.1$, respectively. Note the accumulation of error which is expressed geometrically by the broken lines getting further and further away from the exponential graph, most obviously of course for the larger value of Δt, but things are not particularly better for the smaller one.

The problem with Euler's method can be expressed as follows: when passing directly from a point $P_0 = (t,x)$ on the graph of a solution to a neighbouring point $P_1 = (t + \Delta t, x(t + \Delta t))$ we really ought to move along a *secant* of the graph, but according to Euler's method we actually move along the tangent at P_0. If for example the function $r(t,x)$ is increasing with t in the neighbourhood of P_0, corresponding to the solution graphs being convex there, then the tangent slope $r(t,x)$ used to project the x value by (A.68) will systematically underestimate the scant slope, and we get a picture of accumulating error as illustrated by Example A.24 (see figure opposite).

We will describe an improvement of Euler's method resting on the following idea: the slope α_{sec} of the secant P_0P_1 has a value in between the tangent slopes at the end-points, $\alpha_0 = r(P_0)$ and $\alpha_1 = r(P_1)$, respectively. It can be proved that α_{sec} is in general close to the arithmetical mean of the two tangent slopes, i.e., for Δt small we have with a good accuracy



$$\alpha_{sec} \approx \frac{1}{2}\cdot(\alpha_0 + \alpha_1). \tag{A.139}$$

(For a parabola (A.139) holds regardless of Δt). Since we do not know the exact position of P_1 we cannot calculate α_1, the tangent slope at P_1. What we *can* do is to use the simple Euler principle (A.68) to pass from P_0 to another point Q and calculate the tangent slope $r(Q)$ of the solution graph passing through there; that graph is not the one we wanted to stay at but there is reason to believe, cf. the above figure, that for Δt still being small $r(Q)$ is much closer to $\alpha_1 = r(P_1)$ than is $\alpha_0(P_0)$, implying that the mean

$$\frac{1}{2}\cdot(r_0 + r(Q))$$

is a much better approximation of α_{sec} that is α_0. Therefore, after having used Q in the process of calculating α_{sec} with a good approximation we return to P_0 and leave this point with the corrected secant slope, to arrive at a point R which we may hope is considerably closer to the 'true' neighbouring point P_1 than would be Q. The entire process is then iterated to move on from P_1 to P_2, from P_2 to P_3, etc.

To sum up: a single step in the iteration process has three components:

(1) from $P_0 = (t,x)$ pass provisionally to $Q = (t+\Delta t, x+\alpha_0\Delta t)$ where $\alpha_0 = r(t,x)$

(2) calculate $r(Q)$ and subsequently $\alpha_{sec} = {}^1\!/_2(\alpha_0 + r(Q))$,

(3) from $P_0 = (t,x)$ pass to $R = (t+\Delta t, x+\alpha_{sec}\Delta t)$.

We could also say that the principle used to project the solution function is the following modification of Eq. (A.68):

$$x(t+\Delta t) = x(t) + \alpha_{sec}\Delta t, \tag{A.140}$$

where α_{sec} is approximated as mentioned above.

This method, termed Euler's method of the second order or 'Euler's Improved Method', can be shown to lead to much better approximations of solutions of a given differential equation than does the simple Euler's method, as is also confirmed by practice.

Example A.25

Let us return to the situation in Example A.24, i.e., to the differential equation $dx/dt = x$ and the solution $x = x(t)$ determined by $x(0) = 1$ which was found to be $x(t) = e^t$. Continuing the calculations in Example A.24 by applying Euler's Improved Method we consider an arbitrary point $P_0 = (t,x)$ of the solution graph and its Euler neighbour point $Q = (t+\Delta t, x+x\Delta t)$. Since $r(t,x)$, we have $\alpha_0 = x$ and $r(Q) = x+x\Delta t$ from which we get $\alpha_{sec} = {}^1\!/_2(x + x + x\,\Delta t) = x\cdot(1+{}^1\!/_2\,\Delta t)$, and (A.140) becomes

$$x(t+\Delta t) = x(t)+x(t)\cdot\left(1+\frac{1}{2}\cdot\Delta t\right)\Delta t = x(t)\cdot\left(1+\Delta t+\frac{1}{2}\cdot\Delta t^2\right). \tag{A.141}$$

Iteration n times of (A.141) yields

$$x(t+n\cdot\Delta t) = x(t)\cdot\left(1+\Delta t+\frac{1}{2}\cdot\Delta t^2\right)^n. \tag{A.142}$$

By taking $t = 0$, $\Delta t = 1/n$ (and recalling that $x(0) = 1$) we get from (A.142):

$$x(1) = (1 + 1/n + 1/(2n^2))^n. \tag{A.143}$$

The quantity on the right hand side of (A.143) turns out to converge essentially faster than that of (A.138) to the true value of $x(1)$, i.e., to $e = 2.718$. For example, for $n = 5$ we get $1.22^5 = 2.703$, and for $n = 10$ we get $1.105^{10} = 2.714$.

