

Biogeochemical Models

S.E. Jørgensen

Emeritus Professor, Copenhagen University, Denmark

E-mail: soerenorsnielsen@gmail.com

OUTLINE

2.1 Advantages and Properties of Biogeochemical Models	13	2.4 Ecological and Environmental Biogeochemical Models	33
2.2 Modeling Elements	16	References	38
2.3 The Modeling Procedure	19		

2.1 ADVANTAGES AND PROPERTIES OF BIOGEOCHEMICAL MODELS

Among the modeling types represented in this book, the biogeochemical models are the most applied model type. The journal *Ecological Modelling* started in 1975 and about two-thirds of all papers published in the journal during the 1970s were biogeochemical models. Today, this model type is still the most applied one. Despite the competition with many new model types, about one-third of the papers published in *Ecological Modelling* still belong to this type. In the 1970s, about 10–12 biogeochemical models were annually published in the journal, while today more than 100 of the annually published models in the journal are biogeochemical models.

This dominance of biogeochemical models is easy to understand, as the model type offers the user several advantages. First of all, the model is easy to develop. It is based on the mass conservation principles, which is expressed easily by differential equations. Fig. 2.1 illustrates the idea behind the use of differential equations for the state variables—it means the variables that are chosen to express the state of the modeled system. In mathematics, the

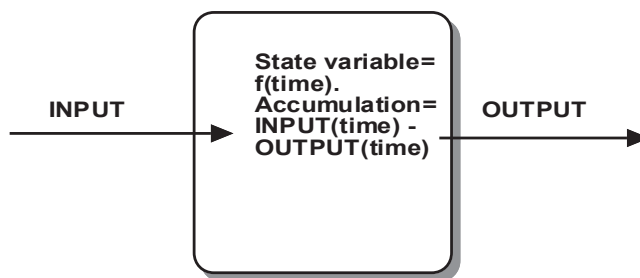


FIGURE 2.1 The idea behind the use of differential equations is illustrated. The differential equation accounts for the increase of a state variable due to what is denoted in the figure accumulation for a selected time step. The accumulation is input – output. Theoretically in mathematics, the time step is infinitely small, but when the equation is solved numerically by use of computers, we are selecting a time step. The shorter the time step, the closer is the solution to the mathematical solution.

differential equations are solved analytically, while the equations are solved numerically by computers by use of the equation accumulation = inputs – outputs. A time step is selected for the model calculations by computers. The shorter the time step, the closer will the computer calculations come to the real time variations of inputs and outputs. It is recommended to test different time steps and use the longest time step that would not give any significant change of the model results by decreasing the time step. Significant changes are of course evaluated relative to the accuracy of the observations that are used as basis for the development of the model. The processes determining the inputs and outputs to the state variables, $C = f(\text{time})$, must, however, be formulated as an algebraic equation. [Table 2.1](#) gives an overview of the most applied process equations:

1. a constant flow rate—also denoted zero-order expression: $dC/dt = k$ ($t = \text{time}$)
2. a first-order rate expression, where the rate is proportional to a variable, for instance a concentration of state variables: rate = $dC/dt = k \times C$. This expression corresponds to exponential growth. The following expression is obtained by integration $C(t) = C_0 \times e^{kt}$
First-order decay has the rate = $dC/dt = -k \times t$ and $C(t) = C_0 \times e^{-kt}$.
3. a second-order rate expression, where the rate is proportional to two variables simultaneously.
4. a Michaelis-Menten expression or Monod kinetics known from kinetics of enzymatic processes. At small concentrations of the substrate the 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 are determined by a limiting nutrient according to Liebig's minimum law. The so-called Michaelis–Menten constant 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, while it is close to a zero-order rate expression at high concentrations. Notice furthermore that the rate is regulated from a first-order to a zero-order expression more and more as the concentration increases.

TABLE 2.1 Process Rate Equations

Expression	Mathematical Formulation	Application of the Process Rate Expression
Zero order	Rate = $k = \text{constant}$	Supply is constant f. inst. in film kinetics
First order	Rate = $k \times \text{variable}$	Decomposition of organic matter, decay of radioactive components, exponential population growth
Second order	Rate = $k \times \text{conc1} \times \text{conc2}$	Chemical and biochemical reactions, where the process is based on a reaction of two different components
Monod kinetics	Rate = $k \times \text{st.var.}/(\text{st.var.} + k_m)$	Plant growth by limiting nutrient (Liebig's law) and growth of organisms or populations limited by the food source, f. inst. grazing
Logistic growth	Rate = $k \times \text{st.var.} \times (1 - \text{st.var.}/\text{carrying capacity})$	Growth, where the rate at high values of the st.var. is regulated by another regulation factor
Conc. gradients	Rate = $k \times dC/dx$	Diffusion processes

5. a first-order rate expression with a regulation due to limitation by another factor, for instance the space of the nesting areas. It is expressed by introduction of a carrying capacity or upper limit for the state variables. The general first-order expression is applied regulated by the following factor: $(1 - \text{concentration}/\text{carrying capacity})$. When the concentration reaches the carrying capacity, the factor becomes zero and the growth stops. This process of rate expression is denoted logistic growth. These two growth expressions are often applied in population dynamic models, but may also be applied in biogeochemical models for instance to express the growth of an organism.
6. rates governed by diffusion often use a concentration gradient dC/dx to determine the rate, as it is expressed in Fick's laws: rate = $k \times (dC/dx)$ (Fick's First Law).

Table 2.1 summarizes the information about the applications of these six expressions: for which processes these equations are most often used. Most processes of ecological relevance are covered with these six expressions, although there of course are a few processes that will require another mathematical formulation. More than 90% of ecologically relevant processes in modeling may presumably be covered by these equations.

