2 Concepts of Modelling

CHAPTER OUTLINE

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 are presented, a tentative modelling procedure is given. The steps in the modelling procedure are discussed in detail and they include: model conceptualization, mathematical formulation, parameter estimation and calibration, sensitivity analysis, and validation. This chapter focuses on model selection or the selection of model components, processes, equations, and in particular, model complexity. Various methods to select "close to the right" complexity of the model are presented. Several model formulations are always available, and to choose among these will require that sound scientific constraints are imposed on the model. Many different model types with different advantages and disadvantages are available. The selection of the best model type for a well-defined ecological or environmental management problem will be discussed in Chapter 3, where an overview of the available model types will be presented. A mathematical model usually requires the use of a computer and a computer language. The selection

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of a computer language is not discussed here, because there are many possibilities and new languages emerge from time to time. In the models used as illustrative examples, STELLA (c) (High Performance Systems) software is applied.

2.2. Modelling Elements

In its mathematical formulation, an ecological model has five components:

1. **Forcing functions or external variables:** 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. If certain forcing functions are varied, then 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, due to the human impact on ecosystems, are called *control functions*, because it is in our hands to change them. The control function in ecotoxicological models is, for instance, the discharge of toxic substances to the ecosystems; in eutrophication models it is discharge of nutrients. Other forcing functions of interest could be climatic and natural external variables, which influence the biotic and abiotic components and the process rates. In contrast to the control functions, they are not controllable by humans. By using models we will be able to address the crucial question: Which changes in the control functions are needed to obtain well-defined conditions for a considered ecosystem?
2. **State variables:** Describe, as the name indicates, the state or the conditions 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, then 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 are the concentrations of nutrients and phytoplankton. When the model is used in a management context, the values of the state variables simulated by changing the controllable forcing functions provide model results that contain the direct and indirect relations between the forcing functions and the state variables.

3. **Mathematical equations:** 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. However, this does not imply 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 and/or the problem. Some modellers refer to the description and mathematical formulation of processes as submodels. The most applied process formulations are presented by a short overview in Section 2.3.
4. **Parameters:** Coefficients in the mathematical representation of processes. They may be considered constant for a specific ecosystem or part of an ecosystem for a certain time, but they may also be a function of time or vary spatially. In causal models, the parameter will have a scientific definition and a well-defined unit, for instance, the excretion rate of cadmium from a fish — the unit could be mgCd/(24h * kg of fish). Many parameters are indicated in the literature as ranges not constants, but even that is of great value in the parameter estimation as will be discussed further in the following text. 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 this book. Furthermore, the applications of parameters as constants in our models are unrealistic due to the many feedback systems 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 varying parameters according to ecological principles seems a possible solution to the problem, but further development in this direction is absolutely necessary before we can achieve an improved modelling procedure that reflects the processes in real ecosystems. This topic will be further discussed in Chapter 10.

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, which will be treated in more detail in the next section. The verbal model is, however, difficult to visualize so it is translated into a more convenient *conceptual diagram*, which contains the state variables, the forcing functions, and how these components are interrelated by mathematical formulations of processes. The conceptual diagram shows how the previous modelling elements 1 through 3 are related and connected.

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 un-ionized form of ammonia), nitrogen in phytoplankton, nitrogen in zooplankton, nitrogen in fish, nitrogen in sediment, and nitrogen in detritus. The state variables in this conceptual diagram are indicated as boxes connected by processes (indicated as arrows).

The forcing functions are outflows and inflows, concentrations of nitrogen components in the inflows and outflows, solar radiation, and the temperature (not shown in the diagram), which influence all of the process rates. The processes are formulated using quantitative expressions in the mathematical part of the model. Three significant steps in the modelling procedure need to be defined in this section before we go into the modelling procedure in detail. These are verification, calibration, and validation.

1. *Verification* is a test of the *internal logic* of the model. Typical questions in the verification phase include: Does the model behave as expected and intended? Is the model long-term stable, as one should expect in an ecosystem? Does the model follow the law of mass conservation, which is often used as the basis for the differential equations of the model (as discussed in the next section)? Is the use of units consistent? Verification is, to some extent, a subjective assessment of the model behavior and will continue during the model use before the calibration phase.

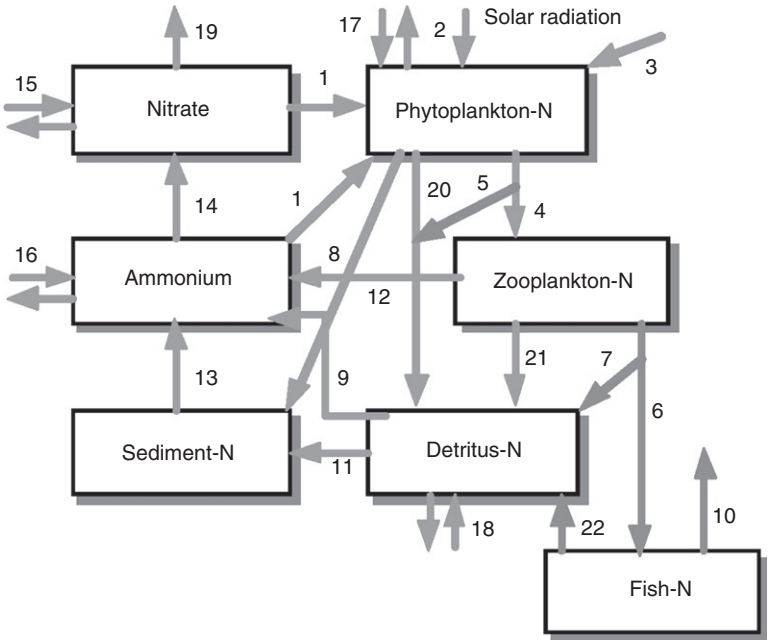

FIGURE 2.1 The conceptual diagram of a nitrogen cycle in an aquatic ecosystem. The processes are (1) uptake of nitrate and ammonium by algae; (2) photosynthesis; (3) nitrogen fixation; (4) grazing with loss of undigested matter; (5), (6), and (7) predation and loss of undigested matter; (8) settling 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; and (20), (21), and (22) mortality of phytoplankton, zooplankton, and fish.

2. *Calibration* is an attempt to find the best agreement between the computed and observed data by variation of some selected parameters. It may be carried out by trial and error or by using software developed to find the parameters that best fit between observed and computed values. In some static and simple models, which contain only a few well-defined or directly measured parameters, calibration may not be required, but it is generally recommended to calibrate the model if observations of a proper quality and quantity are available.
3. *Validation* must be distinguished from verification. Validation consists of an objective test to show how well the model output fits 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 reasonably and accurately

represents the cause-effect relationship of the real system. The model exhibits predictive validity if its predictions of the system behavior reasonably align with observations of the real system. The selection of possible objective tests will be dependent on the purposes 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, then they may be given different weights.

Further detail on these three important steps in modelling will be given in the next section where the entire modelling procedure is presented as well as additional information given in Sections 2.4–2.7.

2.3. The Modelling Procedure

A tentative modelling procedure is presented in this section. The authors have successfully used this procedure numerous times and strongly recommend that all steps of the procedure are used very carefully. To make shortcuts in modelling is not recommended. Other scientists in the field have published other slightly different procedures, but detailed examination reveals that the differences are only minor. The most important steps of modelling are included in all the recommended modelling procedures.

Always, the initial focus of research is the definition of the problem. This is the only way in which the limited research resources can be correctly allocated.

The first modelling step is therefore a *definition of the problem*. This 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.

Systems thinking is important in this phase. You must try to grasp the big picture. The focal system behavior must be interpreted as a product of dynamic processes, preferably described 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 in the first attempt, so there is no need to aim for perfection in one step. The procedure should be considered as an iterative process and the main requirement is to get started (Jeffers, 1978).

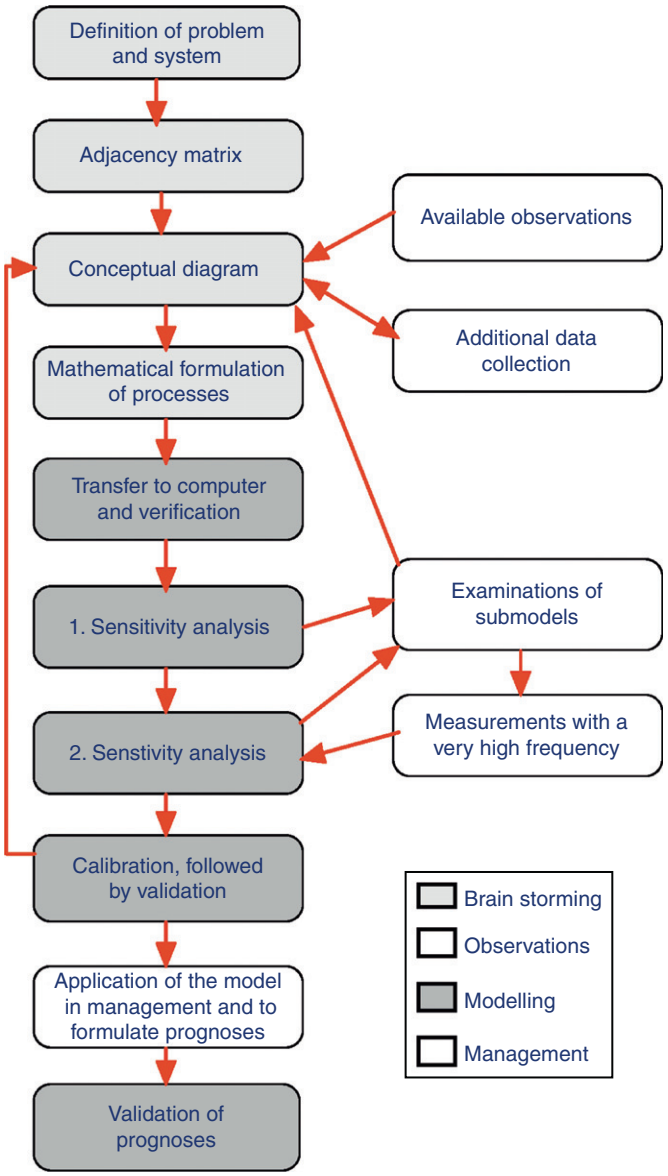

FIGURE 2.2 A tentative modelling procedure is shown. Ideally, as mentioned in the text, one should determine the data collection based on the model, not the other way around. Both possibilities are shown because models in practice have often been developed from available data, supplemented by additional observations. This diagram shows that examinations of submodels and intensive measurements should follow the first sensitivity analysis. Unfortunately, many modellers do not have the resources to do so and instead have bypassed 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. The diagram shows that modelling should be considered an iterative process.

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 behavior of a real system, but this is not necessarily true. Additional factors are involved, but a more complex model has more parameters and increases the level of uncertainty because parameters have to be estimated either by field observations, laboratory experiments, or calibrations, which again are based on field measurements. Parameter estimations are never completely without errors, and the errors are carried through into the model contributing to its uncertainty. The problem of selecting the *right model complexity* will be further discussed in Section 2.8. This is a problem of particular interest for modelling in ecology because ecosystems are very complex, but it does not imply that an ecological model to be used in research or environmental management should be very complex. It depends on the ecosystem and the problem.

A first approach to the data requirement can be made at this stage, but it is most likely to be changed later once experience with the verification, calibration, sensitivity analysis, and validation has been gained. Development of an ecological model should be considered an iterative process.

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 *data quality and quantity*.

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

Adjacency matrix for the model in Figure 2.1

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

In this example, the adjacency matrix is made from the conceptual diagram for illustrative purposes, but in practice it is recommended to set up the adjacency matrix 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, then there should be a link between sediment-N and detritus-N. If the lake is shallow, then 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, which is to get the very first overview of the state variables and their interactions. The adjacency matrix can be considered as a checklist to assess which processes of all the possible linkages actually realized should be included in the model.

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 from Figure 2.1. This diagram will provide 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; that is, to let the conceptual model or even some first more primitive mathematical models determine the data at least within some given economic limitation. 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 application of these methods is limited.

The conceptual diagram in Figure 2.1 indicates the state variables as boxes; for instance, nitrate, and the processes as arrows between boxes. The forcing functions are symbolized by arrows to or from a state variable like 15 and 16. It is possible to use other symbols for the modelling components.

The STELLA software will be used to illustrate the development of models throughout this book. It uses boxes for state variables (compartments), thick arrows with a symbol of a valve for the processes (connections), thick arrows coming or going to a cloud for the forcing functions (which require

a constant, an equation, a table, or a graph), and a thin arrow to indicate the transfer of information or variables (controls such as forcing function, parameter, and/or a state variable calculated by an algebraic expression from another state variable and so on). See Figure 2.3.

There are other symbolic languages for development of conceptual diagrams, for instance, Odum's energy circuit language. It has more symbols than STELLA, so it is more informative but also more time-consuming to develop. For an overview of the most used symbolic languages including Odum's energy circuit language, see Jørgensen and Bendoricchio (2001).