To compare the two methods, as they perform in this particular but characteristic case, we can arrange the following table of the results in Example A.24 and the present example:

Method	Δt	Value	Deviation × 10^3
Euler	0.2	2.488	230
Euler	0.1	2.594	124
Improved Euler	0.2	2.703	15
Improved Euler	0.1	2.714	4
(true value)		2.718	

Even Euler's Improved Method is not much used in practice. So, why did we take the trouble of going through it, if not meticulously then at least in some detail? Because the methods that *are* actually used in computer programs and elsewhere to solve numerically differential equations—and that eventually means to do the hard calculation work of an important class of the ecological models this volume is all about—are generally based on the same idea as Euler's Improved Method, namely to refine the process of projecting the solution by (A.140), minimizing the error committed when using a specific approximation of the secant slope. One such method is named after *Runge and Kutta* who deduced an ingenious weighted average of four different r values leading to a very close approximation of the secant slope. And there are other methods. The purpose here was not to teach the reader to do the work the computer will have to do anyway, but merely to provide a decent amount of understanding of what goes on when the computer 'integrates' a differential equation/an entire model. You can now relax and let the computer take over again.

A final remark concerns the accuracy of a model under investigation. Since practical modelling is liable to imminent deviations from reality for several reasons: the model is never quite adequate, the exact parameter values are not known, measurements are uncertain, etc., and since these deviations are often larger than the error introduced by using, e.g., Euler's method to solve the system numerically, why bother to use a more sophisticated method? The answer is that there is no reason to introduce an extra source of error: integrating the equations by a method with no detectable computing error makes us sure to get a true picture, if not of how reality behaves, then at least of how the *model* behaves.

ACKNOWLEDGEMENT

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APPENDIX 2

Definition of Expressions, Concepts and Indices

Acceptable daily intake (ADI)—the estimate of the amount of a substance in food or drinking water, which can be ingested per day over a lifetime by humans without appreciable health risk. ADI is normally used for food additives. The applied unit is usually mg/(kg body weight × 24 h).

Acid–base reactions—processes in which one or more hydrogen ions are transferred.

Adaptation—the response of an organism to changing environmental conditions.

Adverse effect—the change in morphology, physiology, growth, biochemistry, and/or development of lifespan of an organism which results in impairment of the functional capacity or impairment of the capacity to compensate for additional harmful effects of other environmental influences.

ATP—adenosine triphosphate, a relatively simple molecule that carries an energy bond. ATP is used to transfer energy from where it is produced by catabolism to where it is needed.

Anabolism—the biochemical construction of organic compounds from inorganic matter or simple organic compounds.

Bioconcentration factor (BCF)—the ratio of the examined chemical substance concentration in the test organisms to the concentration in the test medium, water (or air), at steady state.

Biodegradability—indicates the ability of microorganisms to decompose a specific compound or a specific water sample to inorganic components. Biodegradability may be expressed as biological half life, as a first-order kinetic coefficient, or as the biological oxygen demand relative to the theoretical oxygen demand understood as the oxygen demand needed for a complete decomposition.

Biological half life ($t_{1/2}$)—the time needed to reduce the concentration of a chemical in environmental compartments or organisms to half the initial concentration by various biological processes (biodegradation, metabolism or growth).

Biological oxygen demand—measures the amount of organic matter in a water sample as mg oxygen consumed per litre by microorganisms over a period of time often indicated as days.

Biomagnification factor (BMF)—measure of the tendency of a compound to be taken up through the food. It is the concentration of a chemical compound in a living organism divided by the concentration of the chemical compound in the food at steady state.

Body burden—concentration of a toxic substance in an organism, usually expressed as mg/kg dry matter.

Carnivores—meat-eating organisms.

Catabolism—decomposition of organic matter to simpler molecules. Energy is released by catabolism and utilized by the organism.