This short overview of processes equation used to express the input and outputs to the selected state variables demonstrates another advantage by biogeochemical models: the applied expression build, in most cases, on causality. The equations are rooted in the quantification of real ecological processes.

There are several modifications of the expressions in Table 2.1. For instance, sometimes a threshold concentration tr is used, in the Michaelis–Menten expression. The concentration (state variable) is replaced by the concentration $- tr$. The concentration has therefore to exceed tr to generate any rate. For grazing and predation is often used to multiply the

Michaelis–Menten expression by $(1 - \text{concentration}/\text{carrying capacity})$ similar to what is used in the logistic growth expression. It implies that when the food is abundant (concentration is high) another factor determines the growth for instance the space or the nesting area. These modifications are often used for development of a eutrophication model.

The equations contain, however, also constants as it is called most often in ecological modeling parameters and unfortunately they are frequently not known with low standard deviations, as they are biological constants in contrast to physical–chemical parameters that can be found with low standard deviation in physical–chemical handbooks. The biological parameters are dependent on a number of influential factors that may vary significantly from case to case. For instance the growth rates expressed by the unit $1/24$ h for well-defined species vary from ecosystem to ecosystem because the factors that influence the growth rate—for instance the presence of stones, the shelter, the presence of other organisms, the meteorological conditions—are different and the complexity is too high to take all these factors into account. The influence of these factors could be described sometimes but that would inevitably introduce other parameters which would only add to the uncertainty. The biological parameters require in most cases that they are calibrated by a comparison of model results with observations. It implies, however, a disadvantage of the model type, namely that the accuracy of the model is dependent on good observations. To achieve a model with a low standard deviation, it is important to have good observations. Consequently, the cost of developing a good biogeochemical model is mainly determined by the cost of providing quantitatively and qualitatively a good data base of observations to be used for calibration and validation.

Because this model type has been widely applied, applicable software is available to develop the model—relatively easily, which of course should be considered a significant advantage by the application of biogeochemical models.

The next sections will present the modeling elements followed by a section showing how to develop biogeochemical models. The proposed procedure should be considered as general for all model types. If the same steps are not applied in detail for all model types, then the considerations on how to develop the best reliable model are also given for all model types, in general. These two sections are based on the widely applied textbook by [Jørgensen and Fath \(2011\)](#).

2.2 MODELING ELEMENTS

In its mathematical formulation, an ecological model has five components ([Jørgensen and Fath, 2011](#)):

1. *Forcing functions, or external variables*, are functions or variables of an external nature that influence the state of the ecosystem. In a management context the problem to be solved can often be reformulated as follows: if certain forcing functions are varied, how will this influence the state of the ecosystem? The model is used to predict what will change in the ecosystem when forcing functions are varied with time. The forcing functions due to the human impact on ecosystems are called *control functions* because it is in our hands to change them. The control functions in ecotoxicological models are, for instance, discharge of toxic

substances to the ecosystems, and in eutrophication models are 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. They are in contrast to the control functions not controllable by man. By using models we will be able to address the crucial question: which changes of 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 most important organisms. In eutrophication models, the state variables will be the concentrations of nutrients and phytoplankton. When the model is used in a management context, the state variable values 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* are used to represent the biological, chemical, and physical processes. They describe the relationship between the forcing functions and state variables and between two or more state variables. The same type of process may be found in many different environmental contexts, which implies that the same equations can be used in different models. This does not imply, however, that the same process is always formulated by use of the same equation. Firstly, the considered process may be better described by another equation because of the influence of other factors. Secondly, 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 modelers refer to the description and mathematical formulation of processes as submodels. The most applied process formulations are presented by a short overview earlier in this chapter. Most of the applied equations build on causality, which means that they are quantifications of real ecological (physical, chemical, and biological) processes.
4. *Parameters* are 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 $\text{mg Cd}/(24 \text{ h} \times \text{kg of fish})$. Many parameters are not indicated in the literature as constants but as ranges, but even that is of great value in the parameter estimation, as will be discussed further in 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 biogeochemical modeling, but also in the applications of other model type—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 feedbacks in real ecosystems. The flexibility and adaptability of ecosystems is inconsistent with the application of constant parameters in the models. A new generation of models that attempts to use parameters varying according to ecological principles seems a possible solution to the problem, but a further development in this direction is absolutely necessary

before we can achieve an improved modeling procedure reflecting the processes in real ecosystems. This topic will be further discussed in Chapter 7.

5. *Universal constants*, such as the gas constant and atomic weights, are also used in many 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 modeling procedure, which will be treated in more detail in the next section. The verbal model is, however, difficult to visualize and it is, therefore, more conveniently translated into a *conceptual diagram*, which contains the state variables, the forcing functions, and how these components are interrelated by mathematical formulations of processes. The conceptual diagram shows with other words how the modeling elements 1–3 are related and connected.

