

Chapter 2

Model Formulation

Model formulation is the step where our knowledge of a natural system is translated in mathematical form. It involves two steps: the construction of a conceptual model and the formulation of this conceptual model into mathematical equations.

We start by choosing the main components (state variables) and the flows that describe exchange of matter, energy or momentum, between them. We show that, based on the principle of *conservation*, the conceptual model equations simply express the rate of change of the state variables as the sum of all the flows that enter minus all flows that leave the compartment. This is conveniently depicted as a conceptual diagram or a flow chart, where the state variables are depicted by boxes, which are connected by arrows symbolising the flows.

In the next step, the flows are formulated explicitly as mathematical expressions. Although ecological systems are complex and cross many different levels (from cell to organism to an entire ecosystem), the processes share many features and can therefore be expressed with similar mathematical expressions. A number of basic and very simple rules apply. The most important one is that an ecological interaction (flow) can be written as the product of a maximal rate times the compartment performing the work, and, if appropriate, one or more limitation and inhibition terms.

Although the distinction is somewhat artificial, we discuss separately how to formulate ecological and chemical interactions, and how inhibition can be mathematically represented. We demonstrate that there exist several ways in which model equations can be coupled. Finally we discuss the forcing functions (driving variables) that are commonly used in ecological models.

2.1 Conceptual Model

At the stage of conceptual model formulation, we determine the model complexity. For practical as well as aesthetic reasons, a model should be as simple as possible, but not simpler (this quote has been ascribed to Einstein). The largest intellectual challenge of modelling consists in the creative simplification of a scientific problem, in such a way that no great injustice is done to realism.

The choice of modelled components and processes involves a subtle balance between realism and complexity. If knowledge is poor, then the model will be unable to contain many details. The more we know about a system, the more complex the model can be. However, the most complex model is not necessarily the most effective! Ecologists who have spent half their career studying all the details of a particular process, have a hard time accepting that neglecting, rather than incorporating, most of this knowledge will lead to better models. Yet, the will to make simplifications is the first step to becoming a modeller.

Note also that model complexity must depend on the problem to be solved. Thus, for one system, many different models may exist, all addressing different questions.

A conceptual model can be represented in a conceptual diagram or flow chart (Fig. 2.1) which contains the following components:

The **state variables** (or dynamic variables) are the components that we are interested in. In ecological models they are often the biomasses or densities of organisms, the concentrations of nutrients and so on. State variables are those variables that appear on the left-hand side of the model equations as time derivatives: we specify their rate of change in the model (see later), and after model solution will determine their values in time.

Time derivatives of a state variable represent the ‘speed’ at which the value of the state variable will change over an infinitesimal time period (dt) and are represented as: $\frac{d\text{StateVariable}}{dt}$.

In Appendix B we give a more elaborate definition of the concept.

In a flow chart, the state variables are often denoted by rectangular boxes connected by arrows. The arrows are the **flows or interactions** amongst the various state variables; they represent the external sources and sinks to a state variable, (where source arrows point towards and sinks leave the state variable boxes).

Forcing functions, or external variables, are important external factors that drive or regulate the system. As they are not calculated in the model and are not constant in time, they are generally imposed to (‘forced upon’) the model as a data series. Frequently used forcing functions in ecological models are: light intensity, temperature, flow rates, wind, inputs of toxic substances to ecosystems, rate of harvesting (effort) by humans...

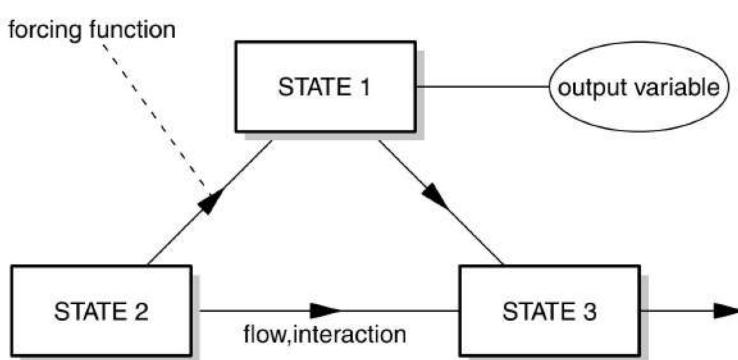


Fig. 2.1 Conceptual model diagram, with the main model components; STATE1, STATE2 and STATE 3 are state variables, connected by flows (arrows)

In addition to state variables, a model generally contains **output variables**. These often relate to measured quantities, and allow comparison of the model to reality. In addition, output variables can be instantaneous rates that one wants to inspect, or long-term averaged rates. They are computed based on other components of the model (forcing functions, state variables, parameters). For instance, algal biomass is a state variable in many aquatic models, but it is usually not measured as such. Chlorophyll, a related and more easily measurable quantity is often used as a proxy to algal biomass instead. In these models, chlorophyll will be an output variable that is calculated based on the state variable algal biomass (using a conversion factor) and that can be compared to the data. Other output variables in these models might be (instantaneous) net algal growth, or yearly averaged primary production, because these are interesting quantities.

Choosing an appropriate **spatial and temporal scale** is equally important at the stage of conceptual model formulation. For instance, in astronomy, one might choose a length scale that allows expressing, in not too large numbers, the distance between the sun and planets, whilst in molecular dynamics, the spatial scale should allow representing the distance separation between the atoms. Our choice of temporal and spatial scale of the model has great repercussion on the choice of processes to represent or not in the model. We will generally only crudely represent processes that fall outside of the model's scale window.

Together with the model components, and the temporal and spatial scales, we also decide about the **model currency**, the elemental composition in which we want to express the state variables. There are many different ways of expressing biomass in models. One can use dry weight or (especially for animals containing large calcareous structures) ash-free dry weight, carbon content, nitrogen content, phosphorus content, protein content, energy equivalents (i.e. energy released upon oxidation) or other measures. Important is to choose a currency that is both accurate and convenient. For instance, in models that describe phosphate, but not nitrate or ammonium, the best choice for biomass of living organisms will be in terms of phosphorus.

2.1.1 The Balance Equation of a State Variable

Most models that we will deal with in this book are concerned with the exchange of mass, energy or momentum. For instance, environmental models may describe:

- Uptake of dissolved inorganic nitrogen by phytoplankton (ecosystem models).
- Conversion of carbohydrates and nutrients into more complex proteins (physiological models).
- Heat transfer from the air to the water column (physical models)
- Transfer of momentum from air to sea by the action of the wind on the water (turbulence models)

One of the most powerful laws when studying such interactions is the **conservation law**. This law states that neither mass, energy nor momentum can be created or lost by ordinary means, i.e. flows of these quantities have to come from known sources, or go to known sinks. Stated otherwise, any flux entering some state variable should either accumulate in this state variable, or lead to another state variable or to a known sink.

When this principle applies, i.e. the state variable is expressed in mass, energy or momentum, we can state the **balance equation** for the state variable as:

$$\frac{d\text{StateVariable}}{dt} = \text{sources} - \text{sinks} \quad (2.1)$$

It expresses that a state variable can only change in time when there is either an external input (source) or an external output (sink), i.e. material flows into or out of the state variable.

Consider the following simple model (Fig. 2.2): two state variables (SV1 and SV2) are connected with one flow (F1); F0 is a flow from the external world to state variable 1 (SV1), whilst F2 leaves state variable 2 to the external world. The conservation law states that any increase in mass (or energy, momentum) of state variable 2, due to F1 induces an equally large decrease in the magnitude of state variable 1. The total mass in the model (sum of SV1 and SV2) changes due to F0 and F2.

We may write the balance equations, representing the rate of change of the state variables as:

$$\begin{aligned} \frac{d\text{SV1}}{dt} &= F_0 - F_1 \\ \frac{d\text{SV2}}{dt} &= F_1 - F_2 \end{aligned} \quad (2.2)$$

We now use the conservation of mass principle to test whether the model makes sense. The easiest test is by making total mass budget calculations. If the model conserves mass, then the total mass in the model should change only due to flows

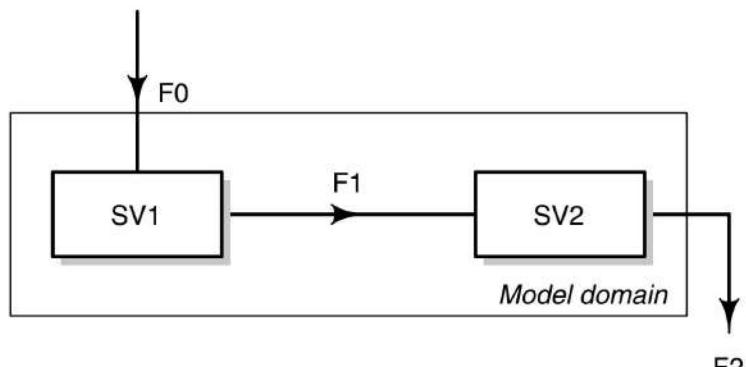


Fig. 2.2 Illustration of the balance equation of state variables. See text for details

External world

from and to the external world. In the simple model example total mass changes as:

$$\frac{dSV1}{dt} + \frac{dSV2}{dt} = F0-F1+F1-F2 \\ = F0-F2 \quad (2.3)$$

Total mass changes only due to flows connecting the model domain with the external world, therefore, the model is mass conserving.

Note: the conservation principle does not apply to all conceivable state variables. Many ecological models use individuals as their currency. In many models (e.g. predator-prey models), individuals is a proxy for mass and in these cases the conservation principle still holds. However, in other models transfer of mass is not considered. For instance, in population models, newborns may be generated in the youngest age class, depending on numbers in the reproductive age classes, without conservation: the numbers in the reproductive age classes do not decrease because they have given rise to newborns.

In this book, we mainly deal with models for which the conservation principle does hold. Yet, you may find examples of non-conservative models in Chapter 9 (structured population models) and Chapter 3 (cellular automata models).