For each state variable, a differential equation is constructed: accumulation = inputs − outputs. For detritus-N in Figure 2.1, the inputs are the processes 20 + 5 +21 + 7 + 22 +18 (in) and the outputs are the processes 11 + 9 + 18 (out). The differential equations are solved analytically in mathematics, but it is rarely possible with most ecological models because they are too complex. The differential equations are therefore solved

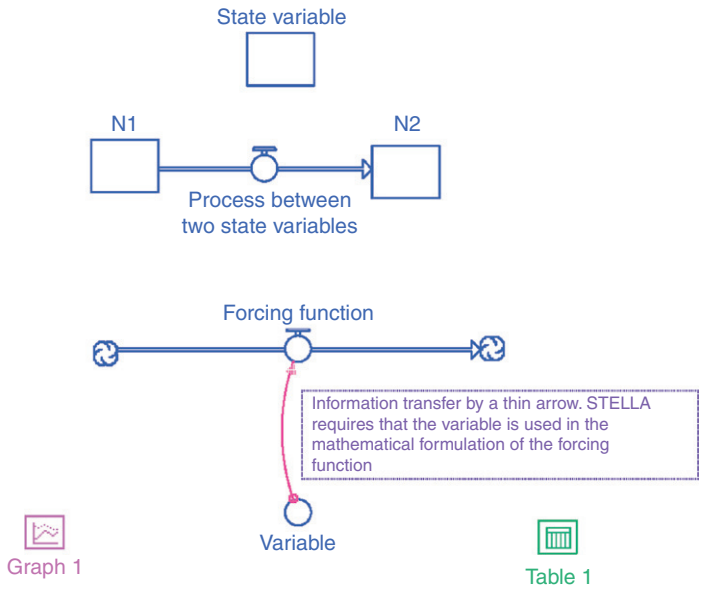

FIGURE 2.3 The symbols applied to erect a conceptual diagram using STELLA. State variables are boxes for which differential equations are erected as accumulation = inputs − outputs. Processes are thick arrows with the valve symbol. Forcing functions are thick arrows starting or ending as a cloud. Circles are variables in general. Graph 1 and Table 1 indicate that the results can be presented as graphs or as tables.

numerically within the computer software. A time step is selected for the model calculations. The shorter the time step, the closer the computer calculations come to the real-time variations of inputs and outputs, but the shorter the time step, the longer the simulation takes to run. It is recommended to test different time steps and use the longest time step that does not significantly change the model results by decreasing the time step further. The term "significant changes" is evaluated relative to the accuracy of the observations used as basis for the development of the model.

The STELLA software develops the differential equations directly from the conceptual diagram, which is input on the main user interface. The time derivative of the state variables will be equal to all the inputs = all process arrows going into the state variables minus all outputs = all process arrows going out from the state variables. The processes must, however, be formulated as an algebraic equation.

The next step is formulating 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. The ecological literature contains mathematical formulations of most ecological processes, but a short overview of the most applied mathematical equations is presented here. More than 95% of all ecologically relevant processes can be formulated mathematically by one of the following six equations:

1. A constant flow rate, also denoted zero order expression:

$$\frac{dC}{dt} = k_1 \tag{2.1}$$

2. A first-order rate expression, where the rate is proportional to a variable such as a concentration of a state variable:

$$\frac{dC}{dt} = k_1 C \tag{2.2a}$$

This expression corresponds to exponential growth and the following solution can be obtained by integration:

$$C(t) = C_0 e^{k_1 t} \tag{2.2b}$$

This is often used to for modelling population growth (see Chapter 5). Decomposition processes and radioactive decay can also be approximated as first order reactions, in which the rate is negative.

3. A second-order rate expression occurs when the rate is proportional to two state variables simultaneously, for instance:

$$\frac{dC_1}{dt} = k_2 C_1 C_2 \tag{2.3}$$

4. This is a first-order rate expression with a regulation due to environmental constraints, for instance, space or resources.

$$\frac{dC}{dt} = k_4 C\left(1 - \frac{C}{K}\right) \tag{2.4}$$

where K is the carrying capacity. When the concentration reaches the carrying capacity the factor becomes zero and the growth stops. This process rate expression is denoted logistic growth and it is illustrated in more detail in Chapter 5. These two growth expressions are both extensively applied in population dynamic models.

5. A Michaelis-Menten expression or Monod kinetics known from enzymatic processes in biochemistry is given by:

$$\frac{dC}{dt} = \frac{k_3 C}{(C + k_m)} \tag{2.5}$$

Where k_3 is the maximum reaction rate and k_m is the Michaelis constant. At small concentrations of the substrate, this process rate is proportional to the substrate concentration, while the process rate is at maximum and constant at high substrate concentrations where the enzymes are fully utilized. The same expression is used when the growth rate of plants is determined by a limiting nutrient according to Liebig's minimum law. The Michaelis-Menten's constant, k_m, or the half saturation constant, corresponds to the concentration that gives half the maximum rate. At small concentrations of substrate or nutrients, the rate is very close to a first-order rate expression, whereas it is close to a zero order rate expression at high concentrations. Notice, that the rate is regulated from a first-order to a zero order expression more and more as the concentration increases.

6. A rate governed by diffusion often uses a concentration gradient to determine the rate as it is expressed in Fick's First Law:

$$\frac{dC}{dt} = k_5 \frac{dC}{dx} \tag{2.6}$$

There are several modifications of these six expressions. For instance, a threshold concentration tr, is often used in the Michaelis-Menten expression. The concentration (state variable) is replaced by the concentration –tr. The concentration therefore has to exceed tr to generate any rate. For grazing and predation processes, the Michaelis-Menten's expression is often multiplied by (1 − concentration/carrying capacity) similar to what is used in the logistic growth expression. It implies that when food is abundant (concentration is high) another factor determines and limits the growth such as space or nesting area. These modifications will be used in Chapter 7 for development of a eutrophication model.

Once the system of mathematical equations is available, model *verification* can be carried out. As pointed out in Section 2.2, this is an important step, which unfortunately is omitted by some modellers. The next section presents the details of this modelling step.

2.4. Verification

The next step of the modelling procedure includes verification, which is a test of the internal model logic. Crucial questions about the model are asked and answered by the modeller. Verification is to some extent a subjective assessment of the behavior of the model.

Findeisen et al. (1978) gave 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 a rigid step-by-step procedure, but rather as an iterative operation, which must be repeated a few times. The model is first given realistic parameters from the literature, then it is calibrated coarsely, and finally 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 be satisfactory.

It is recommended at this step that answers to the following questions are provided:

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 state variable values remain 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 also can be recommended for finding the initial values if they are not measured or known by other means. This question presumes that real ecosystems are long-term stable, which is not necessarily the case.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, show a certain pattern in their fluctuations. The simulation period should be long enough to allow the model to demonstrate any possible instability.
2. **Does the model react as expected?** For example, if the input of toxic substances is increased, then we should expect a higher concentration of the toxic substance in the top carnivores. If this is not so, then it shows that some formulations may be wrong and these should be corrected. This question assumes that we actually know at least some behavior of the ecosystem, which is not always the case. In general, playing with the model is recommended at this phase. Through such exercises the modeller gets acquainted with the model and its reactions to perturbations. Models should generally be considered 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 model's behavior. If the modeller is satisfied with the accordance between model and observations, then the model is accepted as a useful description of the real ecosystem — at least within the framework of the observations. This part of the verification is based upon more subjective criteria. Typically, the model builder formulates several questions about the model behavior and tests the model response by provoking changes in forcing functions or initial conditions. If the responses are not as expected, then the model structure or equations will have to be changed, 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 sunrise when photosynthesis is included in the model? Will decreased predator concentration in a prey-predator model imply increased prey concentration? Will increased nutrient loadings in a eutrophication model give increased concentration of phytoplankton? Numerous other questions can be asked.

3. **It is also recommended to check all the units 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? Are the parameters used in the model consistent for the type of equations used and do the units match with the available data?
4. **Investigate the statistical properties of the noise in the model.** To conform to 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. If the error sequences do not conform to their desired properties, then this suggests that the model does not adequately characterize all of the more deterministic features of the observed dynamic behavior. Consequently, the model structure should be modified to accommodate additional relationships. To summarize this part of the verification the errors:

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

   Results of this kind of analysis are illustrated in detail in Beck (1987). Notice that this analysis requires good estimates of standard deviations in sampling and analysis (observations).

Notice finally that during verification it is possible to perform multiple scenario analyses or "Gedanken Experiments." For example, we can test a eutrophication model by its response to the following test. We rent a helicopter and buy 100,000 kg of phosphorus fertilizer and drop it instantly to the lake. The experiment could be made at no cost using the model, while it would be very expensive to rent a helicopter and buy 100,000 kg of fertilizer. A major advantage of models is how easy it is to assess the system behavior under a wide array of scenarios.

Model verification may seem very cumbersome, but it is a very necessary step for the model development process. Through the verification one learns the model through its behavior, and the verification becomes an important checkpoint in the construction of a workable model. This also emphasizes the importance of good ecological knowledge of 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 the experience shows that what might seem to be a shortcut will lead to an unreliable model, which at a later stage might require more time to compensate for the lack of verification. It must therefore be strongly recommended to invest enough time in the verification and to plan for the necessary allocation of resources in this important phase of the modelling procedure.

2.5. Sensitivity Analysis

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 parameters, 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 carnivorous insects as a result of the use of insecticides, then one will choose this state variable as the most important one for a sensitivity analysis along with 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:

$$S = [\partial x/x]/[\partial P/P] \tag{2.7}$$

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 the modeller estimates the uncertainty to be about 50%, then a change in the parameters at $\pm 10\%$ and $\pm 50\%$ is chosen and the corresponding change in the state variable(s) recorded. 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 behavior and low-leverage variables, whose values have minimal impact on the system. Obviously, the modeller must concentrate the effort on improvements of the parameters and the submodels associated with the high-leverage variables. The result of a sensitivity analysis of a eutrophication model with 18 state variables, presented in Chapter 7, is shown in Table 2.1. The sensitivity of the examined parameters by a 10% increase to phytoplankton, s-phyt; to zooplankton, s-zoo; to soluble nitrogen, s-nit; and to soluble phosphorus, s-phos, is shown. These results clearly indicate that the parameters "maximum growth rate of phytoplankton and zooplankton," "mortality of zooplankton," and the "settling rate of

Table 2.1 Results of a $\pm 10\%$ Sensitivity Analysis of the 18 State Variable Model in Chapter 7

Parameter	s-phyt	s-zoo	s-nit	s-phos
Maximum growth rate of phytoplankton	0.488	0.620	-0.356	-0.392
Maximum growth rate of zooplankton	-2.088	-4.002	2.749	4.052
Denitrification rate	-0.19	-0.010	-0.579	0.013
Fish concentration	0.008	0.012	-0.011	-0.014
Rate of mineralization	0.003	0.010	0.038	0.001
Mortality zooplankton	2.063	1.949	-3.479	-3.350
Settling rate	-1.042	-0.0823	0.321	0.388

phytoplankton," are very important parameters to determine accurately because they all have a sensitivity to the most important state variable, the phytoplankton, which is more than 0.5 or 50%, meaning that a change of the parameters by 10% would make a change *of the phytoplankton concentration of more than 50%.* On the other hand**,** the parameters "maximum denitrification rate," the "mortality of fish," and the "rate of mineralization" are significantly less important parameters. They all have a sensitivity of less than 0.1 or 10%. Therefore, they would change the phytoplankton less than 1% if the parameters are changed 10%.

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 changes. Relatively large changes are applied at this stage.
2. The most sensitive parameters are determined more accurately either by a calibration or by other means (see Section 2.9).
3. Under all circumstances, great efforts are made to obtain a relatively well calibrated model.
4. A second sensitivity analysis is then carried out using more narrow 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 on the most sensitive parameters.

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. For example, if the sensitivity shows that it is crucial for the model results to use a more detailed submodel, then this result should be used to change the model correspondingly.

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

It can generally be stated that those submodels, which contain sensitive parameters, are also submodels that are sensitive to the important state variable. 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 intuition, but it is also possible to show that they are correct by analytical methods.

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

2.6. Calibration

The goal of *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. To cover all possible parameters for all possible ecological models including ecotoxicological models, we need to know more than one billion parameters. Therefore, 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 previously mentioned. 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 by 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). Parameter estimation methods must be used when no literature value can be found, particularly ecotoxicological models. See, Jørgensen (1991, 1992a) and Chapter 8. In addition, we must accept that unlike many

physical parameters, ecological ones are not constant but change in time or situation (Jørgensen, 1986, 1992b, 2002). This point will be discussed further in Chapter 10.

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 slightly different values for the parameters from the real, but unknown, values in nature, but the difference may partly account for the influence from the omitted details.
3. Most models in environmental sciences and ecology are "lumped models," which means 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. This will be discussed in more detail in Chapter 10.

A calibration cannot be carried out randomly if more than a couple of parameters have been selected for calibration. If, for instance, 10 parameters have to be calibrated and the uncertainties justify the testing of 10 values for each parameter, the model has to be run 10^{10} times, which is an impossible task. Therefore, the modeller must learn the behavior 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 earlier is redundant. If the automatic calibration should give satisfactory results within a certain frame of time, then it is necessary to calibrate only 6–9 parameters simultaneously. In any circumstances, the narrower

the ranges of the parameters before the calibration gets started, the easier it is to find the optimum parameter set.

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. The model must be calibrated step-by-step to achieve these objectives step-by-step.

If an automatic calibration procedure is applied, then 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:

$$Y = [(\Sigma((X_c - X_m)^2/X_{m,a})/n]^{1/2} \tag{2.8}$$

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 computed during an automatic calibration with the goal to obtain the lowest Y value possible.