Fig. 2.2 illustrates a conceptual diagram of the nitrogen cycle in a lake. The state variables are nitrate, ammonium (which is toxic to fish in the unionized form of ammonia), nitrogen in phytoplankton, nitrogen in zooplankton, nitrogen in fish, nitrogen in sediment, and nitrogen in

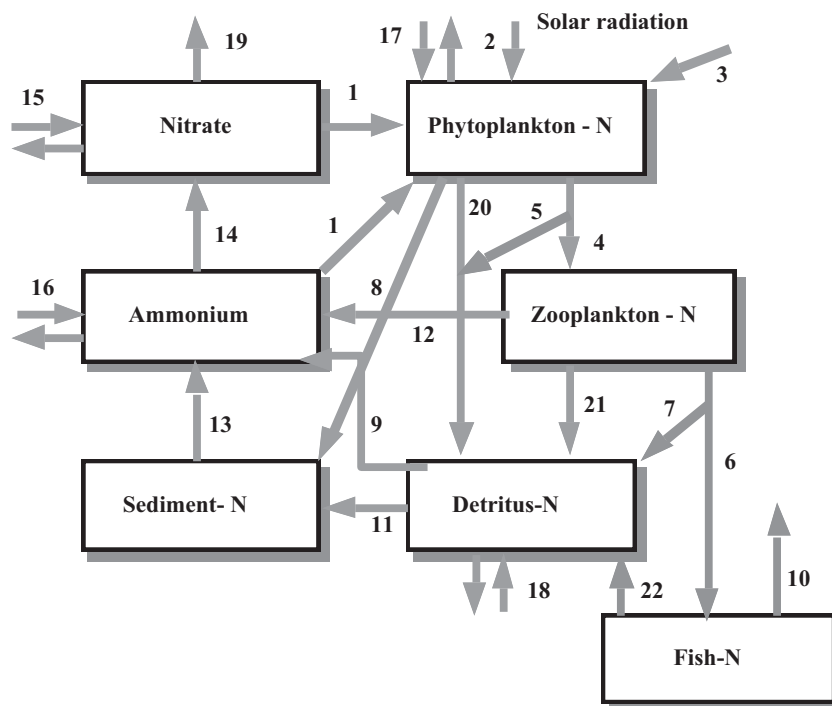


FIGURE 2.2 The conceptual diagram of a nitrogen cycle in an aquatic ecosystem. The processes are (1) uptake of nitrate and ammonium by algae, (2) photosynthesis, (3) nitrogen fixation, (4) grazing with loss of undigested matter, (5)–(7) are predation and loss of undigested matter, (8) settling of algae, (9) mineralization, (10) fishery, (11) settling of detritus, (12) excretion of ammonium from zooplankton, (13) release of nitrogen from the sediment, (14) nitrification, (15)–(18) are inputs/outputs, (19) denitrification, (20)–(22) mortality of phytoplankton, zooplankton, and fish.

in detritus. The state variables are in this conceptual diagram indicated as boxes that are 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, which is not shown in the diagram, but which influences all the process rates. The processes are formulated using quantitative expressions in the mathematical part of the model. Three significant steps in the modeling procedure need to be defined in this section before we go to the modeling procedure in detail. They are verification, calibration, and validation:

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

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 giving the best fit between observed and computed values. In some static models and in some simple models, which contain only a few well-defined, or directly measured, parameters, calibration may not be required, but it is generally recommendable to calibrate the model if observations of a proper quality and quantity are available.

Validation must be distinguished from verification. Validation consists of an objective test on 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 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 aims of the model, but the standard deviations between model predictions and observations and a comparison of observed and predicted minimum or maximum values of a particularly important state variable are frequently used. If several state variables are included in the validation, then they may be given different weights.

Further detail on these three important steps in modeling will be given in the next section where the entire modeling procedure will be presented.

2.3 THE MODELING PROCEDURE

A tentative modeling procedure is presented in this section. The detailed information is given for the development of biogeochemical models, but also other model types follow the general considerations that are presented. The author has used this procedure successfully numerous times and strongly recommends that all the steps of the procedure are used very carefully. To make shortcuts in modeling is not recommended. Other scientists in the field have published other slightly different procedures, but detailed examinations will reveal that the differences are only very minor. The most important steps of modeling

are included in all the recommended modeling procedures for biogeochemical models and to a certain extent for the development of all model types.

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 instead of being dispersed into irrelevant activities. The first modeling step is therefore a definition of the problem and the definition will need to be bound by the constituents of space, time, and subsystems. The bounding of the problem in space and time is usually easy, and consequently more explicit, than the identification of the subsystems to be incorporated in the model.

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 describable by causal relationships. [Fig. 2.3](#) shows the procedure proposed by the author, 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 at perfection in one step. The procedure should be considered as an iterative process and the main requirement is to get started ([Jeffers, 1978](#)).

It is difficult, at least in the first instance, to determine the optimum number of subsystems to be included in the model for an acceptable level of accuracy defined by the scope of the model. Due to lack of data, it will often become necessary at a later stage to accept a lower number than intended at the start or to provide additional data for improvement of the model. It has often been argued that a more complex model should account more accurately for the 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, by laboratory experiments, or by calibrations, which again are based on field measurements. Parameter estimations are never completely without errors, and the errors are carried through into the model and will thereby contribute to its uncertainty. The problem of selecting the right model complexity will be mentioned several times throughout the book. It is a problem of particular interest for modeling in ecology because ecosystems are very complex, but it does not imply that an ecological model to be used in research or environmental management necessarily 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 at a later stage, once experience with the verification, calibration, sensitivity analysis, and validation has been gained. Development of an ecological model should generally 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 [Fig. 2.2](#) can be used to illustrate the application of an adjacency matrix in modeling.