2.1.2 Example: Conceptual Model of a Lake Ecosystem

Consider a conceptual model of a whole lake. The model contains 6 state variables: Phytoplankton (PHYTO), zooplankton (ZOO), detritus (DETRITUS), ammonium (NH_4^+), fish (FISH), and bottom detritus (BotDET). The state variables are connected by 13 flows. There is one forcing function (solar radiation) and one output variable (Chlorophyll). In Fig. 2.3, the conceptual diagram is drawn.

As the model also describes ammonium, it is convenient to take nitrogen as the **model currency**, so the units of all the state variables are concentrations, expressed in mmol N m^{-3} . The law of conservation of mass applies to the balance equations of all state variables.

The components typically change seasonally, in a time window of one to a few years, so a day will be a suitable model **time unit**, and consequently, all rates will be expressed per day.

As we are not interested in spatial patterns of ecosystem changes within the lake, the **spatial scale** chosen is the entire lake.

Based on the model diagram (Fig. 2.3), we use the flows that describe exchange of matter between the state variables to generate the **conceptual model equations**. These equations simply relate the rate of change of the state variables to the flows.

For instance, the statement:

$$\frac{d\text{NH}_4^+}{dt} = f11+f10 + f4-f1 \quad (2.4)$$

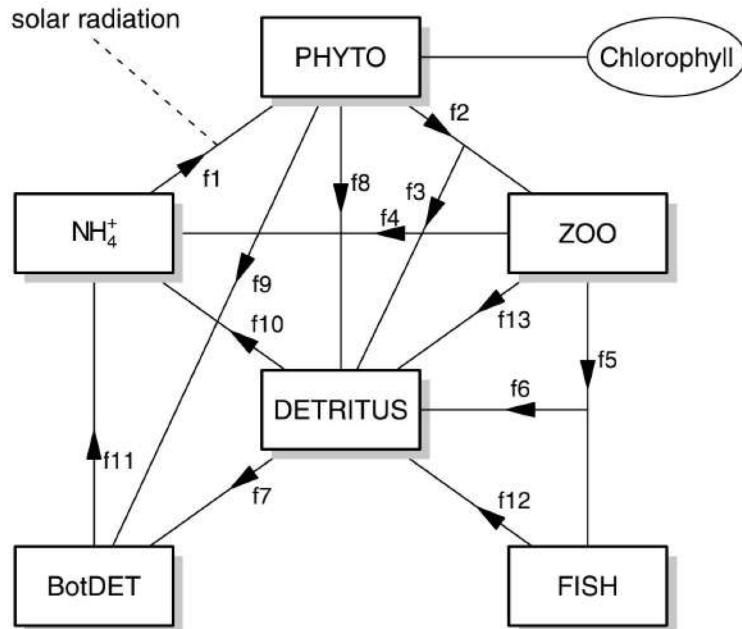


Fig. 2.3 Conceptual diagram of the lake ecosystem model. State variables are denoted by rectangular boxes, flows with arrows, forcing functions with a dashed line and the output variable with an ellipse

states that the ammonium concentration will increase as a result of mineralization of bottom detritus (flow 11), mineralization of suspended detritus (flow 10) and excretion of zooplankton (flow 4). It will decrease due to uptake by phytoplankton (flow 1).

With the state variable NH₄⁺ expressed in mmol N m⁻³, and the time unit of days, the rate of change, dNH₄/dt, is expressed in mmol N m⁻³ day⁻¹. Consequently, all flows are also expressed in mmol N m⁻³ day⁻¹.

The full conceptual model describes the rate of change of all state variables. The rate of change is simply the sum of all flows that enter the compartment minus all the flows that leave the compartment:

$$\begin{aligned}
 \frac{d\text{PHYTO}}{dt} &= f_1 - f_2 - f_8 - f_9 \\
 \frac{d\text{ZOO}}{dt} &= f_2 - f_3 - f_4 - f_5 - f_{13} \\
 \frac{d\text{DETRITUS}}{dt} &= f_3 + f_8 + f_6 + f_{12} + f_{13} - f_7 - f_{10} \\
 \frac{d\text{FISH}}{dt} &= f_5 - f_6 - f_{12} \\
 \frac{d\text{BOTTOMDETRITUS}}{dt} &= f_7 + f_9 - f_{11} \\
 \frac{d\text{NH}_4^+}{dt} &= f_{11} + f_{10} + f_4 - f_1
 \end{aligned} \tag{2.5}$$

2.1.3 Conservation of Mass and Energy as a Consistency Check

We now use the conservation law to check whether the model makes sense and is correctly solved (more about this later). Already at the stage of the conceptual model, we may test whether any flux leaving some state variable actually accumulates in another state variable, or leads to a known sink. The easiest way to test that is either by making mass budget calculations or by calculating the total load.

1. *Total load* can be used as a check when there is no external source or sink compartment. This is the case in the example of Section 2.1.2, where all arrows (flows) connect state variable boxes, no arrow points from or to the outside world. Then, total mass should be constant, and we can easily check for that by calculating the rate of change over time of the sum of all components:

$$\begin{aligned}
 & \frac{d[\text{PHYTO} + \text{ZOO} + \text{DETRITUS} + \text{FISH} + \text{BOTTOMDETRITUS} + \text{NH}_4^+]}{dt} \\
 &= \frac{d\text{PHYTO}}{dt} + \frac{d\text{ZOO}}{dt} + \frac{d\text{DETRITUS}}{dt} + \frac{d\text{FISH}}{dt} + \frac{d\text{BOTTOMDETRITUS}}{dt} + \frac{d\text{NH}_4^+}{dt} \\
 &= f1 - f2 - f8 - f9 + f2 - f3 - f4 - f5 - f13 + f3 + f8 + f6 + f12 + f13 - f7 - f10 \\
 &\quad + f5 - f6 - f12 + f7 + f9 - f11 + f11 + f10 + f4 - f1 \\
 &= 0
 \end{aligned} \tag{2.6}$$

If mass is not conserved in this calculation, i.e. when the sum of all flows is not zero, we have an error. Every error, no matter how small, should be traced back.

2. *Mass budget* calculation is often the only available method when there is an external sink or source compartment. For instance, in pelagic ecological models that have carbon as their currency, it is not customary to include CO₂ as a state variable, as it is rarely limiting primary production. Nevertheless, CO₂ acts as a source of modelled carbon through photosynthesis, and as a sink of modelled carbon through biological respiration (that is, CO₂ is an external sink and source of C). In such models, the total amount of carbon in the model will generally not be constant. Through mass budget analysis, we inspect if the sum of all rate of changes and external sinks and sources are zero.

To illustrate the point, we have made a different model for our lake, this time expressed in carbon as the model currency, but essentially containing the same fluxes (Fig. 2.4). There are 5 flows that connect the model with the outside world (in this case CO₂, which is not modelled). They are the primary production flow (f1), a source, and four respiration flows (f4, f10, f11, f14), which remove carbon from the modelled system (sinks). The rate of change of the state variables can be easily written as:

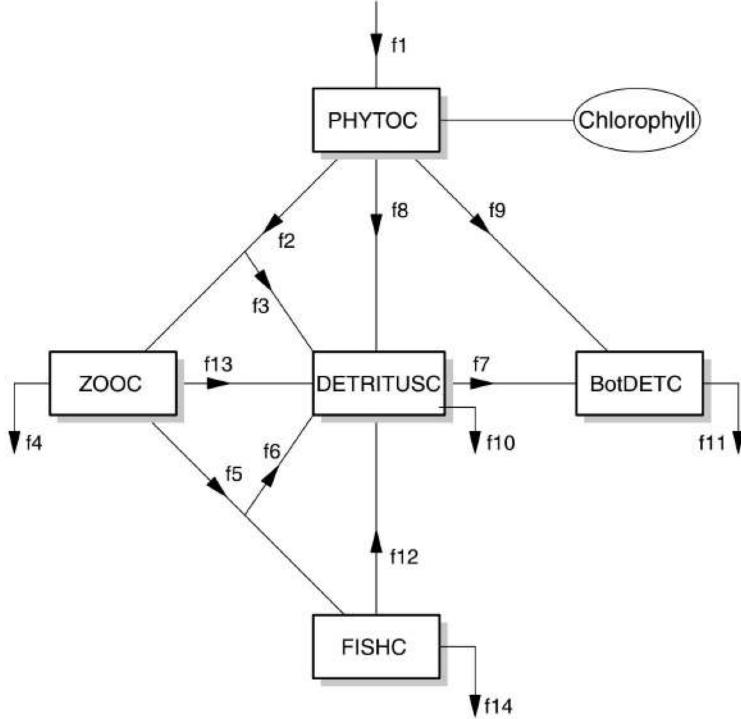


Fig. 2.4 Conceptual diagram of the lake ecosystem model, now expressed in units of carbon. Note the presence of flows from and to the outside world (f1,f4,f10,f11 and f14)

$$\begin{aligned}
 \frac{d\text{PHYTOC}}{dt} &= f_1 - f_2 - f_8 - f_9 \\
 \frac{d\text{ZOOC}}{dt} &= f_2 - f_3 - f_4 - f_5 - f_{13} \\
 \frac{d\text{DETRITUSC}}{dt} &= f_3 + f_8 + f_6 + f_{12} + f_{13} - f_7 - f_{10} \\
 \frac{d\text{FISHC}}{dt} &= f_5 - f_6 - f_{12} - f_{14} \\
 \frac{d\text{BOTTONDETRITUSC}}{dt} &= f_7 + f_9 - f_{11}
 \end{aligned} \tag{2.7}$$

while the mass budget can be written as:

$$\begin{aligned}
 &\frac{d[\text{PHYTOC} + \text{ZOOC} + \text{DETRITUSC} + \text{FISHC} + \text{BOTTONDETRITUSC}]}{dt} \\
 &= \frac{d\text{PHYTOC}}{dt} + \frac{d\text{ZOOC}}{dt} + \frac{d\text{DETRITUSC}}{dt} + \frac{d\text{FISHC}}{dt} + \frac{d\text{BOTTONDETRITUSC}}{dt} \\
 &= f_1 - f_2 - f_8 - f_9 + f_2 - f_3 - f_4 - f_5 - f_{13} + f_3 + f_8 + f_6 + f_{12} + f_{13} - f_7 - f_{10} + \\
 &\quad + f_5 - f_6 - f_{12} + f_7 + f_9 - f_{11} \\
 &= -f_4 - f_{10} - f_{11} - f_{14} + f_1
 \end{aligned} \tag{2.8}$$

As this is simply the sum of the external input- external outputs, we conclude that mass is conserved in the model.