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

If it is impossible to calibrate a model properly, then it is not necessarily due to an incorrect model. Instead, it may be due to the poor data quality, which is crucial for calibration. It is also of great importance that the *observations reflect the system dynamics*. If the objective of the model is to give a good description of one or a few state variables, then it is essential that the data 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. This rule has unfortunately 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) showed 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 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 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, then the *estimation methods* mentioned later in this Section 2.9 and in Chapter 8 may be used. For some crucial parameters it may be recommended 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. The estimation methods and the determination of the parameters by experiments should focus mainly on the most sensitive parameters.
4. An *intensive data collection program* for the most important state variables should be used to provide a better estimation for the most crucial parameters. For further details see Section 2.9.
5. First, at this stage, the *calibration* should 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 to get acquainted with the model

reaction to changes in the parameters. An automatic calibration procedure is used subsequently to polish the parameter estimation.

6. These results are used in a *second sensitivity analysis*, which may give results different from the first sensitivity analysis.
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 previous calibration methods may be used. In some cases, the modeller would repeat steps 6 and 7 one time more and make a third calibration. After this final calibration the model can be considered calibrated and we can go to the next step — validation.

2.7. Validation and Assessment of the Model Uncertainty

The calibration should *always* be followed by a *validation***.** During this step the modeller tests the model against an *independent* data set to observe how well the model simulations fit these data. It may be possible, even in a data-rich situation, to force a wrong model by the parameter selection to give outputs that fit well with the data. It must, however, be emphasized that the validation only confirms the model behavior 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 eutrophication model is tested, it should preferably have data sets for the calibration and the validation that differ by the level of eutrophication. This is often impossible or at least very difficult as it may correspond to a complete validation of the model predictions, which at best 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 modelled ecosystem. 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 considered toxic substances, and a population model by different levels of the populations, and so forth.

If an ideal validation cannot be obtained, then it is still important to validate the model as best as possible. The method of validation is dependent on the model objectives. A comparison between measured and computed data using an objective function Eq. (2) is an obvious test. This is, however, often not sufficient, 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 for the model and the modeller. For instance, if we are concerned with the eutrophication in an aquatic ecosystem, it would be useful to compare the measured and computed maximum concentrations of phytoplankton. The validation discussion can be summarized by the following issues:

1. Validation is always required to get a picture of the model reliability.
2. Attempts should be made to get data for the validation that 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 model objectives.
3. The validation criteria are formulated based on the model objectives 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.

Validation is a very important modelling step because it gives the uncertainty of the model results. It attempts to answer the question: Which model uncertainty should we consider when using the model to develop strategies for environmental management? If we use the model as research tool, then the validation will tell us whether the model results can be used to support or reject a hypothesis. The uncertainty determined by the validation relative to the difference between the hypothesis and the model results will be decisive. In Chapter 7, a eutrophication model with 18 state variables will be applied as a case

study to demonstrate how the validation results can be used to assess the expected uncertainty of the prognoses developed by the model.

The validation result can also be used to consider the model revisions that would be needed to reduce the uncertainty. In our effort to improve the model, we should ask the following pertinent questions:

1. What is the uncertainty of the observations (measurements)? If the uncertainty of the model is not very different from the uncertainty of the observations, then it will probably be beneficial to get more reliable observations with less uncertainty.
2. Do the observations represent the system dynamics? If not, then more frequent monitoring should be considered for some period to capture the system dynamics. See the discussion of this question in Section 2.9.
3. Are some important processes or components missing or described wrongly in the model? In this context, as previously mentioned, it is important to set up a mass and/or energy balance to reveal the most important processes and sources.

It is recommended to give a sufficiently comprehensive answer to question 3 and eventually use the model experimentally to find the best answer. It is quite easy in most cases to replace important equations by other expressions or add new components or processes and so on. Such experiments are very elucidating for the importance of formulations and inclusion of processes. Small changes in process equations that make big changes in the model results uncover the soft points of the model and may inspire additional experiments or observations in situ or in the laboratory, and eventually to further changes of the model.

It should be emphasized that the "ideal" model can never be achieved, but step-by-step by steadily questioning the model and using these three points again and again, we can improve the model quality moving asymptotically toward the ideal model. An ideal model is, however, not necessary to have a useful and powerful tool in environmental management and ecosystem research. A satisfactory calibration and validation with sufficiently low uncertainties to allow application in a defined context would be the general requirement for the pragmatic modeller.

2.8. Model Classes

It is useful to distinguish between various model classes and briefly discuss the selection of model classes.

Pairs of models are shown in Table 2.2. The first division of models is based on the application *scientific and management models*. This initial

Table 2.2 Classification of Models (Pairs of Model Types)

Type of Models	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	Uses matrices in the mathematical formulation
Reductionistic models	Include as many relevant details as possible
Holistic models	Uses 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
Nonlinear models	One or more of the equations are not first degree
Causal models	The inputs, states, and the outputs are interrelated by using causal relations
Black-box models	The input disturbances effect 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)

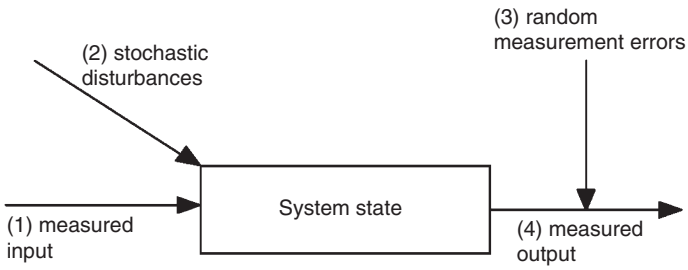

FIGURE 2.4 A stochastic model considers (1), (2), and (3), while a deterministic model assumes that (2) and (3) are zero.

distinction guides the objectives of the model development toward either research or application orientation and influences the choice of which processes and state variables to emphasize.

The next pair is *stochastic and deterministic models*. A stochastic model contains stochastic input disturbances and random measurement errors, as shown in Figure 2.4. If they are both assumed to be zero, then the stochastic model will reduce to a deterministic model provided 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 knowledge of the present state and future measured inputs. Stochastic models are not frequently applied in ecology.

The third pair in Table 2.2 is *compartment and matrix models*. Some modellers refer to compartment models as models based on the use of compartments in the conceptual diagram, while other modellers distinguish between the two model classes entirely by the mathematical formulation as indicated in Table 2.2. Both model types are applied in ecological modelling, although the use of compartment models is far more pronounced.

The classification of *reductionistic and holistic models* is based upon 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 behavior, believing that the properties of the system are the sum of the details. A holistic modeller will abstract some detail to capture broader scale patterns. The bridge between these bottom-up and top-down approaches is spanned by the use of hierarchical models that include lower level micro-scale interactions constrained by higher level macro-scale processes.

Most problems in environmental sciences and ecology may be described by dynamic models, which use 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 around the steady state are described by use of a dynamic model, while the steady state can be described by use of a static model (see Figure 2.5), which can be reduced to algebraic equations.

Some dynamic systems have no steady state; for instance, systems that show limit cycles. This situation obviously requires a dynamic model to describe the system behavior. In this case, the system is always nonlinear, although there are nonlinear systems that have steady states.

A static model assumes, consequently, that all variables and parameters are time independent. 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 by seasonal and diurnal variations may be utilized by the state variables to obtain higher average values.

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

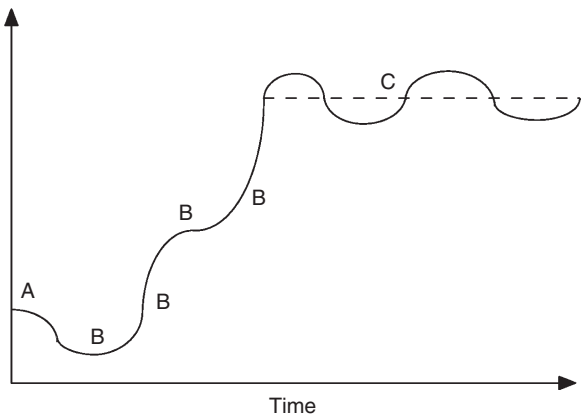

FIGURE 2.5 Y is a state variable expressed as a function of time. A is the initial state and B the transient states. C oscillates around a steady state. The dotted line corresponds to the steady state that can be described by a static model. The transient state requires the use of a dynamic model.

variations in the three orthogonal directions. 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 behavior. The black-box model deals only with what is measurable at the boundary: the input and the output. The relationship may be found by a statistical analysis. If, on the other hand, the processes are described by model equations that represent the relationships, then the model will be causal.

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

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

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

$$dy/dt = a^{*}y^{b} + c^{*}y^{d} + e \tag{2.9}$$

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

$$dy/dt = a^{*}y^{b} + c^{*}y^{d} + e + g(t) \tag{2.10}$$

The pairs in Table 2.2 may be used to define the type of model that is most applicable to solve a given problem. It will be further discussed

Table 2.3 Model Identification

Model Types	Organization	Pattern	Measurements
Biodemographic	Conservation of genetic information	Life cycles of species	Number of species or individual
Bioenergetic	Conservation of energy	Energy flow	Energy
Biogeochemical	Conservation of mass	Element cycles	Mass of concentrations

in the next section, where a practical model classification will also be presented.

Table 2.3 shows another way to classify models. The differences among the three model types are the choice of components used as state variables. If the model describes a number of individuals, species, or classes of species, then it is called *biodemographic*. A model that describes the energy flows is *bioenergetic* and the state variables will typically be expressed in kJ or kJ per unit of volume or area. *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.

The problem, the ecosystem characteristics, and the available database should be reflected in the choice of model class. The two model classifications presented earlier 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 5, Section 5.4.

If the model is developed on the basis of a database that has limited quality and/or quantity, then the model should have relatively low complexity. A dynamic model is generally more demanding to calibrate and validate than a static model. Therefore, the latter type would often be selected in a data-poor situation, provided 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 (estimate) one (otherwise unknown) parameter. Chapter 6 shows how a steady-state model can be developed and used to get a

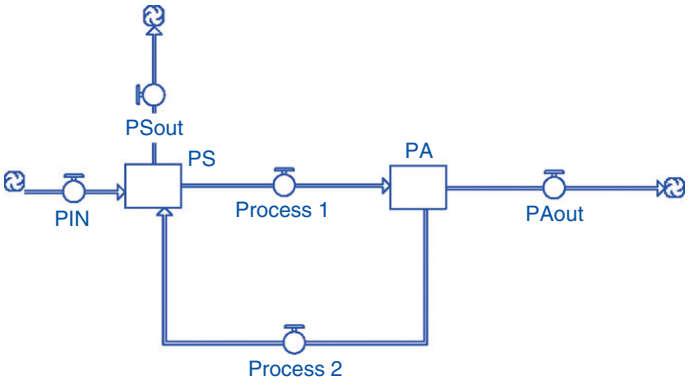

FIGURE 2.6 A conceptual diagram of a simple model with two state variables, PS and PA, is shown. PIN is a forcing function. (1) and (2) are processes.

good overview of an ecological situation, even in a relatively data-poor situation.

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 Figure 2.6, the following differential equations are valid:

$$\mathrm{dPS/dt} = \mathrm{PIN} + \mathrm{Process(2)} - \mathrm{Process(1)} - \mathrm{PS} * \mathrm{Q/V} \tag{2.11}$$

$$\mathrm{dPA/dt} = \mathrm{Process(1)} - \mathrm{PA} * \mathrm{Q/V} \tag{2.12}$$

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) 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, where k and k′ are two parameters.

The corresponding steady-state model gives us two equations:

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

that 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 apply differential equations because the time variations are important.

It is known that ecosystems are adaptable. Over time, species can change their properties to meet changing conditions (i.e., change of forcing functions or disturbances). If the changes are major, then 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 nonstationary, time-varying differential equations. They are often called structurally dynamic models (SDMs; see Jørgensen, 1986, 1997, 2002), because they are able to predict the changes in properties of the biological components. Chapter 10 covers this model type and its application. Structurally dynamic models are distributed models, because the parameters are considered functions of time and space. While distributed models in most cases are 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 simulate change in the structure (shifts in parameter values). 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 adaptation. Therefore, models without dynamic structure often give unreliable results, particularly if the forcing functions are significantly changed.

In Chapter 3, an overview of the model types that are available for the development of ecological models is presented. The choice of model type for development in a particular situation depends on the different mathematical methods, different goals, and different applications and may also use different types of databases. While the model classes are characterized by a difference in one property only (e.g., steady state vs. dynamic state and mass flows vs. energy flows), the different model types are significantly different. They have been developed to solve some fundamental modelling problems in ecology during the last couple of decades, including: (1) How do we account for the individuality of organisms? (2) How do we account for adaptation and shifts in species composition? (3) What model approach is best when our data set is uncertain (i.e., fuzzy)? (4) How can we make an effective model from a very heterogeneous database? (5) How can we improve model parameter estimation? We have solved these problems by development of several different model types that have expanded the range and application of ecological models in many different directions.

2.9. Selection of Model Complexity and Structure

The literature of environmental modelling contains several methods that are applicable to the selection of model complexity. References can be given to the following papers devoted to this question: Halfon (1983, 1984, 1986), Halfon, Unbehauen, and Schmid (1979), Costanza and Sklar (1985), Bosserman (1980, 1982) and Jørgensen and Mejer (1977).