CF—is the ratio of the examined chemical substance concentration in the test organisms to the concentration in the test medium, water (or air), at steady state, assuming that only the medium (and not, e.g., the food) is contaminated. In practice, it is very close to the same value as BCF. In addition it is difficult to have a medium that is contaminated without contaminating the food.

COD—chemical oxygen demand expressed as the amount of oxygen in mg/l necessary to decompose a specific compound or a specific water sample by a chemical, most often dichromate. Permanganate is also used as oxidator, and the result is in this case indicated as the permanganate number, expressed either as the normal COD as mg oxygen/l or as potassium permanganate/l.

Critical body burden—the concentration in an organism which is critical for the organism. It is suggested that it be found as the critical concentration in the medium (for instance LC_{50}) × BCF.

Critical range—the range of concentrations in mg/l below which all organisms live for 24 hr and above which all die. Mortality is expressed as a fraction indicating the death rate (e.g. 3/4).

DOC—dissolved organic carbon.

Ecosphere—the living organisms and their physical–chemical environment, i.e., the part of the earth where organisms may be found.

HCp—the harzadous concentration for $p\%$ of the species, derived by a statistical extrapolation procedure.

Herbivores—plant-eating organisms.

ICp—the inhibiting concentration to produce an inhibiting effect of $p\%$.

LC_{50} (lethal concentration fifty)—a calculated concentration which, when administered by the respiratory route, is expected to kill 50% of a population of experimental animals during an exposure of a specified duration. Ambient concentration is expressed in mg per litre.

LCn (lethal concentration n)—a calculated concentration which, when administered by the respiratory route, is expected to kill $n\%$ of a population of experimental animals during an exposure of a specified duration. Ambient concentration is expressed in mg per litre.

LD_{50} (lethal dose fifty)—a calculated dose of a chemical substance which is expected to kill 50% of a population of experimental animals exposed through a route other than respiration. Dose concentration is expressed in mg per kg of body weight. the LD_{50} has often been used to classify toxicity between chemical compounds. The following classification may be used—oral LD_{50} to rat, expressed in mg/kg body weight: highly toxic < 25; toxic > 25 and < 200; harmful > 200 and < 2000.

LD_n (lethal dose n)—a calculated dose of a chemical substance which is expected to kill n% of a population of experimental animals exposed through a route other than respiration. Dose concentration is expressed in mg per kg of body weight.

LOEC—the abbreviation for lowest observed effect concentration. The LOEC is generally reserved for sublethal effects but can, in principle, also be used for mortality which is usually the most sensitive effect observed.

MAC (maximum allowable concentration)—a value in accordance with environmental legislation. Often dependent on time. This relation may be expressed as follows: $\log C = 1.8 - 0.7 \log t + 0.068 \log t2$, where C is the MAC (in mg/m^3) and t is the time (in hours).

Metabolism—catabolism and anabolism.

NC (narcotic concentration), NC_{50}—median narcotic concentration.

No effect level(NEL)—implies that test animals have remained in good condition. In most experiments, blood and urine tests are performed. The urine tests include specific gravity, pH, reducing sugars, bilirubin, and protein. The blood tests include haemoglobin concentration, packed cell volume, mean corpuscular Hb content, a white and differential cell count, clotting function, and the concentration of urea, sodium, and potassium. Control tests for hematological examination were made on the group of animals before exposure. No effect level in this context means: no toxic signs; autopsy: organs normal, blood and urine tests (if made): normal.

No observed effect concentration (level): NOEC (NOEL)—is defined as the highest concentration (level) of a test chemical substance to which the organisms are exposed that does not cause any observed and statistically significant adverse effects on the organisms compared with controls.

Oxidation state—a concept that provides a way to keep track of electrons in redox processes according to certain rules.

POM—particulate organic matter.

ppb —parts per billion. For water this is presumed to be μg/l, for air μl/m^3 and for soil μg/kg (dry matter), unless another unit is indicated.

ppm—parts per million. For water this is presumed to be mg/l, for air μl/l and for soil mg/kg (dry matter), unless another unit is indicated.

Predicted environmental concentrations (PEC)—the concentration of a chemical in the environment, calculated primarily with the use of models on the basis of available information about its properties and application pattern.

Predicted no effect concentration (PNEC)—the environmental concentration below which it is probable that an unacceptable effect will not occur according to predictions.