2.1.4 Dimensional Homogeneity and Consistency of Units.

Not only mass conservation, but also consistency of units is an important technique to check the consistency of a model. To introduce it we must make the distinction between *quantities* and *units*, where the units are the numerical dimensions of a certain quantity. In addition, there is a distinction between *primary* (or fundamental) and *derived* quantities and units.

The fundamental units and quantities, consistent with the Système International (SI) are:

- Unit meter (m) for quantity length
- Unit kilogram (kg) for quantity mass
- Unit second (s) for quantity time
- Unit Kelvin (K) for quantity temperature
- Unit mole (mol) for quantity amount of substance

A quantity is taken as primary if it can be assigned a standard of measurement independent of that chosen for the other fundamental quantities.

Derived quantities and units are expressed as a function of the primary quantities and units. Examples:

- Unit m^2 for quantity area
- Unit $m\ s^{-1}$ for quantity velocity
- Unit $mol\ m^{-3}$ for quantity concentration
- Unit $N = kg\ m\ s^{-2}$ for quantity force

Units can be manipulated just as numbers, using the simple rules of multiplication and division.

For example, the units of mass-specific energy, Joule kg^{-1} can be written in primary units as follows: with Joule = $kg\ m^2s^{-2}$, joule $kg^{-1} = (kg\ m^2s^{-2})kg^{-1} = m^2s^{-2}$.

An equation is *dimensionally homogeneous* and has *consistent units* if the units and quantities on two sides of an equation balance.

- It is not allowed to add, for instance, length to area, or concentration to flux in one equation (dimensional homogeneity).
- Moreover, it is not allowed to add grams to kilograms, or to add $mol\ m^{-3}$ to $kg\ m^{-3}$ (consistency of units).

We can use the principle of dimensional homogeneity and consistency of units in two ways:

- To test whether an equation makes sense
- To derive the (unknown) units of a quantity.

As an example of the latter, consider the mathematical equation which expresses the extinction of light in a water column (Lambert-Beer law):

$$\frac{dI}{dz} = -\lambda \cdot I \quad (2.9)$$

where I is light intensity, expressed in $\mu\text{mol m}^{-2} \text{ s}^{-1}$ (or, equivalently, $\mu\text{Einst m}^{-2} \text{ s}^{-1}$), z is depth (m), dI/dz is the rate of change of light with depth and λ is a first-order decay coefficient, known as the extinction coefficient.

Dimensional analysis readily shows that units of λ must be reciprocal to units of z , therefore must be equal to m^{-1} :

$$\frac{\text{Units}(I)}{\text{Unit}(z)} = \text{Unit}(\lambda) \cdot \text{Unit}(I) \quad (2.10)$$

which, after removing the common terms on the left and right hand side:

$$\frac{1}{\text{Unit}(z)} = \text{Unit}(\lambda) \quad (2.11)$$

with Unit of $z = \text{m}$, units of λ must equal m^{-1} .

The analytical solution of the Lambert-Beer equation, expressing light intensity as a function of depth is:

$$I_z = I_0 e^{-\lambda z} \quad (2.12)$$

Where I_0 is the light intensity at depth 0 (the air-water interface).

As exponents can only be taken of dimensionless quantities, it again follows that the units of λ and depth must balance.

2.2 Mathematical Formulations

In the previous Section (2.1), we wrote the model as a set of conceptual balance equations. These express the rate of change of a state variable as a function of sources and sinks (the flows). The remaining problem is to write a mathematical expression for each of the flows in terms of the state variables.

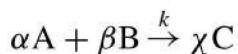
In this step of model building, we make use of relationships from the literature, or from theoretical considerations. Most typically, an interaction or flow is written as a function of the state variables, forcing functions and parameters. The parameters are coefficients that control model processes but do not change in the model. Some parameters are very well known (gas constants, atomic weights...), whereas others are only known approximately, e.g. the maximal grazing rate of zooplankton, the sinking rate of phytoplankton.

In the following two sections we take a closer look at how to express ecological interactions and chemical reactions. We start with chemical reactions, as these are generally simpler to formulate.

2.3 Formulation of Chemical Reactions

2.3.1 The Law of Mass Action

Consider first the example in Fig. 2.5B, where substance A reacts with substance B to give substance C, in the reaction:



Reaction rates are generally expressed using the law of mass action. This law states that the rate of the reaction is proportional to a power of the concentrations of all substances taking part in the reaction:

$$\text{ReactionRate} = k \cdot [A]^\alpha \cdot [B]^\beta \quad (2.13)$$

where k is the proportionality constant (units of conc $^{1-(\alpha+\beta)} t^{-1}$) and α and β are integer powers. Note that the constants α and β are also the stoichiometric constants in the reaction equation. This is generally the case, but not always.

The hypothesis behind this formulation is that this type of elementary reaction will occur only if the molecules collide. The probability for a molecule of A to collide with a molecule of B is proportional to the concentrations of A and B, so the total number of collisions will be proportional to $[A] \cdot [B]$. If more than one molecule of A is participating in the reaction (e.g. $\alpha = 2$), the probability of an A-B complex to collide a second time with an A molecule is again proportional to A, so finally the number of A-A-B complexes formed per unit of time is proportional to $[A]^2 \cdot [B]$. The reasoning can be simply extended for other values of α and β .

Also note our use of square brackets ($[]$). This is standard notation for concentrations in chemistry, so, as long as we deal with chemical models only, we will stick to this formalism. However, it is very awkward for biological quantities, thus we do not use this notation for biological models.

The *order* of the reaction is the sum of the powers.

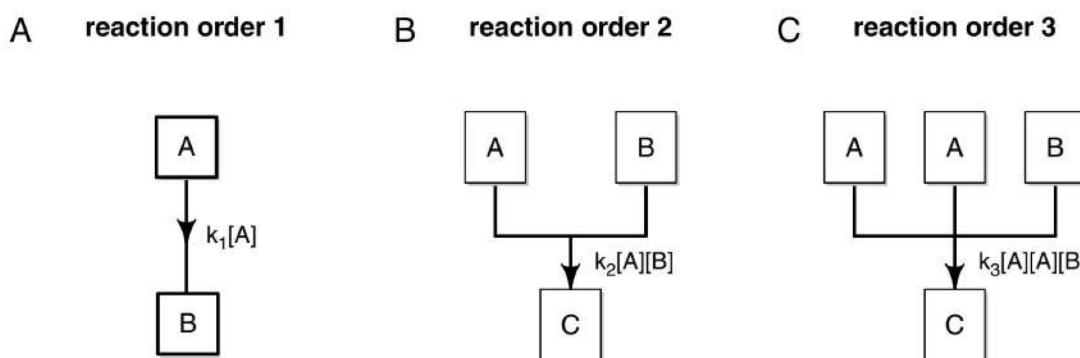


Fig. 2.5 Chemical reactions of different orders and the reaction rates

- In **first-order reactions**, the reaction rate is proportional to the concentration of one substance (Fig. 2.5.A):

$$R1 = k_1 \cdot [A] \quad (2.14)$$

- **Second-order reactions** arise either by the interaction of two substances or they are second order of the concentration of one substance (Fig. 2.5.B).

$$\begin{aligned} R2 &= k_2 \cdot [A] \cdot [B] \\ R2 &= k_2 \cdot [A]^2 \end{aligned} \quad (2.15)$$

- Sometimes the order of the reaction formulation is lower than would be expected based on the reaction equation. This happens when one of the reactants is always present in a concentration that far exceeds that of the other reactant (water is an extreme example). In such a case, the reaction rate can be simply written as a function of the concentration of the limiting reactant only.

A special case appearing as a result of this reduction of order are **zero-order reactions**. Here the reaction rate is assumed to be constant and independent of the reactant(s). Obviously, such a formulation can only be used when the reactants are always present in sufficient quantities, and the reaction rate itself is limited by some other factor, e.g. the availability of reactive surfaces catalyzing the reaction. A model using zero-order reaction for substances in short supply can be very wrong: it will predict that the reaction will continue even when the reactant has zero concentration!

2.3.2 Example: A Simple Chemical Reaction

As stated above, the powers are determined by the stoichiometry of the reaction. Consider the following reversible chemical reaction (Fig. 2.6 A), where one mole of substance C reacts with 2 moles of substance D to form one mole of E; the forward reaction has reaction rate constant k_1 ; the backward reaction rate constant k_2 .

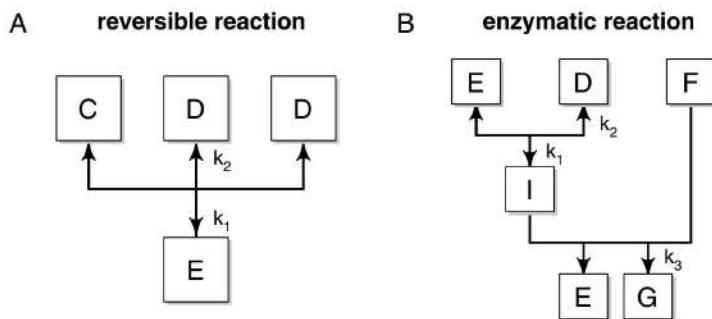


The differential equation that describes the rate of change of E is:

$$\frac{d[E]}{dt} = -k_2 \cdot [E] + k_1 \cdot [C] \cdot [D]^2 \quad (2.17)$$

Where the concentration of D is raised to the power 2 because two molecules of D are needed per molecule of E.