It is clear from the previous discussions in this chapter that selection of the model complexity is a matter of balance. On one hand, it is necessary to include the state variables and the processes essential for the problem in focus. On the other hand, it is important not to make the model more complex than appropriate for the available data set. As Einstein once quipped, "A scientific theory should be as simple as possible, but no simpler." The same applies to models. Our knowledge of processes and state variables together with our data set determine the selection of model complexity. If our knowledge is poor, then the model will include few details and will have a relatively high uncertainty. If we have a profound knowledge of the problem we want to model, then 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 a model can always assist the researcher by synthesizing the present knowledge and by visualizing the system. But the researcher must always present the shortcomings and the uncertainties of the model and not try to pretend that the model is a complete and detailed picture of reality. A model will often be a fruitful instrument to test hypotheses in the hands of the researcher, 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 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 will never be able to develop a model capable of accounting for the complete input-output behavior of a real ecosystem and valid for all frames

(Zeigler, 1976). This ideal 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 to observe 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.

According to this discussion, a model may be made more realistic by adding more connections. Additions of new parameters up to a point do not contribute further to improve the simulation; on the contrary, more parameters imply more uncertainty because of the possible lack of information about the flows the parameters can 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; it only adds to unaccountable uncertainty. These ideas are visualized in Figure 2.7. 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

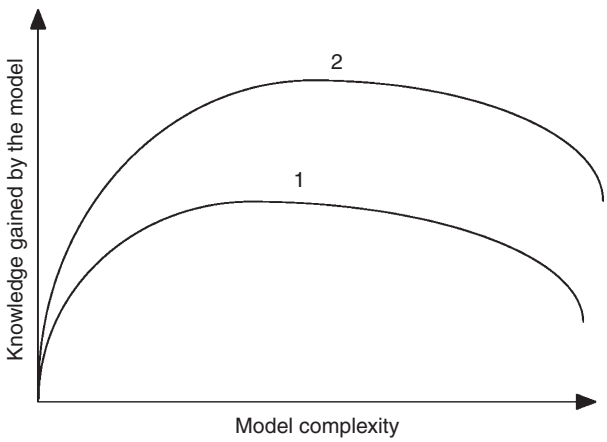

FIGURE 2.7 Knowledge plotted versus model complexity measured by the number of state variables. The knowledge increases up to a certain level. Increased complexity beyond this level will not add to the knowledge gained about the modelled system. At a certain level, the knowledge might even be decreased 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.)*

relation to this figure: How can we select the optimum model complexity and structure for the given understanding for the question at hand?

We will discuss in the following section the methods available to select a good model structure. If a rather complex model is developed, then the use of one of the methods presented in the previous references is recommended, but for simpler models it is often sufficient to select a model of balanced complexity, as discussed earlier.

Costanza and Sklar (1985) have examined 88 different models, and showed that more theoretical discussion behind Figure 2.7 is valid in practice. Their results are summarized in Figure 2.8, where effectiveness is plotted versus articulation (= expression for model complexity). Effectiveness is understood as a product of model results and confidence (i.e., 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 effectiveness are relative. Some other authors may have applied other measures, but it is

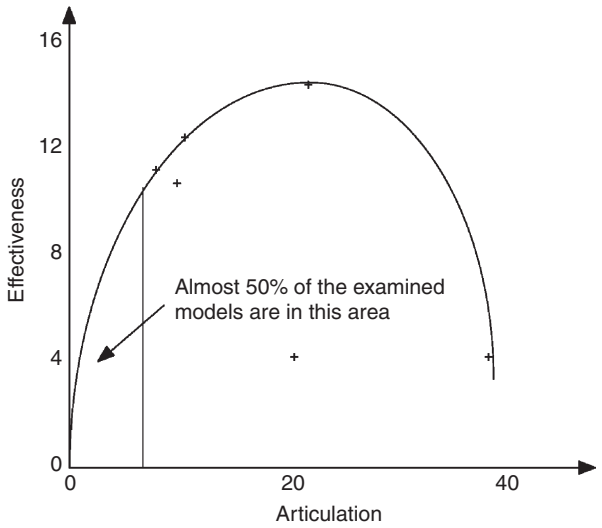

FIGURE 2.8 Plot of articulation index versus effectiveness = articulation*certainty for the 88 models reviewed by Costanza and Sklar (1985). As almost 50% of the models were not validated, they had an effectiveness of 0. These models are not included in the figure, but are represented by the line effectiveness = 0. Notice that nearly 50% of the models have a relatively low effectiveness due to too little articulation, and that only one model had an articulation that was too high, which implies that the uncertainty by drawing the effectiveness frontier as shown in the figure is high at articulations above 25. *(This figure is partly reproduced from Costanza and Sklar, 1985.)*

clearly seen by comparison of Figures 2.7 and 2.8 that they show the same type of relationship.

Selection of the right complexity is of great importance in environmental and ecological models as already stated. The methods presented and discussed in the following section provide an objective procedure to select the correct level of model complexity. However, the model selection always requires that the application of these methods is 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? 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 that the model will always be an extreme simplification of nature. This implies that we cannot make a model of an ecosystem, but we can develop a model of some aspects of that ecosystem.

A parallel to the application of geographical maps (see Section 1.1) can be made again: We cannot make a map (model) of a state with all its details, instead we show some geographic aspects on a certain scale. Therein lays our limitations, which are due to the immense complexity of nature. We have to accept these limitations since we cannot produce a complete model or get a total picture of a natural system. Some kind of map is always more useful than no map, so some kind of model of an ecosystem is better than no model at all. As the map quality improves due to better techniques and knowledge, so does the model of an ecosystem as we gain more experience in modelling and improve our ecological knowledge. We do not need a complete set of details to get a proper overview and a holistic picture; we need some details and we need to understand how the system works on the system level.

Therefore, the conclusion is that although we can never know all of the details needed to make a complete model, we can produce good workable models that expand our knowledge of ecosystems, particularly of their properties as systems. This is completely consistent with Ulanowicz (1979) who 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 that indicates the general trends and take into account the probabilistic nature of the environment.

Furthermore, it seems possible in most situations to apply models as a management tool (Jørgensen et al., 1995). Models should be considered as tools — tools to overview complex systems, and tools to obtain a picture of the systems properties on the system level. Already, a few interactive state variables make it impossible to overview how the system reacts to perturbations or other changes. There are only two possibilities to get around this dilemma: Either limit the number of state variables in the model, or describe the system by use of holistic methods and models, preferably by using higher level scientific laws. See also the discussion about holistic and reductionistic approaches in Sections 2.3 and 2.5. The trade-off for the modeller is between knowing a lot about a little or a little about a lot.

Through a good knowledge of the system, it is possible to set up mass or energy flow diagrams. This might be considered a conceptual model of its own, but the idea is to use the diagram to recognize the most important flows for the model in question. Let us use an energy flow diagram for Silver Springs (Figure 2.9). If the goal of the model is to predict the net primary production for various conditions of temperature and input

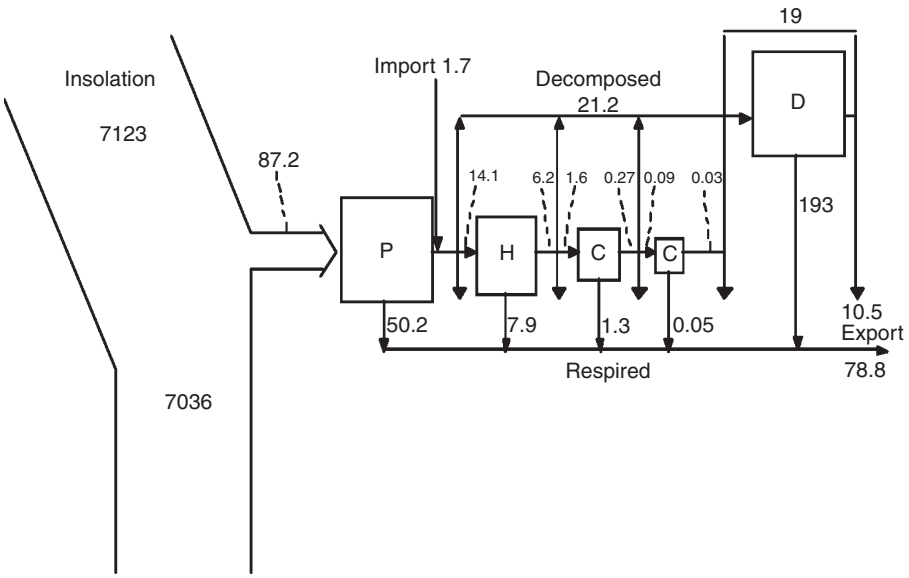

FIGURE 2.9 Energy flow diagram for Silver Springs, Florida. Figures in cal/m^2/year. *(Adapted from H. T. Odum, 1957.)*

of fertilizers, then it is 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 excluded.

As energy flows are different from ecosystem to ecosystem, the selected model should also be different. A general model for one type of ecosystem, for example, a lake, does not exist; on the contrary, it is necessary to adopt the model to the characteristic features of the ecosystem. Figures 2.10 and 2.11 show the phosphorus 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 also different

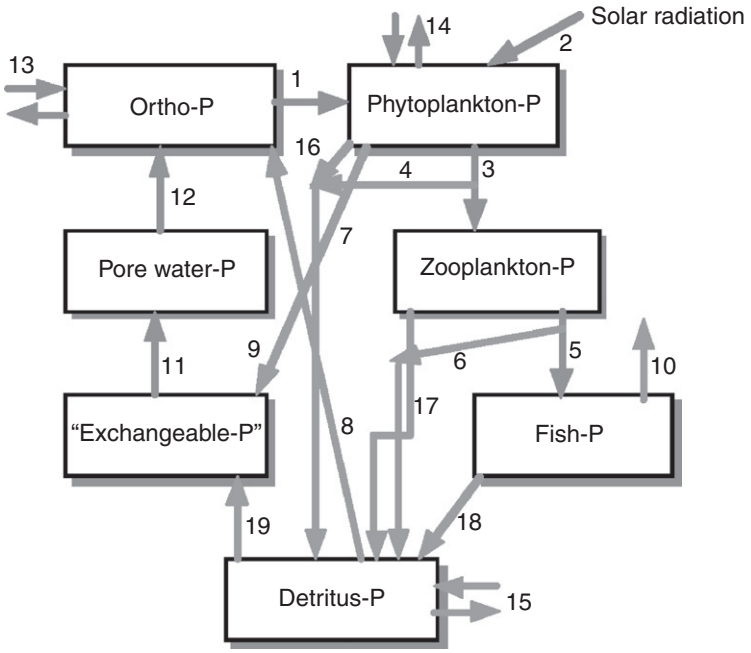

FIGURE 2.10 The phosphorus cycle in an aquatic ecosystem. The processes are (1) uptake of phosphorus by algae; (2) photosynthesis; (3) grazing with loss of undigested matter; (4), (5) predation with loss of undigested material; (6), (7), and (9) settling of phytoplankton; (8) mineralization; (10) fishery; (11) mineralization of phosphorous organic compounds in the sediment; (12) diffusion of pore water P; (13), (14), and (15) inputs/outputs; (16), (17), and (18) represent mortalities; and (19) is settling of detritus.

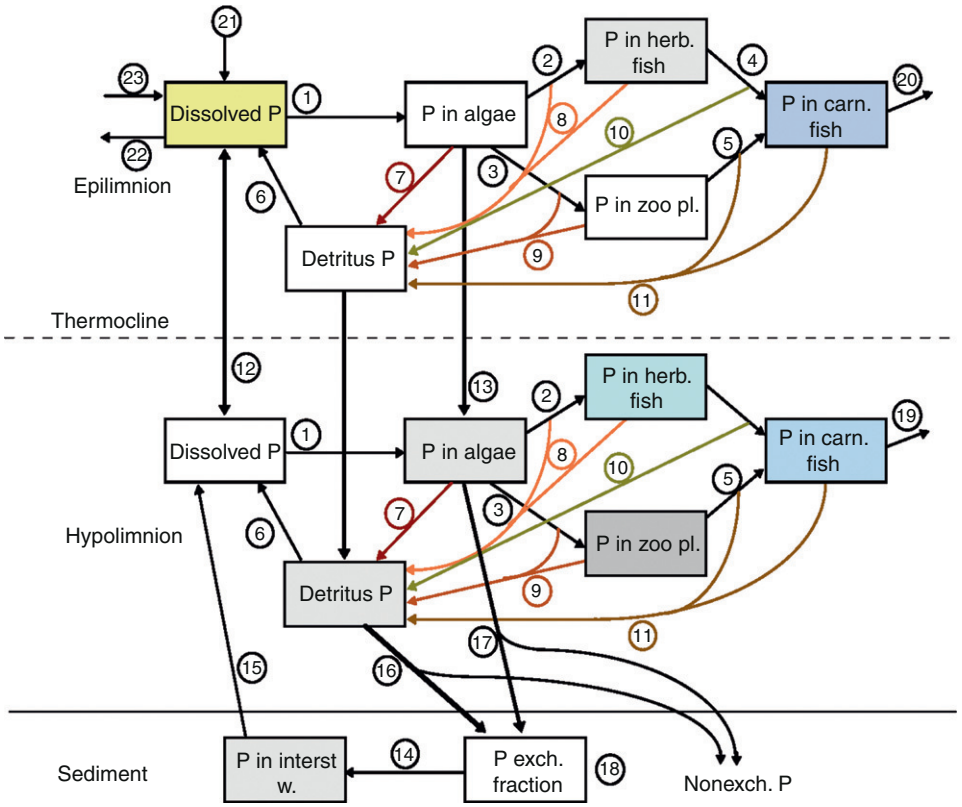

FIGURE 2.11 Eutrophication model of an aquatic ecosystem illustrated by use of P-cycling. Arrows indicate processes. A thermocline is considered. Explanation of numbers are as follows: (1) uptake of phosphorus by algae; (2) grazing by herbivorous fish; (3) grazing by zooplankton; (4), (5) predation on fish and zooplankton, respectively, by carnivorous fish; (6) mineralization; (7) mortality of algae; (8), (9), (10), (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; settling of detritus (16) and algae (17) (hypolimnion-sediment, a part goes to the non-exchangeable fraction); (18) mineralization of P in exchangeable fraction; (19), (20) fishery; (21) precipitation; (22) outflows; and (23) inflows (tributaries).

in the two lakes: 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 wind play an important role. In Lake Balaton, the wind stirs up the sediment, which

consists almost entirely of calcium compounds with 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 are significant. Therefore, an adequate description of the sediment stirring, the adsorption of phosphorous compounds on the suspended matter, and sedimentation must be included in a eutrophication model for this lake.