Predicted no effect level (PNEL)—the maximum level expressed as dose or concentration which, on the basis of our present knowledge, is likely to be tolerated by a particular organism without producing any adverse effect.

Primary producers—the organisms producing organic matter by the use of energy inputs, mainly solar radiation.

Principal component analysis (PCA)—a multivariate technique to derive a set of orthogonal parameters from a large number of properties.

Quantitative structure–activity relationship (QSAR)—the relationships between physical and/or chemical properties of substances and their ability to cause a particular effect or enter into certain processes.

Redox reactions—processes in which one or more electrons are transferred.

Retrospective risk assessment—a risk assessment performed for hazards that began in the past.

Risk–benefit analysis—is the process of setting up the balance of risks and benefits of a proposed risk-reducing action.

Risk quotient—the PEC / PNEC ratio.

Teratogenesis—is the capacity of a substance to cause defects in embryonic and foetal development. Any chemical which can cause these defects is said to be teratogenic

The median tolerance (TLm)—this term has been accepted by most biologists to designate the concentration of toxicant or substance at which $m\%$ of the test organisms survive. In some cases and for certain special reasons, the TL10 or TL90 might be used. The TL90 might be requested by a conservation agency negotiating with an industry in an area where an important fishery exists, and where the agency wants to establish waste concentrations that will definitely not harm the fish. The TL10 might be requested by a conservation agency which is buying toxicants designed to remove undesirable species of fish from fishing lakes.

Threshold-effect concentration (TEC)—the concentration calculated as the geometric mean of NOEC and LOEC. It is equivalent to MATC (maximum acceptable toxicant concentration).

Threshold limit value (TLV)—the concentration in air of a chemical to which most workers can be exposed daily without adverse effects, according to current knowledge.

TOC —total organic carbon expressed, e.g, as kg organic carbon/kg solid. Organic carbon can often be estimated as 50–60% of all organic matter.

Tolerable daily intake (TDI)—the acceptable daily intake established by the European Committee of Food. It is expressed in mg/(person × 24 h), assuming a body weight of 60 kg. TDI is normally used for food contaminants, unlike ADI. *See also* ADI.

Toxicity equivalency factor (TEF)—a factor used in risk assessment to estimate the toxicity of a complex mixture of compounds.

Ultimate median tolerance limit (UMTL)—the concentration of a chemical at which acute toxicity ceases.

Xenobiotic—a man-made chemical not produced in nature and not considered a normal constituent component of a specified biological system.

APPENDIX 3

Parameters for Fugacity Models

Table 1A. Volumes and densities of the unit world

Compartment	Volume (m^3)	Density (kg/m^3)	Organic carbon content (fraction)
Air	6.0×10^{9} (6000 m high)	1.21	–
Water	7.0×10^{6} (10 m deep)	1000	–
Soil	4.5×10^{4} (15 cm deep)	1500	0.02
Sediment	2.1×10^{4} (3 cm deep)	1500	0.04
Suspended sediment	35.0 (5 ppm vol)	1500	0.04
Biota	7.0 (1 ppm vol)	1000	–

Table 1B. Definition of fugacity capacities

Compartment		Definition of Z (mol/m^3 Pa)
Air (subscript A)	$1/RT$	R = 8.314 Pa m^3/mol K T = Temperature (K)
Water (subscript W)	$1/H$ or Cs/Ps	Cs = aqueous solubility (mol/m^3) Ps = vapour pressure (Pa) H = Henry's law constant (Pa m^3/mol)
Soil sorbent (e.g., soil, sediment particles)	$K_{sw} \times \rho/H$	K_{sw} = partition coefficient (l/kg) ρ = density (kg/l)
Biota (subscript F) (l/kg)	$K_{fw} \times d/H$	K_{fw} = bioconcentration factor d = density (kg/l)

Table 2. Volumes of other environments (m^3)

Compartment	Urban	Rural	Lake	Marsh	River
Air	1.0×10^9	6.0×10^9	6.0×10^9	6.0×10^9	1.0×10^9
Water	0	10^5	10^7	1.8×10^6	10^7
Soil	10^5	1.35×10^5	0	10^4	0
Sediment	0	5×10^3	3×10^4	4.5×10^4	5×10^4
Suspended sediment	0	1	50	90	100
Biota	0	0.1	0	18	10
Water area fraction	0	0.1	1.0	0.9	1.0

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