Fig. 2.6 A. Reversible reactions occur in both directions. **B.** An enzymatic reaction, where the enzyme E reacts with substance D to form an intermediate substance I. k_1, k_2, k_3 are the rate coefficients (see text)



The rate of change of D is given by:

$$\frac{d[D]}{dt} = 2 \cdot (k_2 \cdot [E] - k_1 \cdot [C] \cdot [D]^2) \quad (2.18)$$

the multiplication with 2 is because two moles of D are produced per mole of E consumed, and vice versa: two molecules of D disappear for every molecule of E formed.

2.4 Enzymatic Reactions

Enzymatic reactions are crucial to the functioning of organisms. Enzymes catalyze chemical reactions, but take no part in it, in the sense that enzymes are neither produced nor consumed in the reaction. We have depicted the scheme of an enzymatic reaction in Fig. 2.6 B:



One of the reactants, an enzyme, E, chemically reacts with product D forming an intermediary product, I. This intermediary product then in turn enters a reaction with substance F from which the enzyme E is released, together with another product G. The first reaction is reversible with rate coefficient k_1 (forward) and k_2 (backward reaction); the second reaction is irreversible, with rate coefficient k_3 .

In the model of this reaction, there are five state variables, the concentrations of the five substances. The five basic differential equations that define their rate of change are given by:

$$\begin{aligned}
 \frac{d[D]}{dt} &= -k_1 \cdot [E] \cdot [D] + k_2 \cdot [I] \\
 \frac{d[I]}{dt} &= k_1 \cdot [E] \cdot [D] - k_2 \cdot [I] - k_3 \cdot [I] \cdot [F] \\
 \frac{d[E]}{dt} &= -k_1 \cdot [E] \cdot [D] + k_2 \cdot [I] + k_3 \cdot [I] \cdot [F] \\
 \frac{d[F]}{dt} &= -k_3 \cdot [I] \cdot [F] \\
 \frac{d[G]}{dt} &= k_3 \cdot [I] \cdot [F]
 \end{aligned} \tag{2.20}$$

For instance, substance D is produced by the conversion of substrate I, which occurs at rate $k_2 \cdot [I]$; D is consumed by its reaction with the enzyme E, which occurs at a rate $k_1 \cdot [E] \cdot [D]$.

Solving this full set of reactions is awkward. Luckily, under most circumstances it can be simplified considerably. We will derive this simplification mathematically later in the book (Section 8.3.1). Here we simply bring forward the result. Essentially, the reaction can be modelled as a reaction between substances D and F, producing substance G, if the reaction rate formulation is adapted using the so-called Michaelis-Menten kinetics:

$$\frac{d[G]}{dt} = k' [F] \frac{[D]}{[D] + ks} \tag{2.21}$$

where k' and ks are parameters, recalculated from the elementary constants in the full formulation (Eq. 2.20). The Michaelis-Menten kinetics plays an important role in the formulation of biological interactions, as we will see in the next chapters.

2.5 Basic Formulation of Ecological Interactions

Ecological models usually describe the dynamics of organisms, which are significantly more complex than the simple molecules of previous section. Consequently, the formulations of ecological interactions are somewhat different from the chemical reactions. To illustrate why, we start with a simple example.

2.5.1 Example: Flows to and from Phytoplankton in the Lake Ecosystem

We take a closer look at the PHYTO compartment in the lake ecosystem example of Section 2.1.2. Four fluxes are defined in the equation for phytoplankton:

$$\frac{d\text{PHYTO}}{dt} = f_1 - f_2 - f_8 - f_9 \tag{2.22}$$

Here, f_1 is the primary production flux; as this model uses nitrogen as its currency, the primary production is in fact the incorporation of ammonium. The other fluxes are loss fluxes, due to sinking and formation of bottom detritus (f_9), mortality and formation of pelagic detritus (f_8) and ingestion by zooplankton (f_2).

2.5.1.1 A first attempt: first-order reaction?

Focusing on the primary production flux f_1 , we could naively represent this as a kind of chemical reaction (Fig. 2.7A):



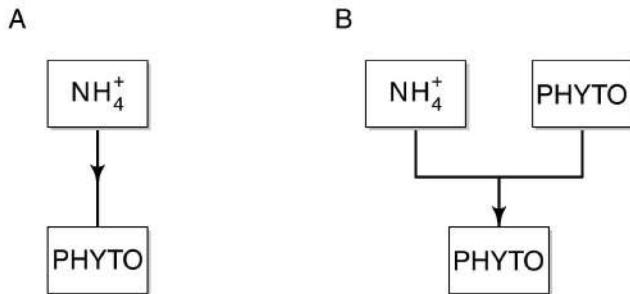
and express the rate of this ‘reaction’, following the law of mass action, as a first-order reaction rate in the ammonium concentration. Now suppose that we have clear water without any phytoplankton, but with a certain concentration of ammonium, then this naïve model tells us that ammonium is going to transform spontaneously into phytoplankton. This *generatio spontanea* used to be a popular concept in biology some centuries ago, but since Pasteur we know that this is a capital mistake. No phytoplankton should be generated when there is no phytoplankton. We conclude that this simple formulation as a first-order chemical reaction is not applicable, and a basic element is missing.

That missing element is the regulation of fluxes by the activity of the organisms themselves. Thus, the formulation should be such that the flux is zero when the organism responsible for this flux has zero concentration (or numbers, biomass, depending on the currency of the model). With ‘the organism responsible for this flux’ we mean the organism that ‘does the work’, whose physiological apparatus (e.g. uptake mechanisms, enzymes) is needed for the reaction to take place. Algae actively pump ammonium from the water into their cell, involve this ammonium in a series of enzymatic reactions, to finally build N-containing organic material, such as proteins. All this would not happen if the full physiological apparatus of the algae would not be present and would not be working in a complex, ordered, way.

2.5.1.2 A Second Attempt: Second-Order Reaction?

How does the flux f_1 scale with phytoplankton when it is present? Compare two situations, one with $\text{PHYTO}=0.1 \text{ mmol N m}^{-3}$, and another with $\text{PHYTO}=1 \text{ mmol N m}^{-3}$, everything else (light conditions, ammonium concentration etc.) being the same. In the first situation the phytoplankton in the lake will be producing at a certain rate. This production is divided over all the individual phytoplankton cells, which will each display a certain degree of activity. In the second situation, there are ten times as many phytoplankton cells present, but each cell will find itself in exactly the same external conditions as in the first case. It is, thus, natural to suppose that they will show exactly the same activity. Consequently, the total population of phytoplankton will be ten times as active in the second situation as in the first. We conclude that the rate f_1 should be proportional to the biomass of the phytoplankton, although other terms could also be involved:

Fig. 2.7 Uptake of ammonium by phytoplankton represented as a ‘first-order’ reaction (**A**) and as a ‘second-order reaction’ (**B**)



$$f_1 = a \cdot \text{PHYTO} \dots \quad (2.24)$$

What other terms could be involved in this flux? When there is no ammonium present, nothing can be taken up and the phytoplankton will not grow (note that we do not model any other nitrogen source for phytoplankton). So a logical second attempt at modelling the flux could be to consider the process as a second-order reaction (Fig. 2.7B).

It is difficult to assign ‘stoichiometric coefficients’ to the ‘reactants’ in this reaction, but in the simplest possible approach we could put them equal to one and write for the flux f_1 :

$$f_1 = a \cdot [\text{NH}_4^+] \cdot \text{PHYTO} \dots \quad (2.25)$$

With this formulation, we have found a way to limit the magnitude of the flux when there is no or little substrate.

However, problems remain. It is not a good idea to make the flux directly proportional to ammonium concentration: at a certain concentration of ammonium the phytoplankton will have plenty of nutrients, but will be limited by the intrinsic capacity of its physiological apparatus. With increasing ammonium concentration, the flux f_1 will asymptotically approach this maximum capacity.

2.5.1.3 A Last Attempt: Using a Rate Limiting Term

We solve this problem by defining a *rate limiting term*, i.e. a function $f(\text{NH}_4^+)$ that becomes zero when NH_4^+ is zero, and tends to 1 when ammonium is sufficiently abundant. Below we will see how such a function can be formulated mathematically. The model for flux f_1 now becomes:

$$f_1 = a \cdot \text{PHYTO} \cdot f(\text{NH}_4^+) \dots \quad (2.26)$$

Further terms can be introduced in the formulation of this flux. We note that when there is no light penetrating into the water column (such as would be the case in extremely turbid waters), no algal growth would take place. Again, with plenty of light other factors would become limiting, so that we also have to define

a light-limiting function $g(I)$ (where I is light intensity in the water column) that is zero at zero light, and tends to 1 at high light levels. More details on light limitation are given in Section 2.8.2. This gives us the final formulation for the flux f_1 :

$$f_1 = a \cdot \text{PHYTO} \cdot f(\text{NH}_4^+) \cdot g(I) \cdot \dots \quad (2.27)$$

Can we do the same for the flux f_2 , ingestion of phytoplankton by zooplankton? Again, we first note that without the zooplankton's physiological apparatus, phytoplankton will not transform spontaneously into zooplankton. Further, when zooplankton is ten times as abundant, all else being equal, ingestion will be ten times as high. Thus, flux f_2 is proportional to zooplankton.

It may be limited however by phytoplankton: when phytoplankton is scarce the ingestion will be lowered, but it will not be limited by phytoplankton any more once that component is sufficiently abundant. Thus, we need a limitation function $f'(\text{PHYTO})$ that is zero when PHYTO is zero, and tends to one when PHYTO is sufficiently abundant. This gives us for the flux f_2 :

$$f_2 = b \cdot \text{ZOO} \cdot f'(\text{PHYTO}) \quad (2.28)$$

2.5.2 Maximal Interaction Strength, Rate Limitation and Inhibition

How can we generalize from these examples? In most ecological models that involve interaction between components, the first basic principle is that the component that is performing the *work* controls the *maximal strength* of the interaction. By the 'compartment performing the work', we mean the one whose physiological apparatus is needed for the flux to take place. For respiration, ingestion and mortality, the component that is performing the work is the one that is respectively respiring, ingesting, and dying.