Jørgensen and Mejer (1977, 1979) examined the inverse sensitivity, called the ecological buffer capacity, to select the number of state variables. The concept of ecological buffer capacity is illustrated in Figure 2.12 and is defined as:

$$\beta = \frac{1}{(\partial(\mathrm{St})/\partial \mathrm{F})} \tag{2.13}$$

where St is a state variable and F a forcing function. It is possible to define many different buffer capacities corresponding to all possible combinations of state variables and forcing functions. However, the model scope will often point out which buffer capacity should be in focus. For a eutrophication model, the most sensitive factor 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.

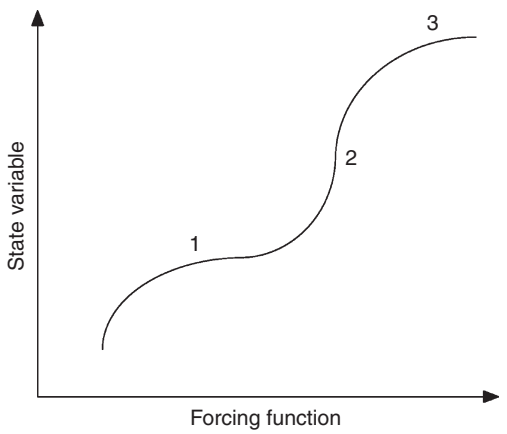

FIGURE 2.12 A relation between a state variable and a forcing function is shown. At points 1 and 3 the buffer capacity is high; at point 2 it is low.

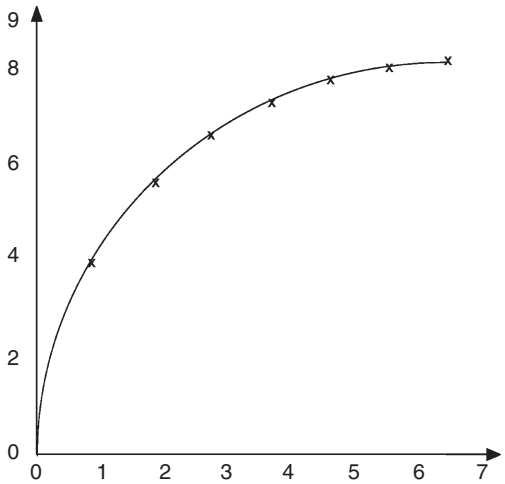

FIGURE 2.13 Illustrates the buffer capacity for a eutrophication model of a shallow Danish lake. In this case, a model with six state variables for each of the important nutrients (C, P, and N) was selected. Adding a seventh state variable representing an additional zooplankton species and an additional phytoplankton species produced only minor changes to the buffer capacity. Other possibilities could also have been tested. In this context it must be pointed out that the buffer capacity does not necessarily increase with the number of state variables as in Figure 2.12. The change in buffer capacity only decreases with the number of state variables when their sequence is selected according to decreasing importance.

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, adding to the uncertainty without contributing to a more accurate model.

Figure 2.13 illustrates 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 — carbon, nitrogen, and phosphorus — was selected. Inclusion of a seventh state variable created only a minor change to the buffer capacity.

Flather (1992, 1996) recommended using Akaike's Information Criterion (AIC), to select a best model from the *a priori* best candidate models:

$$\mathrm{AIC} = \mathrm{n}\log(\mathrm{RSS}/\mathrm{n})^2 + 2\mathrm{K}, \tag{2.14}$$

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. The application of this equation is recommended to select submodels. This equation can also be applied in principle to large models, but not in practice where a comparison of several large models would be too time-consuming.

For other applicable methods used to select the model complexity, see Halfon (1983) and Bosserman (1980, 1982) where the use of the connectivity is presented. Experience shows some model corrections at a later stage will be unnecessary if the model has been calibrated and the validation phase indicates that improvements might be needed. This does not, however, imply 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 at the first instance. The methods presented earlier assist the modeller to exclude some unworkable models, but not necessarily to choose the very best model. Remember, there is no one right model.

2.10. Parameter Estimation

Many parameters in causal ecological models can be found in the literature, not necessarily as constants but as approximate values or

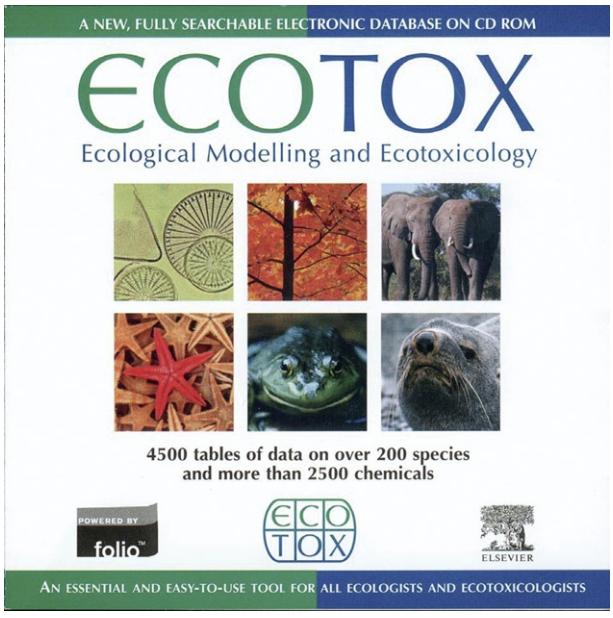

FIGURE 2.14 Jørgensen et al., (2000) contains about 120,000 parameters of interest for ecological modellers.

intervals. Jørgensen et al. (2000) contains about 120,000 parameters of interest for ecological modellers (see Figure 2.14).

However, even if all parameters are known in a model from the literature, calibrating the model is usually required because the biological parameters are only known within ranges. Several sets of parameters are tested by 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.

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 lake dynamics. If it is the scope of the model to predict maximum values and related data for phytoplankton concentrations and primary production, then it is necessary to have a sampling frequency that gives an estimate of the maximum value in phytoplankton concentration and the primary production.

Figure. 2.15 shows characteristic algae concentrations plotted versus time (April 1–May 15) in a hypertrophic lake with a sampling frequency of (1) twice per month and (2) three times per week (denoted as the "intensive" measuring program). The two plots are significantly different and an attempt to get a realistic calibration based on (1) will fail, provided it is the aim to model the day-to-day variation in phytoplankton concentration according to (2). This example illustrates that it is

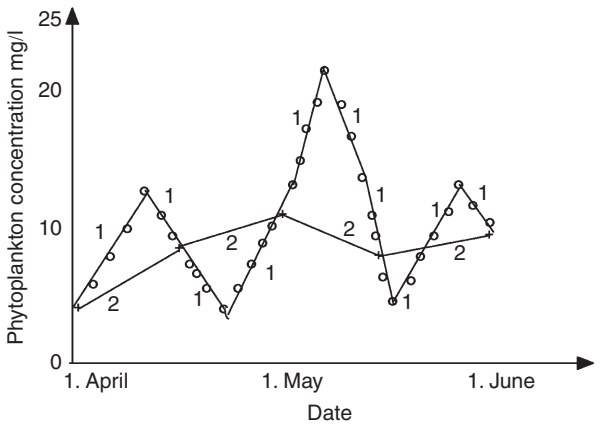

FIGURE 2.15 Algae concentration plotted versus time: (1) = sampling frequency twice a month (+) and (2) = sampling frequency three times a week (*). Note the difference of d(PHYT)/dt between the two curves.

important not only to have data with low uncertainty, but also data sampled with a frequency corresponding to the dynamics of the system.

The rule to match appropriate sampling frequency has often been neglected in modelling eutrophication, 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 samples per week requires too many resources. A combination of an annual sampling program with a frequency of one to three samples per month and an intensive measuring program placed in periods, where different subsystems show maximum changes, is a good basis for parameter estimations.

The intensive measuring program can, as presented next, 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 Figure 2.15. These estimates can be used to set up an overdetermined set of algebraic equations, making the model parameters the sole unknown. An outline of the method runs as follows (see Figure 2.16; for further details, see Jørgensen et al., 1981):

Step 1. Find cubic spline coefficients, $S_i(t_j)$, that is, 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 an n^{th} order polynomium (4th–8th 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: $\psi = (\psi,t,a)$, where a is a parameter.

Step 3. Solve the model equation of the form:

$$\partial\psi(t_j)/dt = f(\psi, \partial\psi/\partial r, \partial^2\psi/\partial r^2, t, a) \tag{2.15}$$

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, then modify the part of the model influenced by a_0 and go to step 1.

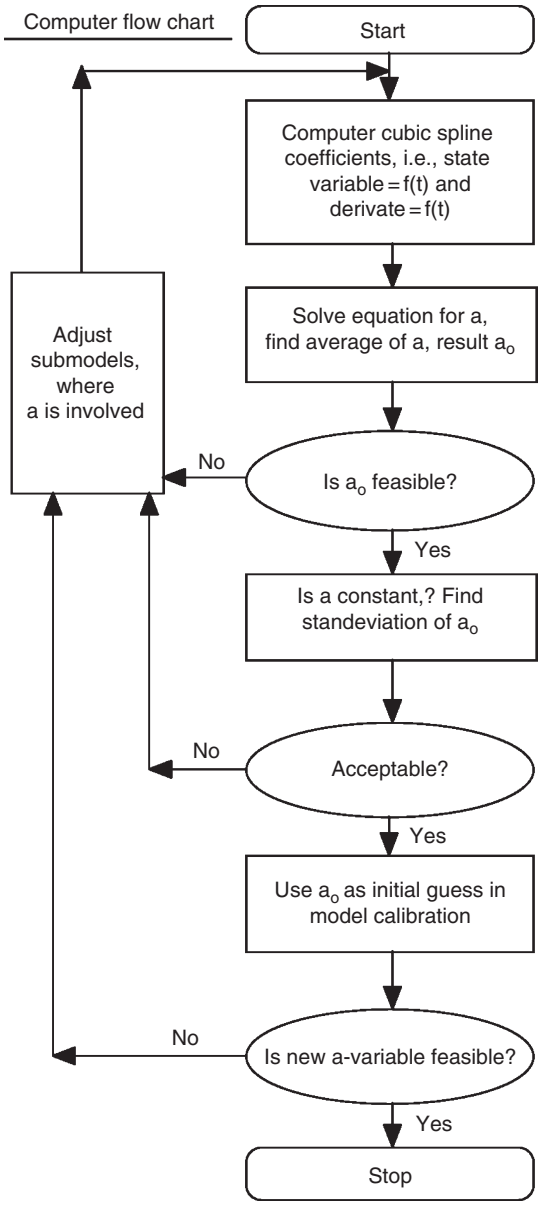

FIGURE 2.16 Computer flow chart of the method applied to estimate parameters by using "intensive measurements."

Step 5. Choose a significance level, and perform a statistical test on constancy of a_0. If the test fails, then 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 such as the one proposed in Eq. (2.2).

Although the model in hand may be highly nonlinear 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. (2.15) is overdetermined. It is easy to smooth the solution, but it is more important to evaluate the constancy of a_0, for example, by variance analysis, test of normality of white noise, and so forth. Information on standard deviation of a_0 around its average value may eventually be used as a 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, 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. (2.15) quite accurately locates the inappropriate terms and constructs in the model. Experience with this method shows it to be a valuable diagnostic tool to single out unfitted model terms.

Since the method is based on cubic spline approximation, it is essential that observations are dense, for example, $t_{j+1} - t_j$ should be small in the sense that local third-degree polynomials should approximate observed values well. It is difficult, in general, to test whether this is fulfilled as the "true" $\psi_i(t)$ function might have microscopic curls that generate oscillating derivates (ψ_i/dt). However, if the method yields basically the same result on a random subset of observations, then it may be safe to assume that $\{s_i(t_j)/dt\}$ represents the true rates on a daily basis. After appropriate adjustment of model equations, an acceptable parameter set a_o 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 mentioned previously are so important. The result of the application of intensive measurements to calibrate the eutrophication model is summarized in Table 2.4, where the difference in parameter estimation is pronounced. It is important to use the parameters determined by intensive measurements before the final calibration.

The illustrated use of intensive measurements for parameter estimation prior to the calibration was based upon 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.

Intensive measurements were used for the 18 state variable eutrophication model presented in Chapter 7. It was possible to determine the maximum phytoplankton growth rate by the previous method to be 1.6 day^{-1} $\pm$10% relative. It was also possible to choose between possible expressions for the temperature influence on the phytoplankton growth.