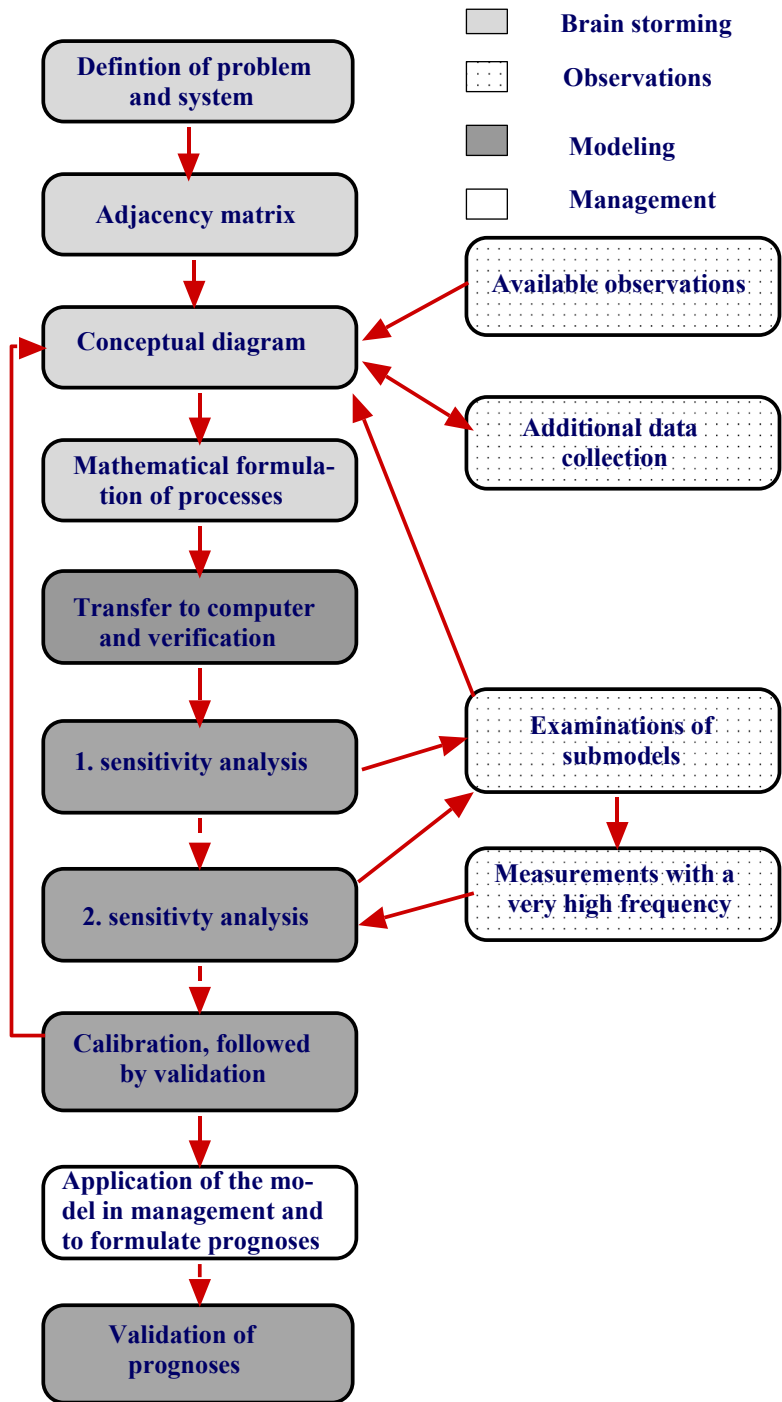


FIGURE 2.3 A tentative modeling procedure is shown. Ideally, as mentioned in the text, one should determine the data collection based on the model, not the other way round. Both possibilities are shown because models in practice have often been developed from available data, supplemented by additional observations. It is shown in the diagram that examinations of submodels and intensive measurements should follow the first sensitivity analysis. Unfortunately, many modelers have not had the resources to do so but have had to bypass these two steps and even the second sensitivity analysis. It must strongly be 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. It shows that modeling should be considered an iterative process.

Adjacency Matrix for the Model in Fig. 2.2

From	Nitrate	Ammonium	Phyt-N	Zoopl-N	Fish N	Detritus-N	Sediment-N
To							
Nitrate	–	0	1	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 modeler 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 nitrogen cycles in all aquatic ecosystems. If resuspension is important there should be a link between sediment-N and detritus-N. If the aquatic ecosystem is shallow, resuspension may be significant, while the process is without any effect in deep lakes. This example illustrates clearly the idea behind the application of an adjacency matrix 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 that actually are realized and should be included in the model.

Once the model complexity, at least as a first attempt, has been selected, it is possible to conceptualize the model as, for instance, in the form of a diagram as shown in Fig. 2.2. It will give information on which state variables, forcing functions and processes are required in the model.

Fig. 2.4 shows a simplification of the procedure illustrated in Fig. 2.3. The more simple procedure in Fig. 2.4 has a more general applicability for all model types.

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

The conceptual diagram in Fig. 2.2 indicates the state variables as boxes, for instance nitrate, and the processes as arrows between boxes, for instance process number one. The forcing functions are symbolized by arrows to or from a state variable, for instance 15 and 16. It is possible to use other symbols for the modeling components.