Maximal interaction strengths are then written as proportional to the concentration of this work component. In other words: maximal interaction strength equals a maximal rate times the concentration of the work component (WORKER).

$$\text{MaxInteraction} = \text{maxRate} \cdot \text{WORKER} \quad (2.29)$$

The rationale behind this rule is quite simple. First, we can note that if there is no one to do the work, no work will be done. Thus, the flux has to be zero when the component responsible for the work is absent. Next, the more workers there are, the more work can be done. So the maximally attainable rate or flux will have to be proportional to the amount of workers (or the concentration of the component responsible for the work).

In many cases, the maximal interaction strengths are not attained endlessly: feedback with the environment may cause a slow-down of the interaction. Thus, the actual interaction strength includes a *rate-limiting term* that reduces the rate.

There are roughly two ways to express these rate-limiting terms:

- as a *functional response*, which explicitly includes the effect of a limiting resource (the source component of the flux).
- as a ‘*carrying capacity*’ term, where the limitation is written as a function of the consumer or sink compartment.

Both types of formulations will be discussed in subsequent chapters.

Sometimes an interaction may be *inhibited* by the presence of some substance (the inhibitor), and this effect is also added to the ecological interaction. An example is an anaerobic process, inhibited by the presence of oxygen.

Summarising then, an ecological interaction (flow) can be written as the product of a maximal rate and the compartment performing the work, and, if appropriate, one or more rate limitation and inhibition terms:

$$\text{Interaction} = \text{maxRate} \cdot \text{WORKER} \cdot \text{RateLimitation} \cdot \text{RateInhibition} \quad (2.30)$$

2.5.2.1 The Compartment Performing the Work

As the notions of the work compartments and maximal strength may be rather abstract, we illustrate the principle with three examples.

Example 1. Resource consumption processes

For consumer-resource interactions, the flux is called ‘consumption’ and the compartment that performs the work is the consumer. A predator for instance needs food and has to perform work to obtain it; the prey does not perform any work in order to be eaten! Thus, the consumption rate is written as:

$$\text{Consumption} = \text{maxRate} \cdot \text{CONSUMER} \cdot \text{RateLimitingTerm} \quad (2.31)$$

where $\text{maxRate} * \text{CONSUMER}$ is the maximal interaction strength.

With CONSUMER expressed as a concentration, the consumption will have units of concentration.time⁻¹, maxRate will have units of t⁻¹ and the rate limiting term will be a dimensionless value between [0,1].

When the rate limiting term equals 0, the consumption rate will be 0, when equal to 1, maximal consumption rate will be achieved.

For a predator grazing on prey (Fig. 2.8 B) we can write:

$$\text{PredationRate} = \text{maxGrazing} \cdot \text{PREDATOR} \cdot \text{RateLimitingTerm} \quad (2.32)$$

The idea behind this functionality is simple: predators or grazers will try to realise growth or reproduction, for which they need food. The higher the predator biomass, the more food is captured, hence the first-order (linear) dependence with respect to

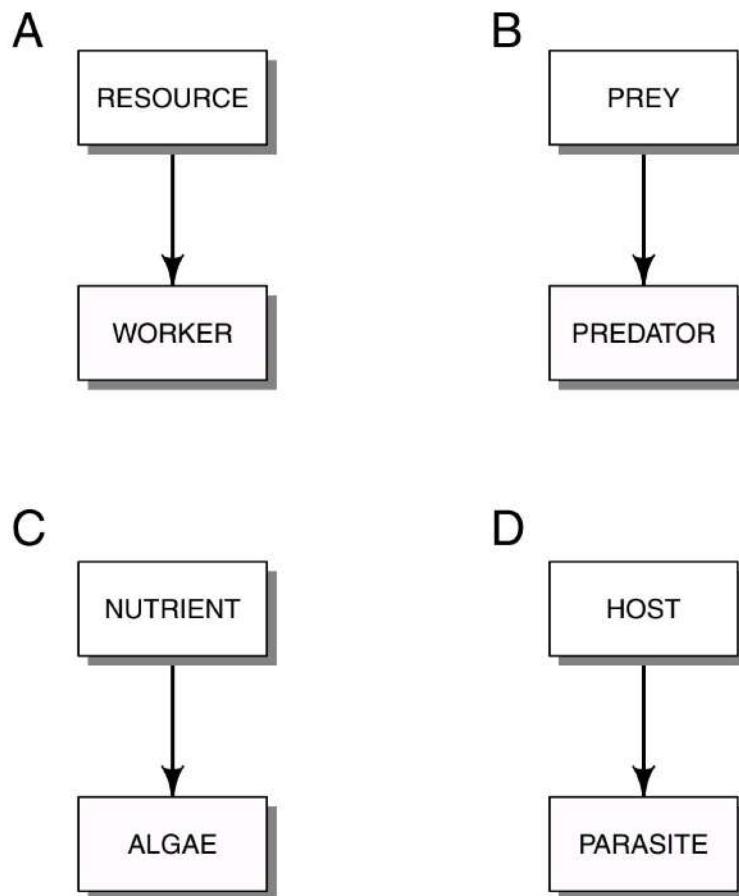


Fig. 2.8 Schematic representation (A) and three examples (B–D) of consumer-resource interactions. The compartment performing the work is the consumer (shaded in grey); the resource sets the rate-limiting term

the predator term. Because the predator must also handle the food and incorporate it into its own biomass or into eggs, there is a limit to the actual rate at which it can take in food, as expressed by the maximal rate coefficient (*maxGrazing*). Under ideal circumstances, the grazing of the predatory population will equal *maxGrazing**PREDATOR, the RateLimitingTerm will attain its maximal value (1). However, when the prey is relatively scarce, the predator will spend more of its time searching for prey. During this time it cannot handle and digest, and the total amount of prey captured and ingested per unit time and per predator will decrease. The maximal grazing rate will no longer be realised, the rate limiting term will have a value less than 1.

Similar dependency applies for algae taking up nutrients (Fig. 2.8 C): algae are performing the work (taking up the nutrients) and thus set the maximal rate; the rate limiting term will be a function of the nutrient concentration:

$$\text{NutrientUptakeRate} = \text{maxRate} \cdot \text{ALGAE} \cdot \text{RateLimitingTerm} \quad (2.33)$$

or for parasites (working compartment) infesting their hosts (rate limiting compartment) (Fig. 2.8 D):

$$\text{InfectionRate} = \text{maxRate} \cdot \text{PARASITES} \cdot \text{RateLimitingTerm} \quad (2.34)$$

Example 2. Biochemical transformations

Many biochemical transformations are mediated by bacteria. Their biomass controls the maximal strength, and the rate limiting term is a function of the substance that is being transformed.

For instance, the hydrolysis of dissolved organic carbon (DOC) with large molecular weight (SEMILABILE DOC) to low molecular weight dissolved organic carbon (LABILE DOC) is a process that is mediated by bacteria (Fig. 2.9 B). The bacteria excrete enzymes that catalyze the hydrolysis outside the bacterial cell. If we choose not to model the details of enzyme excretion, it is straightforward to assume that the enzyme concentration will be proportional to bacterial biomass, and thus, the maximal rate of hydrolysis will be proportional to bacterial biomass.

The flow between semi-labile and labile DOC is then described as:

$$\text{Hydrolysis} = \text{maxHydrolysis} \cdot \text{BACTERIA} \cdot \text{RateLimitingTerm} \quad (2.35)$$

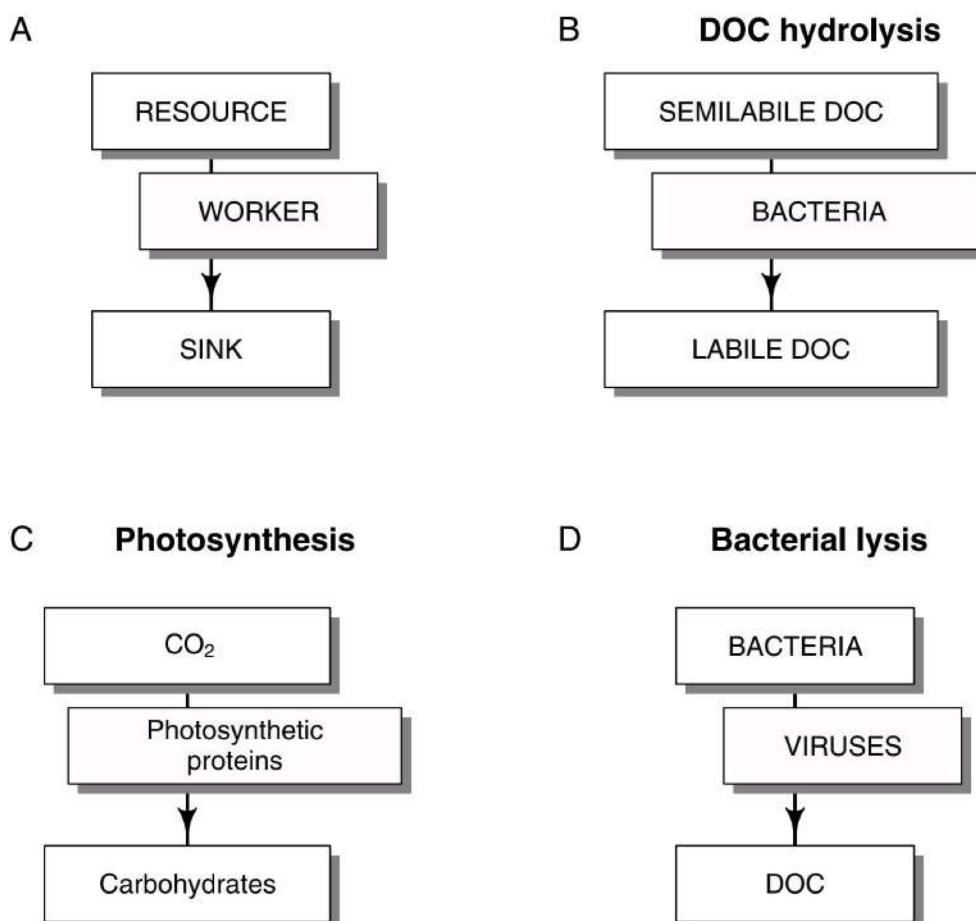


Fig. 2.9 Schematic representation (A) and three examples (B–D) of interactions where the work compartment (shaded box) is neither source nor sink. B. DOC hydrolysis, performed by bacteria. C. Photosynthesis, performed by the photosynthetic apparatus. D. Bacterial lysis performed by viruses

The difference with the previous example is that bacteria do *not* directly consume semi-labile DOC (they are not the sink compartment), but they *do* perform the work for the simple reason that they grow on the products of hydrolysis, the labile DOC.