Measurements and observations *in vitro* were used in the referred case 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. Current record of important state variables is often possible and provides a high number of data, which decreases the standard deviation.

As an example fish growth can be described by use of the following equation:

$$dW/dt = a \times W^b \tag{2.16}$$

where W is the weight, and a and b are constants. In an aquarium or an aquaculture farm it is possible to measure the fish weight over time. If enough data are available, then it is easy by statistical methods to determine a and b in Eq. (2.16). 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 assure the very best growth conditions for the fish. By varying these factors, it is even

Table 2.4 Comparison of Parameter Values

Parameter	Parameter (Symbol)	Unit	Application of Intensive Measurements	Glumsø Lake*	Lyngby Lake*	Literature ranges
Settling rate	SVS = D × 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	0.013l–0.035
Min. N: biomass ratio	FNAmin		0.120.10	0.10	0.10	0.08–0.12
Max.uptake rate N**	UNmax	d^{-1}	0.023 ± 0.005	0.015	0.012	0.0l–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 ± l.05			
Respiration rate**	RC	d^{-1}	0.088	0.13	0.2	0.05–0.25
Mineralization rate P	KDPl0	d^{-1}	0.80 ± 0.47	0.40	0.25	0.2–0.8
Mineralization rate N	KDNl0	d^{-1}	0.21 ± 0.11	0.05	0.15	O.OS–0.3
Max. uptake rate c**	UCmax	d^{-1}	1.21 ± 0.97	0.65	0.40	0.2–1.4

Notes:

*Lyngby and Glumsø lakes have approximately the same biogeochemical characteristics and morphology;

**all parameters related to phytoplankton.

possible to find the influence of the water quality, and the available food on the growth parameters. The results of such experiments can often be found in the literature. Still, the modeller might not find the parameter for the species of interest, nor find the parameters in the literature under the specific conditions in the ecosystem being modelled. In such cases, it may be necessary to use experiments to determine important model parameters. The use of laboratory experiments is advisable also when the literature values for the crucial parameters are too wide for the most sensitive parameters.

However, parameters taken from the literature or resulting from such experiments should be applied with precaution because the discrepancy between the values in the laboratory or even the microcosms and those in nature is much greater for biological parameters than for chemical or physical parameters. The reasons for this can be summarized in the following points:

1. Biological parameters are generally *more sensitive to environmental factors than chemical or physical parameters*. 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*, of which some are quite variable. For instance, phytoplankton growth rate is dependent on the nutrient concentration, but the local nutrient concentration is again very dependent on the water turbulence, which is dependent on the wind stress, and so forth.
3. The example in point 2 shows 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*, then it is not possible to interpret under which circumstances the measurement is valid, because that would require the simultaneous determination 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 phytoplankton biomass cannot be determined by any direct measurement, but it is possible to obtain an indirect measurement by using the chlorophyll concentration, the ATP concentration, the dry matter 1–70μ, and so forth. Still, 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 1–70μ might include other particles (e.g., clay particles). So, it is recommended in practice to apply several of these indirect determinations simultaneously to assure a reasonable estimate. Correspondingly, the phytoplankton growth rate might be determined by the oxygen method or the C-14-method. Neither method determines the photosynthesis; instead they determine the net production of oxygen and the net uptake of carbon, respectively; that is, 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, which is difficult to do accurately.

5. Biological parameters are *influenced by several feedback mechanisms of a biochemical nature*. The past will determine the parameters in the future. For instance, the phytoplankton growth rate 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 (Straskraba, 1980). In other words, it is an approximation to consider parameters as constants. An ecosystem is a soft, flexible system, described with approximations as a rigid system with constant parameters (Jørgensen, 1981, 1992a,b).

The estimation of the settling velocity as a parameter in ecological models may be crucial whether the component is suspended matter or phytoplankton, as it determines the removal rate for a considered component. The sensitivity of this parameter to the phytoplankton concentration in a eutrophication model has been determined to be about -1.0 (see Table 2.3). It means that if the parameter is increased

1%, the phytoplankton concentration will decrease 1% (Jørgensen et al., 1978). Let us therefore use the estimation of the settling rate as another illustration of the needed considerations in our effort to obtain a proper determination of parameters.

Settling velocity may be determined in three ways:

1. Values from previous models found in the literature can be used to give a first estimation of the parameter. Tables 2.5 and 2.6 summarize values found in the literature. As can be seen, these values are indicated as ranges, therefore, it is necessary to calibrate the parameters using measured values for the stated variables.

Table 2.5 Phytoplankton Settling Velocities

Algal Type	Settling Velocity (m/day)	References
Total phytoplankton	0.05–0.5	Jørgensen et al. (1991, 2000);Tetra Tech (1980)
	0.05– 0.2	Di Toro & Connolly (1980); O'Connor et al. (1981); Thomann et al. (1974); Thomann & Fitzpatrick (1982)
	0.02– 0.05	Jørgensen et al. (1991, 2000)
	0.4	Lombardo (1972)
	0.03– 0.05	Scavia (1980)
	0.05	Bierman (1976)
	0.2–0.25	Youngberg (1977)
	0.04– 0.6 *	Jørgensen et al. (2000)
	0.01–4.0	*Jørgensen et al. (2000)
	0.1–2.0 *	Snape et al. (1995)
	0.15–2.0 *	Jørgensen et al. (2000)
	0.1–0.2 *	Brandes (1976)
Diatoms	0.05– 0.4	Bierman (1976); Brandes et al. (1974)
	0.1– 0.2	Jørgensen et al. (2000)
	0.1– 0.25	Tetra Tech (1980)
	0.03– 0.05	Snape et al. (1995)
Diatoms	0.3– 0.5	Jørgensen et al. (2000)
	2.5	Lehman et al. (1975)
	0.02–14.7 *	Jørgensen et al. (2000)
Green algae	0.05– 0.19	Jørgensen et al. (2000)
	0.05– 0.4	Bierman (1976)
Green algae	0.02	Snape et al. (1995)
	0.8	Lehman et al. (1975)
	0.1– 0.25	Tetra Tech (1980)
	0.08– 0.18 *	Jørgensen et al. (2000)
	0.27– 0.89 *	Jørgensen et al. (2000)

Continued

Table 2.5 Phytoplankton Settling Velocities—cont'd

Algal Type	Settling Velocity (m/day)	References
Blue-green algae	0.05– 0.15	Bierman (1976)
	0.08	Snape et al. (1995)
	0.2	Lehman et al. (1975)
	0.1	Jørgensen et al. (2000)
	0.08–0.2	Tetra Tech (1980)
Flagellates	0.5	Lehman et al. (1975)
	0.05	Bierman (1976)
	0.09– 0.2	Tetra Tech (1980)
	0.07–0.39 **	Jørgensen et al. (2000)
Dinoflagellates	2.8–6.0 **	Jøregensen et al. (2000)
Asterionella formosa	0.25– 0.76 **	Jørgensen et al. (2000)
Chaetoceros lauderi	0.46– 1.56 **	Jørgensen et al. (2000)
Chrysophytes	0.5	Lehman et al. (1975)
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)
Melosira agassizii	0.67– 1.87 **	Jørgensen et al. (2000)
Nitzschia seriata	0.26– 0.50 **	Jørgensen et al. (2000)
Rhizosolenia robusta	1.1– 4.7 **	Jørgensen et al. (2000)
R. 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. pseudonana	0.15– 0.85 **	Jørgensen et al. (2000)
T. rotula	0.39– 17.1	Jørgensen et al. (2000)

Notes: Other values used in models.
*Model documentation values;
**literature values.

Table 2.6 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)
Fecal pellets (fish)	23– 666	Jørgensen et al. (2000)

2. Values from calculations based upon knowledge of the size can be used as first estimations. Due to the influence of the many factors previously mentioned, a calibration is also required in this case. This method is hardly applicable for phytoplankton because of their ability to change the specific gravity, but it may be useful for other particles.
3. Measurements *in situ* by use of sedimentation traps. It is possible to determine the distribution of the material in inorganic and organic matter and partly also in phytoplankton and detritus by analysis of chlorophyll (fresh material), phosphorus, nitrogen, and ash. Measurements of phytoplankton settling velocities in the laboratory will unlikely give a reliable value, as they do not consider the various factors *in situ*.

It has been previously pointed out that the *calibration is facilitated significantly if we have good initial estimates of the parameters*. Some estimates might be found in the literature, but it is often only a few compared with the number of parameters needed if we want to model all interesting mass flows in all relevant ecosystems. For the nutrient flows, the parameters known from the literature are the most common species only. If we turn to flows of toxic substances in ecosystems, then 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, then the number of parameters needed is enormous. For example, if we need the interactions of only 10,000 species with the 100,000 substances of environmental interest, the number of needed parameters is $10 \times 10{,}000 \times 100{,}000 = 10^{10}$ parameters. In Jørgensen et al. (2000; see Figure 2.14) 120,000 parameters can be found, and if we estimate that this *Handbook* covers about 10% of the parameters, which can be found in the entire literature, then we know only about 0.012% of the needed 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, and will be discussed in Chapter 8. If needed data cannot be found in the literature, then such relationships are widely used as the second-best approach to the problem.

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

Modern molecular theory provides a sound basis for predicting reliable quantitative data on the chemical, physical, and thermodynamic properties of pure substances and mixtures. The biological sciences are not based upon a similar comprehensive theory, but it is possible, to a certain extent, to apply basic biochemical mechanisms laws to ecology. Furthermore, the very 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 quite similar. All species need, for their fundamental biochemical function, a certain amount of carbohydrates, proteins, fats, and other compounds, and as these groups of biochemical substances are constructed from 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). For example, if we know the uptake rate of nitrogen for phytoplankton, then we can find the approximate uptake rate of phosphorus because the uptake rates must result in a nitrogen-to-phosphorus ratio between 5:1 and 12:1, an average 1:7.

The biochemical reaction pathways are also general, which is demonstrated in all textbooks on biochemistry. The utilization of the chemical energy in the food components is basically the same for microorganisms and mammals. It is, therefore, possible to calculate approximately the energy, E1, released by digestion of food, when the composition is known:

$$\mathrm{E1} = 9\ \text{fat}\%100 + 4(\text{Carbohydrates} + \text{proteins})\%100 \tag{2.17}$$

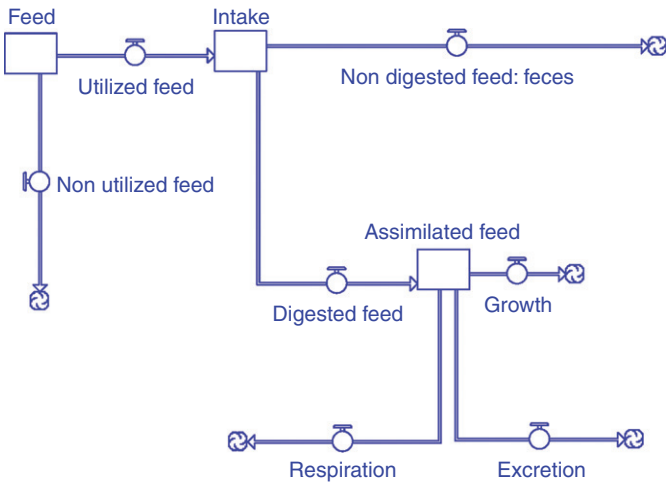

FIGURE 2.17 The principle of a fish growth model. The feed is either utilized or not utilized. The utilized food = the intake is either digested or assimilate and at steady-state intake = nondigested feed (feces) + the assimilated feed. The assimilated feed is used for either growth, excretion, or respiration and at steady state assimilated feed = growth + respiration + excretion (see Jørgensen, 2000).

The law of energy conservation is also valid for a biological system (see Figure 2.17). The chemical energy of the food components is used to cover the energy needs for respiration, assimilation, growth (increase of biomass included reproduction), and losses. As it is possible to set up relations between these needs on the one side with some fundamental properties of the species on the other, it is possible to put a number on the items in Figure 2.17 for different species. This is a general but valid approach to parameter estimation in ecological modelling.

Species surface area is a fundamental property indicating 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. The rate of digestion, the lungs, and hunting ground, are all dependent on the size of the animal and are determinant for a number of parameters.

Therefore, it is not surprising that many parameters for plants and animals are highly related to the size of the organism, 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 characteristic features of the species, but their influence is minor compared with the organism size, and the good estimates provide at least a starting value in the calibration phase.

The conclusion of these considerations is that many parameters are related to simple properties, such as size of the organisms, and that

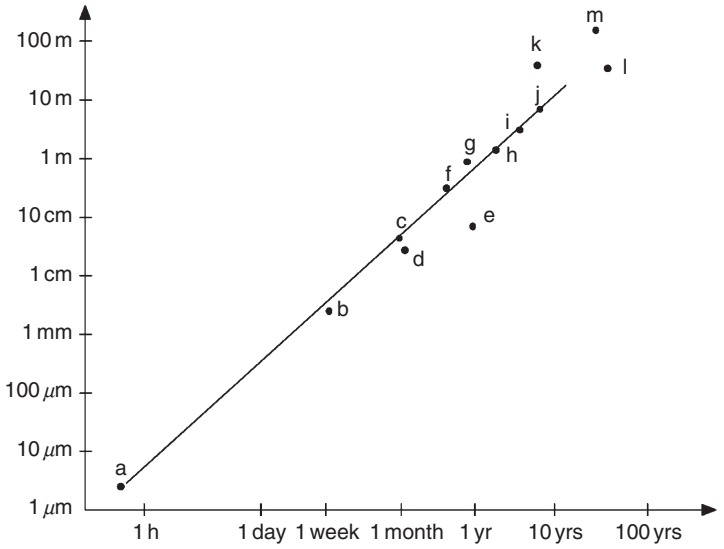

FIGURE 2.18 Length and generation time plotted on log-log scale: (a) pseudomonas, (b) daphnia, (c) bee, (d) house fly, (e) snail, (f) mouse, (g) rat, (h) fox, (i) elk, (j) rhino, (k) whale, (l) birch, (m) fir. See also Peters (1983).

such relations are based upon 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 relationship is illustrated in Figure 2.18. This relationship can be explained using the relationship between size (surface) and total metabolic action per unit of body weight. It implies that the smaller the organism, the greater the specific metabolic activity (= activity/weight). The per capita rate of increase, r, defined by the exponential or logistic growth equations:

$$dN/dt = rN \tag{2.18}$$

respectively,

$$dN/dt = rN(1 - N/K) \tag{2.19}$$

is inversely proportional to the generation time.