The software STELLA, which will be used to illustrate the development of models in several chapters of the book, applies 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

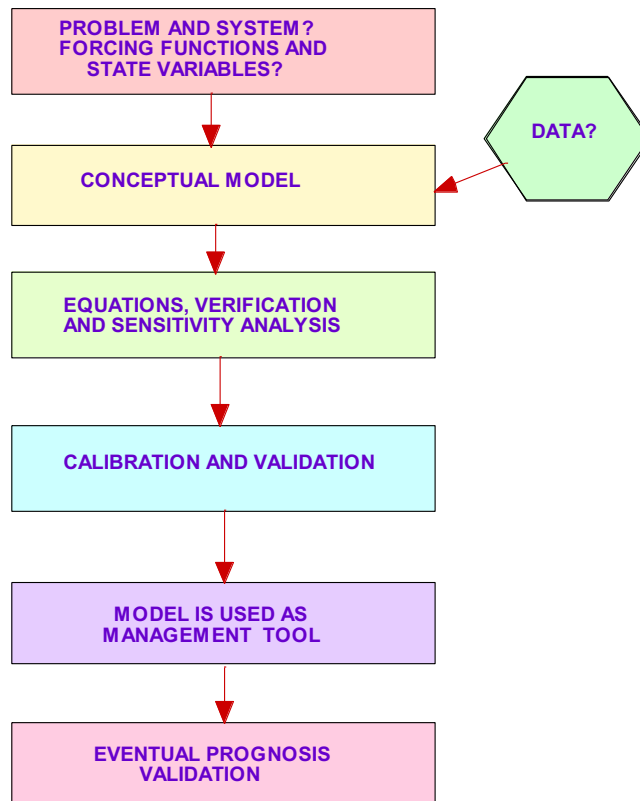


FIGURE 2.4 A slightly simpler model procedure than the one illustrated in Fig. 2.3. It has a more general applicability for all model types.

for the forcing functions (which require a constant, an equation, a table, or a graph), a thin arrow to indicate the transfer of information or variables (Controls—forcing function, parameter, and/or a state variable calculated by an algebraic expression from another state variable and so on); see Fig. 2.5.

There are other symbolic languages for development of conceptual diagrams, for instance Odum's energy circuit language. It has many more symbols than STELLA and is therefore 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 for instance Jørgensen and Bendoricchio (2001).

For each state variable, a differential equation is constructed: accumulation = inputs – outputs. For detritus-N, for instance in Fig. 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 attempted to be solved analytically in mathematics, but it is hardly possible with most ecological models because they are too complex. The differential equations are therefore solved numerically within the computer software. A time step is selected for the model calculations. The shorter the time step, the closer will the computer calculations

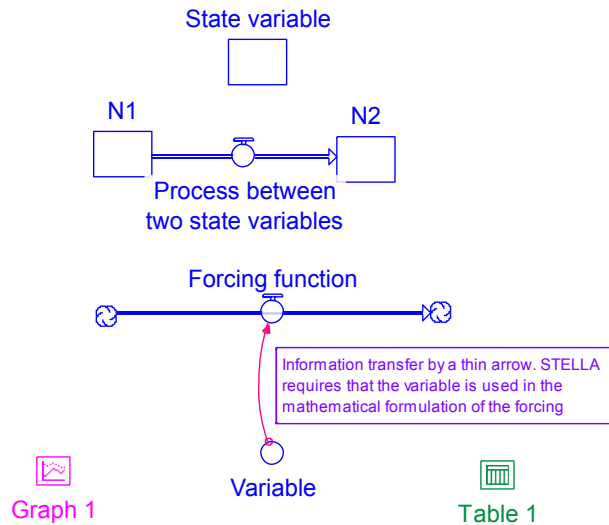


FIGURE 2.5 The symbols applied to erect a conceptual diagram using STELLA. State variables are boxes for which differential equations are erected as accumulation = inputs – outputs. Processes are thick arrows with the symbol of a valve. Forcing functions are thick arrow starting or ending as a cloud. Circles are variables in general. Graph 1 and Table 1 indicate that the results can be presented as graphs or as tables.

come to the real time variations of inputs and outputs; but the shorter the time step, the longer the simulation will take to run. It is recommended as previously mentioned to test different time steps and use the longest time step that would not give any significant change of the model results by decreasing the time step further. The term “significant changes” is of course evaluated relative to the accuracy of the observations that are used as basis for the development of the model.

The software STELLA 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 variable. The processes must, however, be formulated as an algebraic equation; see [Section 2.1](#).

The next steps of the modeling procedure include verification and sensitivity analysis. The latter is covered in the next section. Verification is a test of the internal model logic. Crucial questions about the model are asked and answered by the modeler. Verification is to some extent a subjective assessment of the behavior of the model.

[Findeisen et al. \(1978\)](#) give 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. The sequence verification, sensitivity analysis, and calibration must consequently 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 pertinent 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. A sufficiently long simulation period should be selected 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 modeler 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 modeler's intuition and knowledge of the models behavior. If the modeler 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 to a certain extent 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 BOD₅-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? etc. Numerous other examples can be given.

3. Are the applied units correct? 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?

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

To summarize this part of the verification:

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

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

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 chopper and buy 100,000 kg of phosphorus fertilizer and drop it instantly into a lake. The experiment could be made at no cost using the model, while it would be very expensive to rent a chopper and buy 100,000 kg of fertilizer. A major advantage of models is the ease 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 verification, one learns to know the model through its behavior, and the verification is furthermore 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 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 modeling procedure.

Sensitivity analysis follows verification. Through this analysis, the modeler 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 modeler wants to simulate a toxic substance concentration in, for instance, carnivorous insects as a result of the use of insecticides, one will obviously choose this state variable as the most important one, maybe besides the concentration of the toxic substance concentration in plants and herbivorous insects. The sensitivity analysis tries to assess the "weak points" of the model: which parameters, forcing functions, and processes should be known better because the model results are very sensitive

to the accuracy of this knowledge. In practical modeling, 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:

$$S = [\partial x/x]/[\partial P/P], \quad (2.1)$$

where x is the state variable under consideration.