In certain physiological models, different types of molecules are modelled. Some molecules ‘perform the work’ and transform other molecules. The example in Fig. 2.9 C for instance, is part of a complex physiological model describing algal growth that we will consider in Section 2.9.2. Through photosynthesis, algae transform CO₂ into low molecular weight carbohydrates, and this work is performed by the photosynthetic apparatus.

Another example of this type of interaction is bacterial lysis induced by viruses (Fig. 2.9 D).

Example 3. Loss processes

Respiration is the process that supplies an organism with the energy required for growth and maintenance. With growth we mean the incorporation of organic matter into the organism’s own tissue and the production of offspring. Maintenance includes the cost of basal, cellular metabolism (to support the body functions) and the cost of regenerating lost material (moults, matter to repair the ageing of the organism,...).

The component performing the work is the animal’s biomass, and maintenance respiration is modelled as proportional to this biomass. Respiration consumes oxygen, and thus a rate limiting term as a function of oxygen is added in a standard formulation. However, for organisms living in a permanently oxic world, oxygen is seldom limiting and the rate limiting term (which is always near to 1) can be dropped from the formulation. Note, however, that this is not true for animals living in environments (e.g. water columns, sediments) with a low oxygen concentration !

Thus the model formulation for maintenance respiration in general is:

$$\text{MaintenanceRespiration} = \text{respirationRate} \cdot \text{BIOMASS} \cdot \text{RateLimitingTerm} \quad (2.36)$$

while the model formulation in permanently oxic environments is:

$$\text{MaintenanceRespiration} = \text{respirationRate} \cdot \text{BIOMASS} \quad (2.37)$$

Maintenance respiration is not the only form of respiration. Whenever organisms feed, they have additional energetic costs, linked to the hydrolysis of organic material in their food and re-assemblage into their own tissues. This ‘growth respiration’ increases with feeding rate. We will see later how to express it mathematically (Section 2.6.1).

2.5.3 One Rate-Limiting Resource, 3 Types of Functional Responses

In the examples of the previous section, the maximal interaction was modulated by a rate limiting term that we did not yet specify.

It is common in ecological models to write this rate limitation term as a function of the *resource* (or source component). Equations that include such functionalities are called *functional response* equations. For example, in the predator-prey equation (Eq. 2.32) we would write the rate limiting term as a function of the prey concentration, for the nutrient uptake equation (Eq. 2.33) as a function of the nutrients, for the hydrolysis example (Eq. 2.35) as a function of semilabile DOC. The idea is simple: if there is a surplus of prey, the predator will be able to consume all it can eat, i.e. it will not be limited by prey availability. In contrast, if prey is very scarce, the predator will be lucky to catch one, hence it will not be able to attain the maximal predation rate.

Essentially, the rate limiting term is a mathematical function that describes how the consumption rate is affected by changes in the resource. It obeys the following rules:

- the rate limiting term is dimensionless and scales between 0 and 1.
- if the resource component is abundant, the rate limiting term is large (approaches 1) and interaction is strong, near to maximum intensity,
- if the resource is scarce, the rate limiting term becomes small (approaches 0) and the effective interaction rate will be low,

Based on considerations of encounter probabilities, searching behaviour and handling time, three types of functional responses can be deduced (Holling, 1959) (Fig. 2.10).

- Functional response *type I*, is also called a linear response. It is expected when consumer and resource encounter each other at random, and therefore it is also called the ‘blundering idiot search strategy’. It also assumes that handling time is negligible. Here the rate limiting term is simply proportional to the resource (R). One parameter (k) describes the functional form. The function is not allowed to exceed 1.

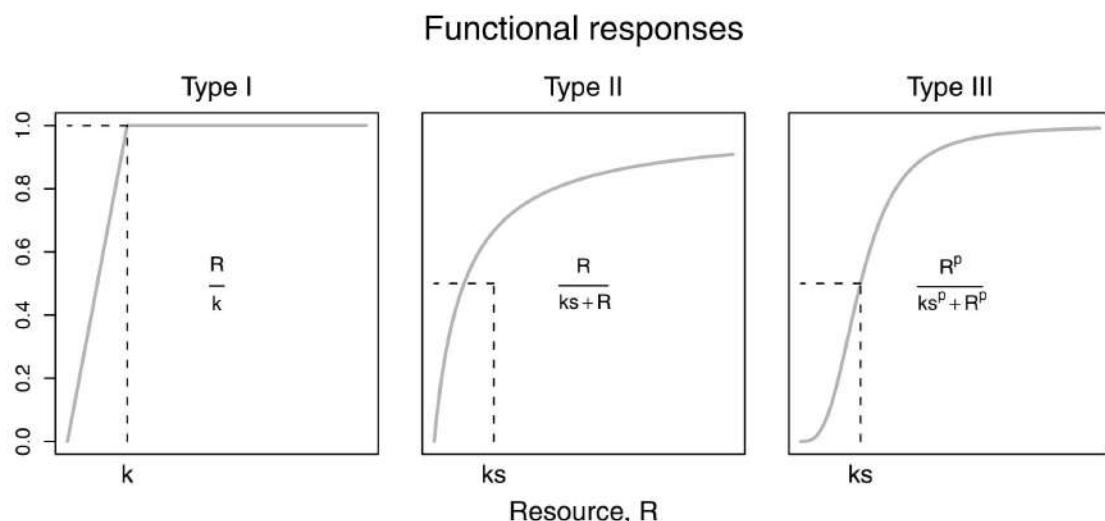


Fig. 2.10 Three types of functional responses. I. linear response. II. Monod or Michaelis-Menten response. III. Sigmoid response

$$\text{RateLimitingTerm} = \text{MIN}\left(\frac{R}{k}, 1\right) \quad (2.38)$$

This type of response is not so often used in ecological models. The discontinuity at the concentration $R = k$ makes it difficult to handle from a mathematical point of view.

- In a functional response *type II*, the rate increases nearly linearly at low resource density, and levels off at higher resource density.

This type of equation is known in enzyme kinetics as a Michaelis-Menten function, and is also frequently called a Monod, or hyperbolic equation. It is the most common form of rate limiting term used in ecological models.

$$\text{RateLimitingTerm} = \frac{R}{R + ks} \quad (2.39)$$

When the resource (R) is scarce, the level of consumption is mainly limited by the ability to take up or find the resource, whereas at high concentrations, the handling time (required to assimilate the resource) becomes the limiting factor. Alternatively, a predator may become satiated and stop feeding. We will derive the Michaelis-Menten formulation for an enzymatic reaction in Chapter 8. To describe the hyperbolic functionality, one parameter is required (ks), which is called the ‘half-saturation constant’. It is the resource concentration where the rate attains 50% of its maximal value. The half-saturation coefficient determines how fast the rate approaches the maximal rate. Low values of ks describe rapidly rising curves, and vice versa.

- In a functional response *type III*, the rate initially increases more than linearly (e.g. related to a learning process, switching to more abundant prey, preferring high-density patches, . . .), after which it levels off. The simplest such function is a sigmoid function:

$$\text{RatelimitingTerm} = \frac{R^p}{R^p + ks^p} \quad (2.40)$$

where ks is, again, the half-saturation concentration, p is a shape factor. The higher its value, the steeper the curve.

2.5.4 More than One Limiting Resource

Many processes are potentially limited by more than one factor. For example, phytoplankton growth requires availability of all the essential elements N,P,C,(Si), . . .

Two empirical solutions are adopted to solve the problem of concomitant limiting factors: the minimum and multiplicative law.

- The *Liebig law of the minimum*, considers that the growth rate will depend only on the factor for which the corresponding growth is lowest, i.e. as a function of the element least in supply

$$\text{RateLimitingterm} = \text{MIN}(\text{LimitingTerm1}, \text{LimitingTerm2}) \quad (2.41)$$

- In contrast, the *multiplicative law* considers that the different factors act simultaneously, as the product:

$$\text{RateLimitingterm} = \text{LimitingTerm1} \cdot \text{LimitingTerm2} \quad (2.42)$$

A common example is algal growth, which is limited both by light availability and nutrient concentrations (assume N, Si). This is often expressed as:

$$\text{RateLimitingTerm} = \text{LightLimitation} \cdot \text{MIN}\left(\frac{\text{N}}{\text{N} + ks_N}, \frac{\text{Si}}{\text{Si} + ks_{Si}}\right) \quad (2.43)$$

where the co-limitation of light and nutrients is described multiplicatively, and where concomitant limitation by inorganic nitrogen and silicate is expressed using the minimum law. Growth limitation on nitrogen and silicate is described with Monod kinetics, with ks_N and ks_{Si} the respective half-saturation constants.