This implies that r is related to the organism size, but, as shown by Fenchel (1974), it actually falls into three groups of organisms: unicellular, poikilotherms, and homeotherms (see Figure 2.19). Thus, the metabolic rate per unit of weight is related to the 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:

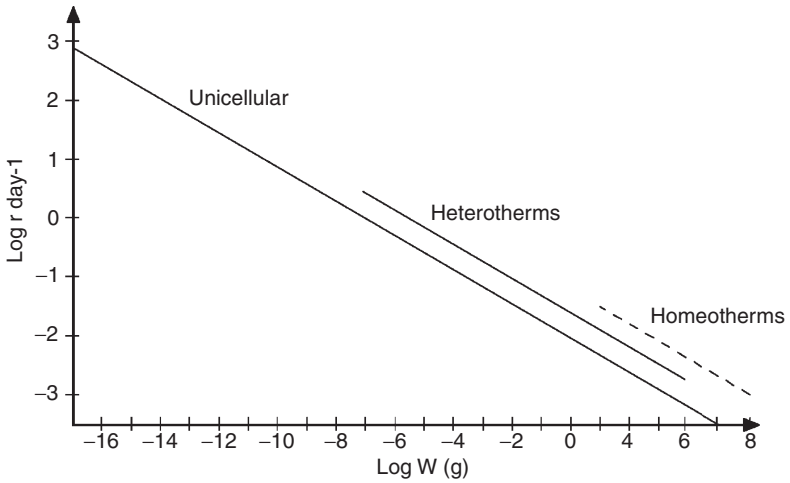

FIGURE 2.19 Intrinsic rate of natural increase against weight for various animals. See also Peters (1983).

$$\text{Respiration} = \text{constant} * \text{W}^{0.80} \tag{2.20}$$

$$\text{Feed Consumption} = \text{constant} * \text{W}^{0.65} \tag{2.21}$$

$$\text{Ammonia Excretion} = \text{constant} * \text{W}^{0.72} \tag{2.22}$$

This is also expressed in Odum's equation (E. P. Odum, 1969, 1971):

$$\text{m} = \text{kW}^{-1/3} \tag{2.23}$$

where k is roughly a constant for all species, equal to about 5.6 $\text{kJ/g}^{2/3}$ 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 of these examples illustrate the fundamental relationship in organisms between size (surface) and the biochemical activity. The surface determines the contact with the environment quantitatively along with the possibility of taking up food and excreting waste substances.

The same relationships are shown in Figures 2.20–2.22, where rates of biochemical processes involving toxic substances are plotted versus size. They are reproduced from Jørgensen (1997, 2002). In these figures, the excretion rate, uptake rate, and concentration factor (for aquatic organisms) follow the same trends as the growth rate. This is not surprising, as excretion is strongly dependent on metabolism and the direct uptake dependent on the surface.

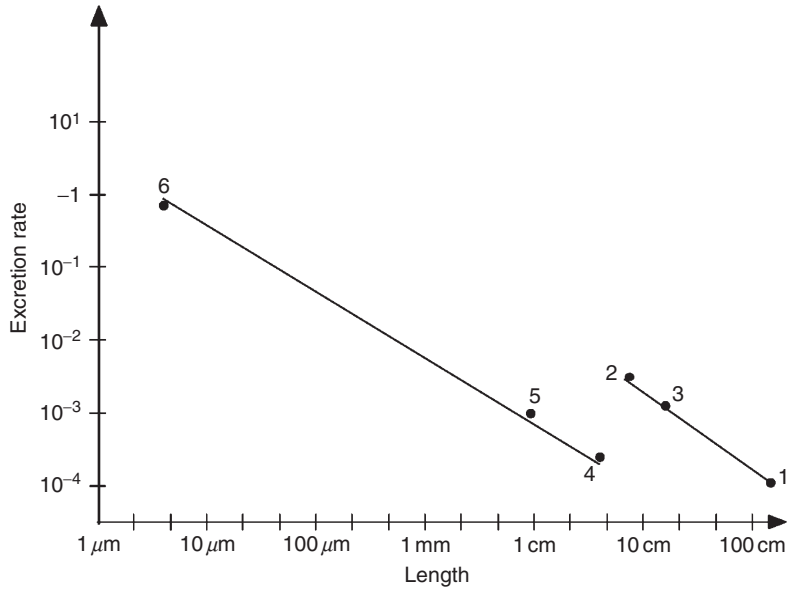

FIGURE 2.20 Excretion of Cd $(24h)^{-1}$ plotted versus the length of various animals: (1) Homosapiens, (2) mice, (3) dogs, (4) oysters, (5) clams, and (6) phytoplankton.

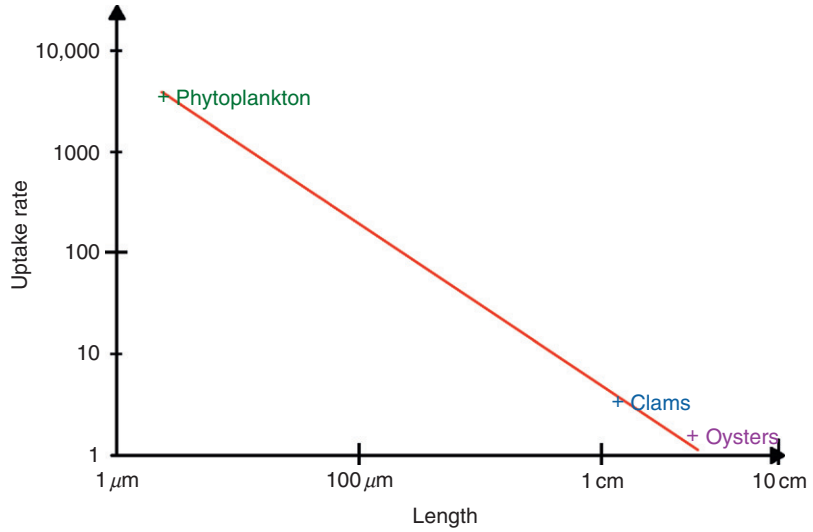

FIGURE 2.21 Uptake rate (μg Cd/g 24 h) plotted against the length of various animals' phytoplankton, clams, and oysters.

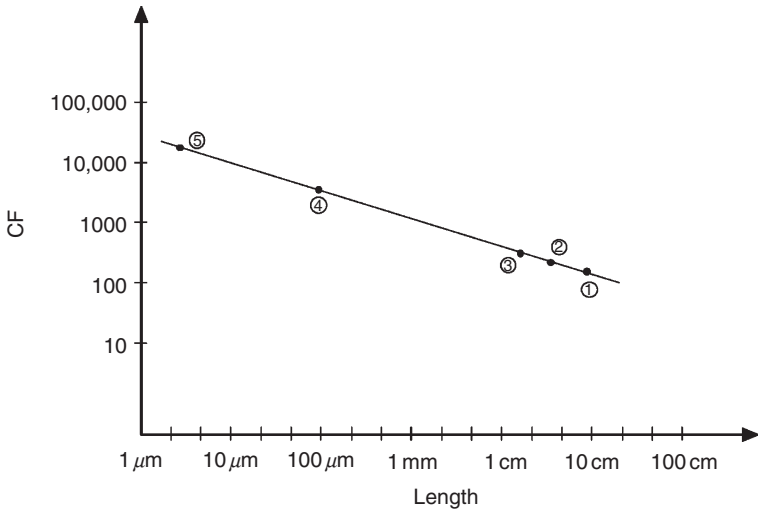

FIGURE 2.22 CF (concentration factor >= to the ratio concentration in organism to the concentration in water>) for Cd versus size: (1) goldfish, (2) mussels, (3) shrimps, (4) zooplankton, (5) algae (brown-green).

In spite of all these methods to estimate parameters, it may still be necessary to accept that a parameter is only known within some unacceptable large range. In such cases, applying a Monte Carlo simulation of the parameter within the known range should be considered. The concentration factor indicating concentration in the organism vis-á-vis concentration in the medium also follows the same lines (see Figure 2.20). 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 Figure. 2.20 seems reasonable. Intervals for-concentration factors are indicated here for some species according to the literature (Jørgensen et al., 1991, 2000).

The *allometric principles***,** illustrated in Figures2.18–2.22, can be generally applied to find process rates, provided these parameters are available for the element or compound under consideration (because the slope is known). However, it is preferable to know several species to control the validity of the graph. When plots similar to Figures 2.18–2.22 are constructed, it is possible to read unknown parameters when the size of the organism is known.

It was mentioned earlier that model constraints could be used to estimate unknown parameters. The chemical composition of an organism

was applied to illustrate this principal method. The topic model constraints are covered further 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 a shift in species composition presented. This constraint has also been applied to estimate unknown parameters, as shown in Chapter 10, after the more basic theory has been presented.

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

A. Examine the literature to find the range of as many model parameters as possible. It is recommended to use Jørgensen et al. (2000), which contains about 120,000 parameters.
B. Examine processes *in situ* or in the laboratory to assess unknown parameters.
C. Apply an intensive observation period to reveal the dynamic processes in the model. Use the method described in Figures 2.15 and 2.16 to find unknown parameters. This method often makes it possible to indicate parameters within relatively narrow ranges.
D. Apply allometric principles to find unknown parameters for the organisms included in the model as well as 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 based on a translation of the chemical structure to the properties of the compound. This method will be presented in detail in Chapter 10, Section 10.6.
F. Use the model constraints to estimate an unknown parameter or to control an uncertain parameter (e.g., how exergy can be used to determine parameters in Chapter 10, Section 10.3).
G. Apply calibration of submodels and/or the entire model. The better the data, the more certain and reliable results the calibration will offer.

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, as well all feedbacks, adaptations, regulations, and the entire evolutionary process.

Jørgensen (1997, 2002) introduced the application of the uncertainty principle of quantum physics in ecology. In nuclear physics, uncertainty is caused by the observer of the incredibly small nuclear particles, while 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 relation is linear or nonlinear. Correspondingly, the relations among three components will require 3*3 observations for the shape of the plane. If we have 18 components we would correspondingly need 3^{17} 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 relation in ecology (Jørgensen, 1990):

$$10^5 * \Delta x / \sqrt{3^{n-1}} \leq 1 \tag{2.24}$$

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

The 100 million observations could also be used to give a very exact picture of one relation. Costanza and Sklar (1985) talked about the choice between the two extremes: knowing "everything" about "nothing" or "nothing" about "everything" (see Section 2.9). The former refers to the use of all the observations on one relation to obtain a high accuracy and certainty, while the latter refers to the use of all observations on as many relations as possible in an ecosystem. How we can obtain a balanced complexity in the description will be further discussed in the next section.

Equation (2.18) formulates a practical uncertainty relation, but, the possibility that the practical number of observations may be increased in the future cannot be excluded. More and more automatic analytical equipment is emerging on the market. This means that the number of observations invested in one project may be one, two, three, or even several magnitudes larger in the future. Yet, a theoretical uncertainty relation can be developed. If we go to the limits given by quantum

mechanics, then the number of variables will still be low compared to the number of components in an ecosystem.

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

$$\Delta s * \Delta p \geq h/2\pi \tag{2.25}$$

where Δs is the uncertainty in determining the position, and Δp is the uncertainty of momentum. According to this relation, Δx of Eq. (2.24) 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:

$$\Delta t * \Delta E \geq h/2\pi \tag{2.26}$$

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

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

$$173 * 10^{15} * 4.5 * 10^{9} * 365.3 * 24 * 3600 = 2.5 * 10^{34} J, \tag{2.27}$$

where 173 $*10^{15}$ W is the energy flow of solar radiation. Δt would, therefore, be in the order of 10^{-69} seconds. Thus, an observation will take 10^{-69} seconds, 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:

$$4.5 * 10^{9} * 365.3 * 3600/10^{-69} \approx of 10^{85}. \tag{2.28}$$

This implies that we can replace 10^5 in Eq. (2.24) with 10^{60} since

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

If we use $\Delta x = 1$ in Eq. (2.28) we get:

$$\sqrt{3^{n-1}} \leq 10^{60} \tag{2.29}$$

or $n \leq 253$.

From these very theoretical considerations, we can clearly conclude that we will never have enough observations to describe even one ecosystem in complete detail. An ecosystem is a middle number system, which means that the number of components are not as high as the number of gas molecules in a room, but that it may be as high as 10^{15}–10^{20}. Unlike the gas molecules in a room, all of these components are different, while there may be only 10 to 20 different types of gas molecules in a room.