The relative change in the parameter value is chosen based on our knowledge of the certainty of the parameters. If, for instance, the modeler estimates the uncertainty to be about 50%, 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 modeler 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, that is presented in [Jørgensen and Fath \(2011\)](#), is shown in [Table 2.2](#). It is used here to illustrate how to interpret the results of a sensitivity analysis. 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 indicate clearly that the parameters "maximum growth rate of phytoplankton and zooplankton," "mortality of zooplankton," and the "settling rate of 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 5%. On the other hand, the parameters "maximum denitrification rate," "mortality of fish," and "rate of mineralization" are significantly less important parameters. They all have a sensitivity of less

TABLE 2.2 Results of a Sensitivity Analysis of a 18 State Variable Model

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

than 0.1 or 10%. Therefore, they would change the phytoplankton less than 1% if the parameters are changed by 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 great changes are applied at this stage.
2. The most sensitive parameters are determined more accurately either by a calibration or by other means.
3. Under all circumstances, great efforts are made to obtain a relatively good calibrated model.
4. A second sensitivity analysis is then carried out using 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 given 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 further in 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. But, on the other hand, it is not necessary to have a sensitive parameter included in a submodel to obtain a sensitive submodel. A modeler 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.

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, however, to know more than one billion parameters. It is therefore obvious that in modeling there is a particular need for *parameter estimation methods*. This will be discussed further in Chapter 11, where methods to estimate ecotoxicological parameters based upon the chemical structure of the toxic compound are briefly presented. Notice in this context, that ecotoxicological models are biogeochemical models that focus on toxic and ecotoxicological compounds in the environment, but they use entirely the principles of biogeochemical models.

In all circumstances, it is a great advantage to give even approximate values of the parameters before the calibration gets started, as already mentioned above. It is, of course, much easier to search for a value between 1 and 10 than to search between 0 and $+\infty$. Even where

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

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

1. Most parameters in environmental science and ecology are not known as exact values. Therefore, all literature values for parameters (Jørgensen et al., 1991, 2000) have a certain uncertainty. Parameter estimation methods must be used when no literature value can be found, particularly ecotoxicological models, see, for instance, Jørgensen (1991, 1992a) and Chapter 11. In addition, we must accept that unlike many physical parameters, ecological ones are not constant but rather changing in time or situation (Jørgensen, 1986, 1992b, 2002). This point will be discussed further in Chapter 7, where the structurally dynamic model type is presented in detail.
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 as touched on. This will be discussed in more detail in Chapter 7.

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 to cover all combinations, which is an impossible task. Therefore, the modeler 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 above is redundant. If the automatic calibration should give satisfactory results within a certain frame of time, then it is necessary to calibrate only six to nine parameters simultaneously. Under any circumstances, it will become easier to find the optimum parameter set, the narrower the ranges of the parameters are before the calibration gets started.

In the trial-and-error calibration, the modeler has to set up, somewhat intuitively, some calibration criteria. For instance, you may want to simulate accurately the minimum oxygen

concentration for a stream model and/or the time at which the minimum occurs. When you are satisfied with these model results, you may then want to simulate the shape of the oxygen concentration versus time curve properly, and so on. You calibrate the model step by step to achieve these objectives step by step.

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

$$Y = \left[\left(\sum ((x_c - x_m)^2 / x_{m,a}) \right) / n \right]^{1/2} \quad (2.2)$$

where x_c is the computed value of a state variable, x_m is the corresponding measured value, $x_{m,a}$ is the average measured value of a state variable, and n is the number of measured or computed values. Y is followed and computed during the automatic calibration and the goal of the calibration is to obtain as low a Y -value as possible. Often, the modeler is, however, more interested in a good agreement between model output and observations for the one or two most important state variables, and less interested in a good agreement with other state variables. Therefore, one may choose weights 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 and considering the toxic substance concentrations in plants, herbivorous insects, and soil to be of less importance. Therefore, a weight of 10 is applied for the first state variable and only one for the subsequent three.

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

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

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

1. Find as many parameters as possible from the literature; see in this context [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 needed.
2. If some parameters cannot be found in the literature, which is often the case, the estimation methods mentioned in detail in [Jørgensen and Fath \(2011\)](#) and partially in Chapter 10 may

be used. For some crucial parameters, it may be recommendable 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 by use of 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 above-mentioned calibration methods may be used. In some cases, the modeler would repeat the 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.

The calibration should *always* be followed by a validation. By this step the modeler tests the model against an *independent* set of data 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 condition 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, which differ by the level of eutrophication. This is often impossible or at least very difficult as it may correspond to a complete validation of a prognosis, which at the 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 modeled 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, etc.

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 objectives of the model. A comparison between measured and computed data by use of an objective function (2.2) 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 modeler. 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 discussion of the validation can be summarized by the following issues:

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

Validation is a very important modeling step because it will give 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 a research tool, the validation will tell us whether the model results can be used to support or reject a hypothesis. The uncertainty determined by the validation relatively to the difference between the hypothesis and the model results will be decisive. In Chapter 8 of [Jørgensen and Fath \(2011\)](#), a eutrophication model with 18 state variables is 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 systems dynamics.
3. Are some important processes or components missing or described wrongly in the model? It is in this context, as previously mentioned, important to set up a mass and/or energy balance to reveal the most important processes and sources.
4. It is recommended to give a sufficiently comprehensive answer to question 3 and eventually use the model experimentally to find the best answer; see the examples of using models experimentally presented in Chapter 10. 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 we can, step-by-step, by steadily questioning the model and using the four points again and again, improve the model quality moving asymptotically toward the ideal model. An ideal model is, however, not necessary to have as 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 modeler.