Sometimes the co-limitation by light and nutrients is described using the minimum law:

$$\text{RateLimitingTerm} = \text{MIN}\left(\text{LightLimitation}, \frac{\text{N}}{\text{N} + ks_N}, \frac{\text{Si}}{\text{Si} + ks_{Si}}\right) \quad (2.44)$$

We will see how light limitation can be expressed in Section 2.8.2.

The two alternatives presented, Liebig's law of the minimum and multiplicative multiple limitation, can be considered as two end-members of a continuum of possible expressions. In the literature many alternatives are presented that express some stronger or weaker form of interaction between different limiting processes.

For predators that have access to different food sources and that can switch from one food to the other (FOOD_i), it is customary to add a certain preference p_i ([0,1]) for each food item. With all $p_i=1$ there is no preference for any of the food items:

$$\text{RateLimitingTerm} = \frac{\sum_i p_i \cdot \text{FOOD}_i}{\sum_i p_i \cdot \text{FOOD}_i + ks_{FOOD}} \quad (2.45)$$

2.5.5 Inhibition Terms

Some processes are inhibited by the presence of a certain substance. The more abundant this inhibitory substance, the lower the rates will be (Fig. 2.11A).

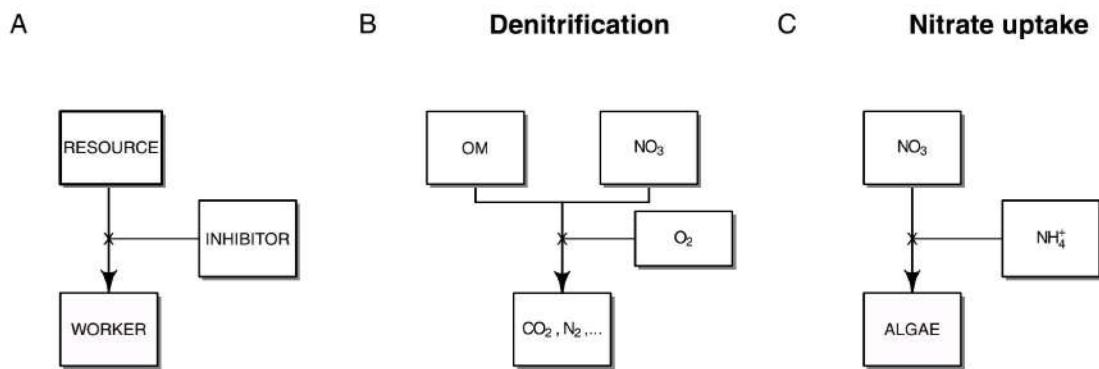


Fig. 2.11 Schematic representation (A) and two examples (B,C) of inhibition. **B.** Denitrification is inhibited in the presence of oxygen. **C.** nitrate uptake by algae is inhibited by ammonium. The compartment performing the work is denoted with a shaded box

2.5.5.1 Example: Denitrification

There are many examples of inhibition in chemical or biogeochemical models, where the occurrence of a reaction is negatively impacted by the concentration of some substance that does NOT play a direct part in the chemical reaction.

For example, the mineralization (respiration) of organic matter with nitrate, called denitrification, is a process that occurs at very low rates in the presence of oxygen: it is inhibited by oxygen (Fig. 2.11B).

A process description of denitrification should take this dependence into account. The simplest solution is to multiply, to the rate term describing nitrate consumption, a dimensionless inhibition term:

$$\text{Inhibition} = 1 - \frac{\text{O}_2}{\text{O}_2 + k_{in O_2}} = \frac{k_{in O_2}}{\text{O}_2 + k_{in O_2}} \quad (2.46)$$

The value of this inhibition term will decrease as the oxygen concentration increases; it has the value 1 at zero oxygen concentrations. The parameter $k_{in O_2}$ is the oxygen concentration at which the rate drops to half of its maximal value.

Assuming that mineralization is first-order with respect to organic matter availability (see above), and that denitrification is limited by nitrate and inhibited by oxygen, the denitrification rate can be expressed as:

$$\text{Denitrification} = r_{max} \cdot \frac{\text{NO}_3}{\text{NO}_3 + k_{sNO_3}} \cdot \frac{k_{in O_2}}{\text{O}_2 + k_{in O_2}} \cdot \text{ORGANICMATTER} \quad (2.47)$$

2.5.5.2 Example: Nitrate and Ammonium Uptake by Algae

Inhibition terms can also be present in biological models.

For example, algae can use ammonium as well as nitrate as a source of nitrogen for their growth (Fig. 2.11 C). However, nitrate has to be reduced before it can be assimilated in algal biomass. As this reduction presents an additional energetic cost

to the algal growth, the algae will take up ammonium preferentially compared to nitrate.

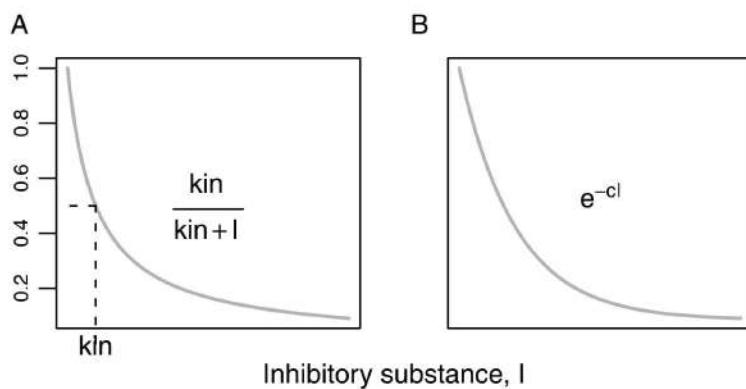
As a consequence, the uptake of nitrate will be negatively impacted by the presence of ammonium. In models that discriminate between these two forms of dissolved inorganic nitrogen, this is generally represented by an inhibition term of nitrate uptake:

$$\text{NitrateUptake} = r_{max} \cdot \frac{\text{NO}_3}{\text{NO}_3 + k_{s\text{NO}_3}} \cdot \frac{k_{in\text{NH}_3}}{\text{NH}_3 + k_{in\text{NH}_3}} \cdot \text{ALGAE} \quad (2.48)$$

In the example above, we used a Monod term (subtracted from 1) to account for the inhibition by ammonium (Fig. 2.12 A). It is more traditional in aquatic modelling to represent the inhibition as an exponential term (Fig. 2.12 B), declining exponentially with increasing ammonium concentration:

$$\text{NitrateUptake} = r_{max} \cdot \frac{\text{NO}_3}{\text{NO}_3 + k_{s\text{NO}_3}} \exp(-InhibitionCt \cdot \text{NH}_3) \cdot \text{ALGAE} \quad (2.49)$$

Fig. 2.12 Often-used inhibition terms in ecological models. **A:** 1-Monod function, **B:** exponential function



2.6 Coupled Model Equations

Models often contain several equations that are coupled either through the interaction between source and sink compartments (Fig. 2.13A) or via stoichiometric relationships (Fig. 2.13B). The coupling of equations is often necessary because fluxes are typically dependent on one state variable for their maximal rate, and on another one for their limitation term.

Below we give three examples of coupled model formulations. Other couplings, e.g. between physical and biological model parts, may also be realised but will not be detailed here.

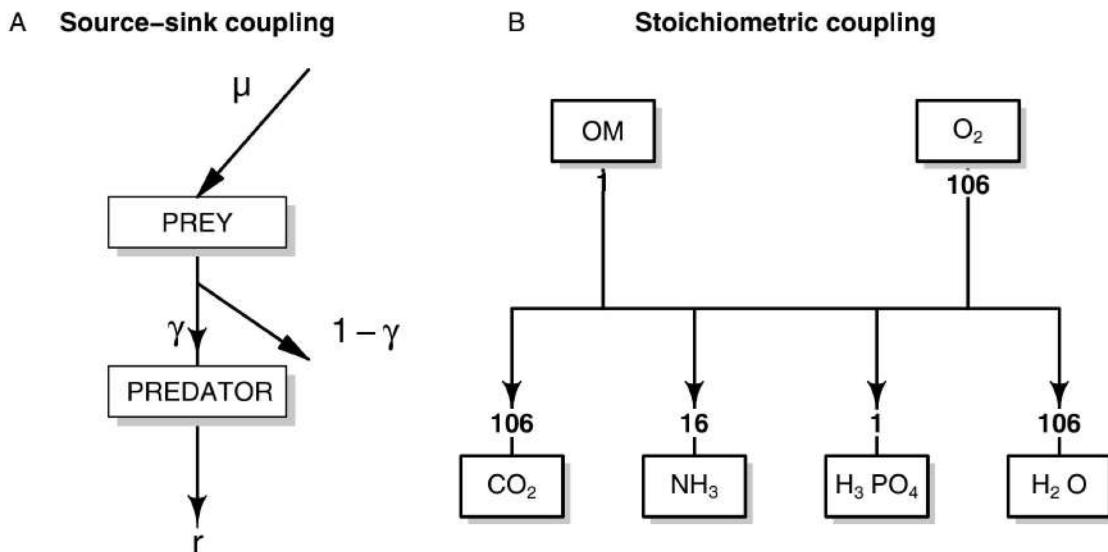


Fig. 2.13 Two examples of coupled equations. **A.** An ingestion flow links the increase of the predator to the decrease of prey and the production of detritus. **B.** The mineralization (respiration) of organic matter (OM) links the oxygen (O_2), carbon (CO_2), nitrogen (NH_3) and the phosphorus cycle (H_3PO_4), according to specific stoichiometric ratios (here: Redfield ratios)

2.6.1 Flows Modelled as Fractions of Other Flows

Not all flows are written as a function of the source and /or sink compartment. Sometimes it is more convenient to express one flow as a function of another flow.