These results agree 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 area 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. Applying the theory of complementarity in ecology, we see that it is important to view the ecosystem from different, complementary angles.

As stated previously, the use of maps in geography is a good parallel to the use of models in ecology. As we have road maps, airplane maps, geological maps, maps in different scales for different purposes, we have many models in ecology of the same ecosystems. We need them all if we want to get a comprehensive view of ecosystems (see Sections 1.1 and 2.9). Furthermore, a map can give an incomplete picture. We can always make the scale larger and larger and include more details, but we cannot get all the details. 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 after the dynamics of the system have changed the "picture."

Another good example comes from physics, in which we need a pluralistic view to 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 describe an ecosystem. We need many models covering different viewpoints. This is consistent with Gödel's Theorem from 1931 (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 every possible detail because that would be the world itself.

Ecosystems must be considered irreducible systems, because it is not possible to make observations and then reduce the observations to more or less complex laws of nature; for instance mechanics. Too many interacting components force us to consider ecosystems as irreducible

systems. It is necessary to use what is called experimental mathematics or modelling to cope with irreducible systems.

Quantum theory may have an even wider application in ecology. Schrödinger (1944) suggested, 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 (1982a, 1985) defined an elementary "particle" of the environment, called an environ — previously Koestler (1967) used the word holon — as a unit that can transfer an input to an output. Patten suggested that a characteristic feature of ecosystems is the network of connections. 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 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) introduced the term infon for the elementary particle of information. He envisaged 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 into a quantum of information. This concept has still not found any application in ecological modelling.

2.12. Modelling Constraints

A modeller is very concerned about the application of the right description of the components and processes in his 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 system properties. Several possible modelling constraints are mentioned next. 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 further discussion will take place in Chapter 10 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 bioenergic 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:

$$E = mc^2 (ML^2T^{-2}), \tag{2.30}$$

where E is energy, m is mass, and c is the velocity of electromagnetic radiation in vacuum ($= 3 * 10^8$ m sec^{-1}). The transformation from matter into energy and vice versa is only of interest for nuclear processes and does not need to be applied to ecosystems; therefore, we might break the proposition down to two more useful propositions, when applied in ecology:

1. Ecosystems conserve matter.
2. Ecosystems conserve energy.

The conservation of matter may mathematically be expressed as follows:

$$dm/dt = \text{input} - \text{output}\ (MT^{-1}) \tag{2.31}$$

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:

$$Vdc/dt = \text{input} - \text{output}\ (MT^{-1}) \tag{2.32}$$

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, then Eq. (2.32) must be changed to:

$$V * dc/dt = \text{input} - \text{output} + \text{formation} - \text{transformation}\ (MT^{-1}) \tag{2.33}$$

The principle of mass conservation is widely used in the class of ecological models called biogeochemical models. Equation (2.26) is set up for the relevant elements, for example, for eutrophication models for C, P, N, and perhaps Si (see Jørgensen, 1976a,b, 1982; Jørgensen et al., 1978).

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

$$A * dma/dt = \text{input} - \text{output} + \text{formation} - \text{transformation}\ (MT^{-1}) \tag{2.34}$$

here A = area and ma = mass per unit of area.

The Streeter-Phelps model (see Chapter 7) is a classical model of an aquatic ecosystem that is based upon conservation of matter and first-order kinetics. The model uses the following central equation:

$$dD/dt + K_a * D = L_o * K_1 * K_T(T - 20) * e^{-K1*t}(ML^{-3}T^{-1}) \tag{2.35}$$

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_o = BOD_5 at time = 0; K_1 = rate constant for decomposition of biodegradable matter; and K_T = constant of temperature dependence.

Equation (2.29) 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 (2.27) are also used in models describing the fate of toxic substances in the ecosystem. Examples can be found in Thomann (1984) and Jørgensen (1991, 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, and growth, including reproduction (see Figure 2.17). If the growth and reproduction are considered as the net production, then it can be stated that:

$$\text{net production} = \text{intake of food} - \text{respiration} - \text{excretion} - \text{waste food} \tag{2.36}$$

The ratio of the net production to the intake of food is called the net efficiency; it 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 excretions because it is much less biodegradable than the normal components in the food. Because of this, 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 2.7. DDT and other chlorinated hydrocarbons have an especially high biological magnification because they have a very low biodegradability and are excreted from the body very slowly, due to dissolution in fatty tissue. These considerations also explain why pesticide residues observed in fish increase with the increasing weight of the fish (see Figure 2.23). As humans are the last link of the food chain, relatively high DDT concentrations have been observed in the human body fat (see Table 2.8).

Table 2.7 Biological Magnification

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 birds2	5	~8,500,000

Source: Data after Woodwell et al., 1967.

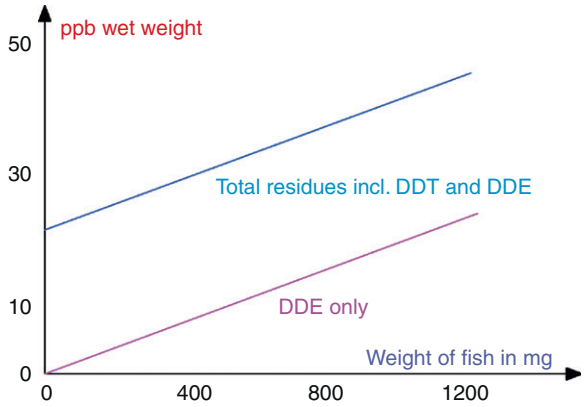

FIGURE 2.23 Increase in pesticide residues in fish as weight of the fish increases. Top line = total residues; bottom line = DDE only. *(After Cox, 1970).*

Understanding the principle of conservation of energy, called the first law of thermodynamics, was initiated in 1778 by Rumford. He observed a large quantity of heat 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 transformed at the expense of another form of energy; in his case 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, Mayer and 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.

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

$$dQ = dU + dW(ML^2T^{-2}) \tag{2.37}$$

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 $\int dU$ is independent on the pathway 1 to 2. The internal energy, U, includes several forms of energy: mechanical, electrical, chemical, magnetic

Table 2.8 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

energy, and so forth. The transformation of solar energy to chemical energy by plants conforms to the first law of thermodynamics (see Figure 2.24):

$$\text{Solar energy assimilated by plants} = \text{chemical energy of plant tissue growth} + \text{heat energy of respiration} \quad (2.38)$$

For the next level in the food chains, the herbivorous animals, the energy balance also can be set up as:

$$F = A + UD = G + H + UD, (ML^2T^{-2}) \quad (2.39)$$

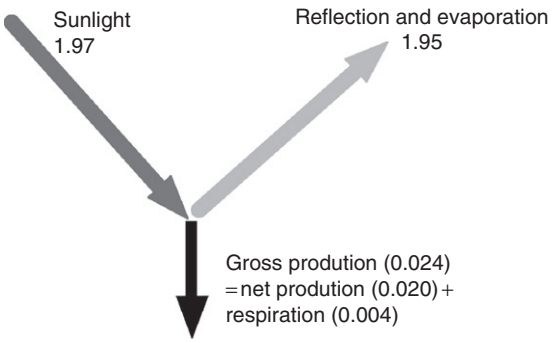

FIGURE 2.24 Fate of solar energy incident upon the perennial grass-herb vegetation of an old field community in Michigan. All values in GJ m-2 y-1.

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

These considerations pursue the same lines as those mentioned in context with Eq. (2.36) and Figure 2.17, where the mass conservation principle is applied. The conversion of biomass to chemical energy is illustrated in Table 2.9. The energy content per g ash-free organic material is surprisingly uniform, as is illustrated in Table 2.9. Table 2.9, part D shows ΔH, which symbolizes the increase in enthalpy, defined as $H = U + p^*V$. Biomass can be translated into energy, 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.

Many biogeochemical models are within *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 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 Mauersberger (1985), who has used this constraint to assess process equations, too. Since the second law of thermodynamics is also valid for ecosystems, it raises the question: How does it apply to ecological processes?

Table 2.9*

A. Combustion Heat of Animal Material

Organism	Species	Heat of Combustion (kcal/ash-free gm)
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
	P. guttifer	-5.706
Spit bug	*Philenus leucopthalmus*	-6.962
Mite	*Tyroglyphus lintneri*	-5.808
Beetle	*Tenebrio molitor*	-6.314
Guppie	*Lebistes reticulates*	-5.823

B. Energy Values in an *Andropogus virginicus*, Old-Field Community in Georgia

Component	Energy Value (kcal/ash-free gm)
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/gm)	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/gm)	ΔH Fat (kcal/gm)	ΔH Carbohydrate (kcal/gm)
Eggs	-5.75	-9.50	-3.75
Gelatin	-5.27	-9.50	

Continued

Table 2.9*—cont'd

Material	ΔH Protein (kcal/gm)	ΔH Fat (kcal/gm)	ΔH Carbohydrate (kcal/gm)
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			-375
Mushroom	-5.00	-9.30	-4.10
Yeast	-5.00	-9.30	-4.20

**Source: Morowitz, 1968.*

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. It means that an ecological model in the initial phase of development has many degrees of freedom. It is necessary to limit the degrees of freedom to develop a workable model.

Many modellers use a comprehensive data set and calibration to limit the number of possible models. Nonetheless, this is a cumbersome method if it is not accompanied by some realistic constraints on the model. Calibration is therefore often limited to give the parameters realistic and literature-based intervals, within which the calibration is carried out, as mentioned in Section 2.10.

But far more would 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. For example: How could the hierarchy of regulation mechanisms be accounted for in the models? Straskraba (1979, 1980) classified models according to the number of levels that the model includes from this hierarchy. He concluded that we need experience with the models of the higher levels to develop structural dynamic models. This is the topic for Chapter 10.

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 for the cooperation

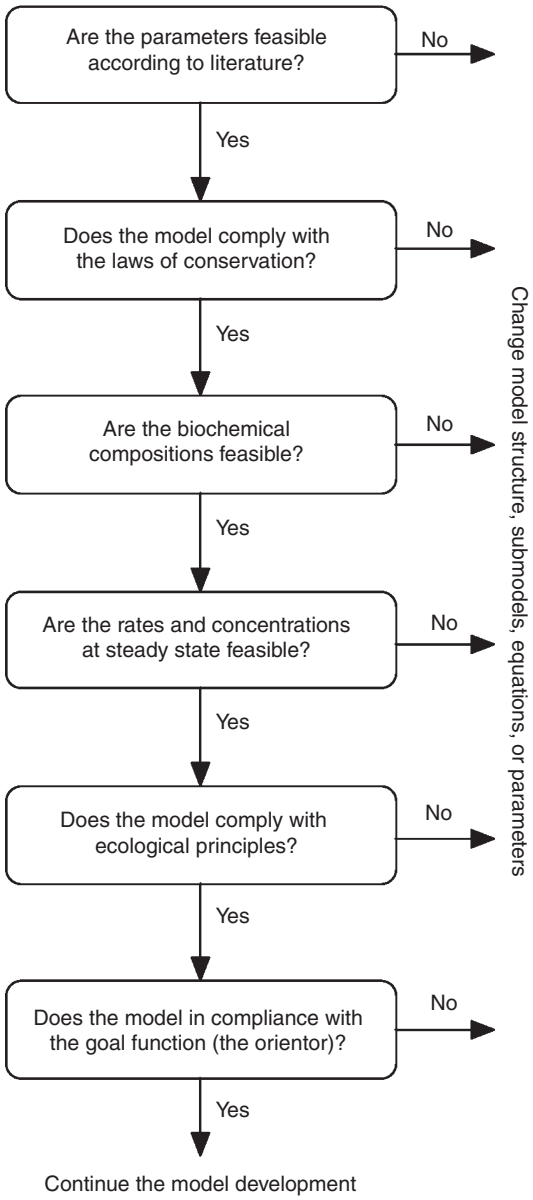

FIGURE 2.25 Considerations on using various constraints by development of models. The range of parameter values is particularly limited by the procedure shown.

among the biological components have been imposed. These rules and principles are the governing laws of ecosystems, and our models should follow these principles and laws.

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

Figure 2.25 summarizes the considerations of using various constraints to limit the number of possible values for parameters, possible descriptions of processes, and possible submodels to facilitate the development of a feasible and workable model. The two last steps of the procedure will be presented in Chapter 10, where the next generation models are developed.

It requires the introduction of variable parameters, governed by a goal function (an orientor). Several possible goal functions have to be introduced before a presentation of structural dynamic models can take place.

Problems

1. Which class of models 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 a length of 20 m.
4. The ammonia excretion for a fish of 500 g is 200 mg/24h. Estimate the ammonia excretion for a fish of 4 kg. What is the excretion rate of a shark of 2000 kg?
5. Set up an adjacency matrix for the models shown in Figure 2.10 and 2.11.

6. Improve the model in Figure 2.5 by adding two more state variables. Which two state variables would probably be most important to add to the present model focused on eutrophication?
7. How often would you determine the phytoplankton concentration, if a model for the diurnal variations of primary production during a month was supposed to be modelled? Would the number of observations be dependent on the season? If yes, why?
8. Set up the equations for a model explaining the accumulation of DDT in fish according to Figure 2.23.
9. How many state variables could a model have, if all the relationships are based entirely on 10,000,000 observations?
10. Develop a model for the biomagnification of a toxic substance through a food chain with primary producers, primary consumers, and secondary consumers.