2.4 ECOLOGICAL AND ENVIRONMENTAL BIOGEOCHEMICAL MODELS

This section attempts to present briefly the history of ecological and environmental modeling and to give an overview of how widely biogeochemical models have been applied. From the history we can learn why it is essential to draw upon the previously gained experience and what goes wrong when we do not follow the recommendations that we have been able to set up to avoid previous flaws.

Fig. 2.6 gives an overview of the history of ecological modeling. The nonlinear time axis gives approximate information on the year, when the various development steps took place. The first models of the oxygen balance in a stream (the Streeter-Phelps model) and of the prey–predator relationship (the Lotka–Volterra model) were developed back in the early 1920s. In the 1950s and the 1960s further development of population dynamic models took place. More complex river models were also developed in the 1960s. These developments could be named the second generation of models.

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

- follow strictly all the steps of the procedure, i.e., conceptualization, selection of parameters, verification, calibration, examination of sensitivity, validation.
- find a complexity of the model, which considers a balance between data, problem, ecosystem, and knowledge.
- a wide use of sensitivity analyses is recommendable in the selection of model components and model complexity make parameter estimations by using all the methods, i.e., literature review, determination by measurement in laboratory or in situ, use of intensive measurements, calibration of submodels and the entire model, theoretical system

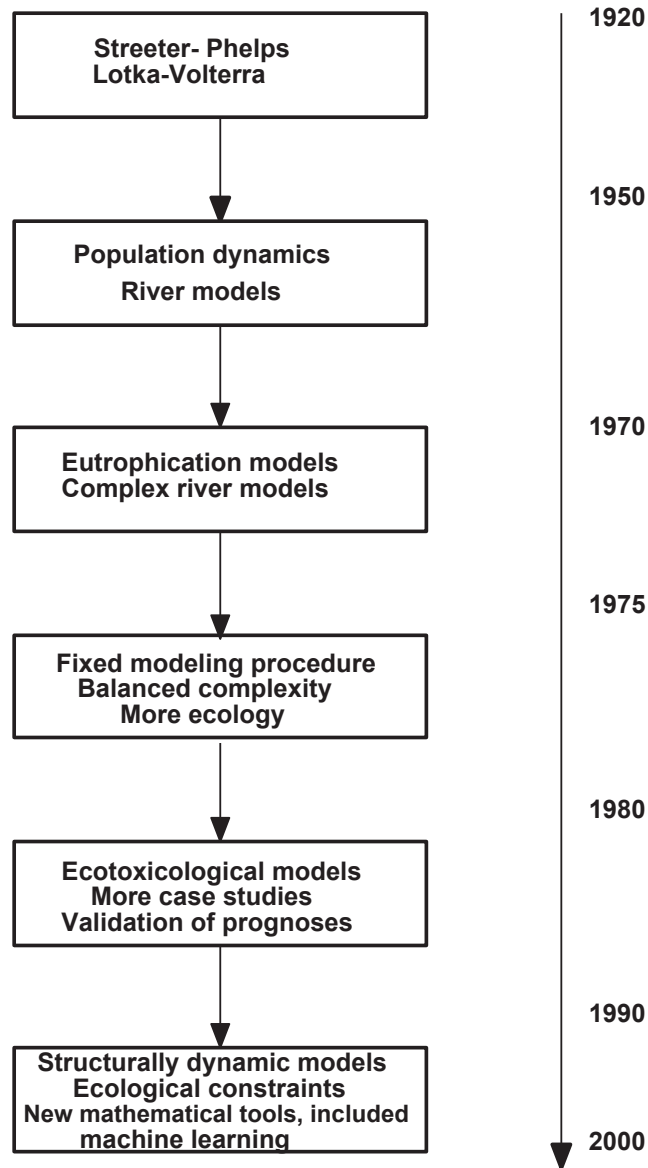


FIGURE 2.6 The development (history) of ecological and environmental models is shown schematically.

ecological considerations and various estimation methods based on allometric principles, and chemical structure of the considered chemical compounds.

Parallel to this development, ecologists became more quantitative in their approach to environmental and ecological problems, probably because of the needs, formulated by

environmental management. The quantitative research results by ecology from the late 1960s until today have been of enormous importance for the quality of the ecological models. They are probably just as important as the development in computer technology.

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

The conclusions from this period may be summarized in the following three points:

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

The shortcomings of modeling were, however, also revealed clearly in the third and fourth phase of modeling. It became clear that the models were rigid in comparison with the enormous flexibility, which was characteristic of ecosystems. The hierarchy of feedback mechanisms that ecosystems possess was not accounted for in the models, which made the models incapable of predicting adaptation and structural dynamic changes. Since the mid-1980s modelers have proposed many new approaches such as (1) fuzzy modeling, (2) examinations of catastrophic and chaotic behavior of models, and (3) application of goal functions to account for adaptation and structural changes. Application of objective and individual modeling, expert knowledge, and artificial intelligence offers some new additional advantages in modeling. It will in the last chapter of the volume discuss when it is advantageous to apply these approaches and what can be gained by their application. All these recent developments could be named the fifth generation of modeling. The model types from this model generation are covered in other chapters of the book.

The most significant development in ecological modeling is, however, that an enormous wide spectrum of models has been developed for a number of ecosystems and a number of environmental problems.

Table 2.3 reviews types of ecosystems, which have been modeled by biogeochemical models up to year 2000. An attempt has been made to indicate the modeling effort by using a scale from 0 to 5. 5 is very intense modeling effort, more than 50 different modeling approaches can be found in the literature; 4, intense modeling effort, 20–50 different modeling approaches can be found in the literature; 4–5 may be translated to class 4 but on the edge of an upgrading to class 5; 3, some modeling effort, 6–19 different modeling approaches are published; 2, few (2–5) different models that have been fairly well studied have been published; 1, one good study and/or a few not sufficiently well-calibrated and validated models; and 0, almost

TABLE 2.3 Biogeochemical Models of Ecosystems

Ecosystem	Modeling Effort
Rivers	5
Lakes, reservoirs, ponds	5
Estuaries	5
Coastal zone	4
Open sea	3
Wetlands	5
Grassland	4
Desert	1
Forests	5
Agriculture land	5
Savanna	2
Mountain lands	
(Above timberline)	1
Arctic and Antarctic ecosystems	2
Coral reef	3
Waste water systems	5
The ecosphere could maybe be added	5

no modeling effort have been published and even not one well-studied model. Notice that the classification is based on the number of different models not on the number of case studies where these models have been applied. In most cases the same models have been used on several cases studies.

Table 2.4 reviews similarly the environmental problems, which have been modeled up today. The same scale is applied to show the modeling effort as in Table 2.3. Table 2.4 covers besides biogeochemical models also models used for management of population dynamics in national parks and steady state models applied as ecological indicators. It is advantageous to apply goal functions in conjunction with a steady state model to obtain a good ecological indication, as proposed by Christensen (1991) and (1992).

The combinations of ecosystems and environmental problems are $16 \times 19 = 304$ and so far most of the 304 different models combining the two classifications can be found in the ecological modeling literature. Some of these combinations have been modeled even very extensively, for instance the climate change (the greenhouse effect) of the entire ecosphere, eutrophication of lakes, oxygen depletion of rivers, and heavy metal and pesticide pollution of grassland and agricultural land.

TABLE 2.4 Models of Environmental Problems

Problem	Modeling Effort
Oxygen balance	5
Eutrophication	5
Heavy metal pollution, all types of ecosystems	4
Pesticide pollution of terrestrial ecosystems	4–5
Other toxic compounds include ERA	5
Regional distribution of toxic compounds	5
Protection of national parks	3
Management of populations in national parks	3
Endangered species (includes population dynamic models)	3
Ground water pollution	5
Carbon dioxide/greenhouse effect	5
Acid rain	5
Total or regional distribution of air pollutants	5
Change in microclimate	3
As ecological indicator	4
Decomposition of the ozone layer	4
Relationships health–pollution	3
Consequences of climate changes	4
Water stress	5

In addition, numerous biogeochemical models have been developed for important processes in ecosystems—models that could be applied as submodels in ecosystem models associated with various environmental problems and models that are developed to understand better the results of combining important ecological processes or to reveal more details of a core part of the ecosystem that is particularly important for the development of the entire ecosystems.

In most of the other chapters, there are illustrative case studies that demonstrate the characteristic features of the model. There are, however, so many illustrations in the literature of this model type, that it seems redundant. Examples and illustrations can be found in Chapter 8 of [Jørgensen and Fath \(2011\)](#). Details are given in this reference for a medium complex eutrophication model (18 state variables), a relatively simple river model (3 state variables), and a wetland model (removal of nutrients by wetlands) with 25 state variables.

References

- Beck, M.B., 1978. Random signal analysis in an environmental sciences problem. *Applied Mathematical Modelling* 2, 23–29.
- Christensen, V., 1991. On ecopath, fishbyte, and fisheries management. *Fishbyte* 9 (2), 62–66.
- Christensen, V., 1992. Network Analysis of Trophic Interactions in Aquatic Ecosystems (Ph. Diss.). Royal Danish School of Pharmacy.
- Findeisen, W., Lastebro, A., Lande, R., Lindsay, J., Pearson, M., Quade, E.S., 1978. A Sample Glossary of Systems Analysis. Working Paper WP-78–12. International Institute for Applied Systems Analysis, Laxenburg, Austria.
- Jeffers, N.R.J., 1978. An Introduction to Systems Analysis with Ecological Applications. E. Arnold 220 pp.
- Jørgensen, S.E., Fath, B., 2011. *Fundamentals of Ecological Modelling*, fourth ed. Elsevier, Amsterdam. 400 pp.
- Jørgensen, S.E., 1986. Structural dynamic model. *Ecological Modelling* 31, 1–9.
- Jørgensen, S.E., 1991. A model for the distribution of chromium in Abukir Bay. In: Jørgensen, S.E. (Ed.), *Modelling in Environmental Chemistry*, vol. 17. Elsevier, Amsterdam.
- Jørgensen, S.E., 1992a. Parameters, ecological constraints and exergy. *Ecological Modelling* 62, 163–170.
- Jørgensen, S.E., 1992b. Development of models able to account for changes in species composition. *Ecological Modelling* 62, 195–208.
- Jørgensen, S.E., 2002. *Integration of Ecosystem Theories: A Pattern*, third ed. Kluwer Acad. Publ. Dordrecht, Boston, London. 428 pp.
- Jørgensen, S.E., Jørgensen, L.A., Kamp Nielsen, L., Mejer, H.F., 1981. Parameter estimation in eutrophication modelling. *Ecological Modelling* 13, 111–129.
- Jørgensen, S.E., Nors Nielsen, S., Jørgensen, L.A., 1991. *Handbook of Ecological Parameters and Ecotoxicology*. Elsevier, Amsterdam. Published as CD under the name ECOTOX, with L.A. Jørgensen as first editor in year 2000.
- Jørgensen, L.A., Jørgensen, S.E., Nielsen, S.N., 2000. *Ecotox*. CD.
- Jørgensen, S.E., Bendoricchio, G., 2001. *Fundamentals of Ecological Modelling*, third ed. Elsevier, Amsterdam. 628 pp.