Consider, again, the feeding of an organism (predator) on its prey. In previous sections we have seen how to describe this as first-order to predator biomass (the work compartment) and with a rate limiting term depending on the prey concentration:

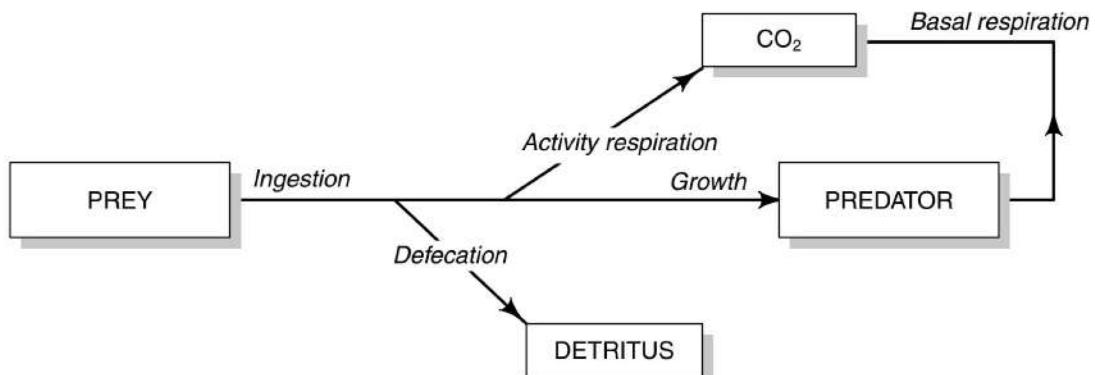


Fig. 2.14 When an organism feeds, it not only provokes a flux from the food to its own biomass, but also to detritus (Defecation) and to $\text{CO}_2 +$ inorganic nutrients (Activity respiration). All these flows are related: an organism can not produce more faeces than the amount of food it ingested. To make the picture complete, the conceptual model also includes basal respiration

$$\text{Ingestion} = \maxIngestion \cdot \frac{\text{PREY}}{\text{PREY} + k_{\text{SPREY}}} \cdot \text{PREDATOR} \quad (2.50)$$

Part of the ingested food will pass through the gut of the predator and be expelled as faeces (Fig. 2.14). The more the organism feeds, the larger this faeces production will be; organisms that do not feed do not produce faeces. As a reasonable approximation, we may write that a fixed fraction of ingested food (p_{Faeces}) will be defecated, which effectively relates faeces production to ingestion.

$$\text{Defecation} = p_{\text{Faeces}} \cdot \text{Ingestion} \quad (2.51)$$

The food that is taken up through the gut of the organism (i.e. the part that is not defecated) will serve organism growth: it will be converted into either structural biomass of the organism or into reproductive tissue. However, conversion of food into tissue is a costly process and the energy required will be delivered by respiration, the so-called activity or growth respiration (Fig. 2.14). The more an organism feeds, the higher this energy requirement, and the higher its respiration. It is usually assumed that a constant fraction (the $growthCost$) of food uptake through the gut is used for respiration:

$$\begin{aligned} \text{Growthrespiration} &= (\text{Ingestion} - \text{Defecation}) \cdot growthCost \\ \text{Growthrespiration} &= \text{Ingestion} \cdot growthCost \cdot (1 - p_{\text{Faeces}}) \end{aligned} \quad (2.52)$$

We may then finally write the food incorporated into structural tissue as:

$$\begin{aligned} \text{Growth} &= \text{Ingestion} - \text{Defecation} - \text{GrowthRespiration} \\ \text{Growth} &= \text{Ingestion} \cdot (1 - growthCost) \cdot (1 - p_{\text{Faeces}}) \\ \text{Growth} &= \text{Ingestion} \cdot \gamma \end{aligned} \quad (2.53)$$

where γ is the growth efficiency.

2.6.2 Coupled Dynamics of Source and Sink Compartments

Still working with a predator and its prey, we will now focus on the dynamic equations for these two state variables. Obviously, the dynamics of a consumer and its resource are connected. Reflecting this, their equations are coupled.

Such coupled equations take into account the feedback between the consumer and resource and therefore make the model more realistic.

Consider for instance the coupled predator-prey dynamics:

$$\begin{aligned}\frac{d\text{PREDATOR}}{dt} &= g \cdot \text{PREDATOR} \cdot \frac{\text{PREY}}{\text{PREY} + k_{\text{SPREY}}} \cdot \gamma - r \cdot \text{PREDATOR} \\ \frac{d\text{PREY}}{dt} &= -g \cdot \text{PREDATOR} \cdot \frac{\text{PREY}}{\text{PREY} + k_{\text{SPREY}}} + \mu \cdot \text{PREY}\end{aligned}\quad (2.54)$$

The grazing of the predator on the prey not only induces a proportional increase in predator biomass, but also reduces the biomass of the prey (first term). As not all of the prey grazed is converted into predator biomass, the grazing is multiplied by parameter γ , the growth efficiency ([0, 1]), in the predator equation.

Note that the growth efficiency parameter γ is used to represent both faeces production flux and growth respiration flux. Similarly, the parameter r in the predator equation represents mortality of the predator, as well as maintenance respiration. In contrast to biogeochemists, who are also interested in detritus, or in CO₂, and therefore separate all these fluxes, theoretical ecologists tend to lump this type of ‘loss processes’ as much as possible.

As the predator biomass increases, so does the predation pressure on its prey. This will slow down the growth of the prey until its biomass eventually decreases. Lower prey biomass will provoke stronger resource limitation, causing slow-down of predator growth and eventual decline of predator biomass, such that the prey biomass may recover.

2.6.3 Stoichiometry and Coupling of Element Cycles

The budgets of several main constituents on earth, e.g. C, N, P, Si are coupled through stoichiometric relations.

The *stoichiometry* of a compound is defined as the proportion of the various quantities.

For instance, in marine algae, the molar ratio of elements is remarkably constant and called the Redfield ratio. Thus, algal organic matter has the composition of

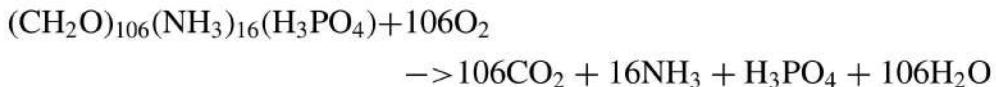


or a stoichiometric C:H:O:N:P ratio of 106:263:110:16:1.

Most marine animals more or less follow this stoichiometric composition of algae. Marine bacteria tend to deviate in composition, with lower C:N ratios.

This interconnectedness of elements provides an additional constraint on mathematical models. Data on the nitrogen cycle can be used to cross-check data or model results on the carbon cycle, as both cycles are intimately linked.

For instance, to oxidise (respire) 106 mole of fresh algal organic matter, 106 mole of oxygen is generally consumed, whereas 16 moles of ammonium, and one mole of phosphate are released. The respiration reaction reads:



This effectively couples the cycles of C, O, N and P.

Models that describe all these elements take into account these changes, using the appropriate stoichiometric ratios.

For instance, with ‘Respiration’ being the amount of organic matter respired, the following terms will pop up in the rate of change of oxygen, ammonium, phosphate, carbon dioxide and organic carbon:

$$\begin{aligned}
 \frac{d\text{O}_2}{dt} &= -\text{Respiration} \cdot OC + \dots \\
 \frac{d\text{NH}_3}{dt} &= \text{Respiration} \cdot NC + \dots \\
 \frac{d\text{PO}_4}{dt} &= \text{Respiration} \cdot PC + \dots \\
 \frac{d\text{CO}_2}{dt} &= \text{Respiration} + \dots \\
 \frac{d \text{ORGANICCARBON}}{dt} &= -\text{Respiration} + \dots \tag{2.55}
 \end{aligned}$$

where $OC = 1$, $NC = 16/106$, and $PC = 1/106$, the stoichiometric ratios of organic matter.

2.7 Model Simplifications

As discussed in Chapter 1, a modeller tries to simplify the world as much as possible. This is not always easy, and particular tricks are sometimes needed to keep a model within reasonable bounds of complexity.

In models involving trophic relations (consumer-resource interactions) the flows are calculated as a function of both consumer and resource. This resource, in turn, may again consume its own resources, etc. – but often we do not want our model to go down all the way to the lowermost level of the food web. In that case we need an expression that approximates the dynamics of the lowermost consumer level in our model as well as possible, without the need to include its resource level explicitly in the model. Often this simplification makes use of a ‘carrying capacity formulation’. (Fig. 2.15A)

Similarly, the highest consumer level in our model may be the prey of a still higher trophic level, but here again we want to stop at some particular level. We will simplify again by modelling the mortality rate of the uppermost trophic level in the model, without the need to explicitly model an even higher trophic level. We call this procedure, with a technical term, *closure* of the model. (Fig. 2.15B)

Sometimes, there exist a number of intermediate links between two compartments that we are not particularly interested in; in that case we may want to suppress

the intermediate compartments and simply model the dynamics as if there were a direct interaction between the end-members. (Fig. 2.16 C)

2.7.1 Carrying Capacity Formulation

In the functional response models discussed previously, the rate limiting term was a function of the resource (the prey for predator-prey relationships, nutrients for algal uptake,...).

In population models, rate limiting feedback terms are often modelled as a function of the *consumer* population density itself. These models are called carrying capacity models. The carrying capacity is the density or concentration above which the growth rate of the consumer becomes negative.

The carrying capacity formulation is an approximation of processes not explicitly included in the model. These processes may be resource limitation, but also competition for space.

The following is a simple example of a model of population growth, with a carrying capacity formulation. It is the logistic equation, sometimes called the Verhulst model, in reference to its creator (Verhulst, 1838)

$$\frac{dN}{dt} = r \cdot N \cdot \left[1 - \frac{N}{K} \right] \quad (2.56)$$

where N , the state variable, is population density, dN/dt is its rate of change, r is maximal net growth rate, also referred to as the intrinsic rate of increase (t^{-1}), K is the carrying capacity, i.e. the maximum population size that can be supported; K has the same units as N . This equation has been so influential in ecological modelling, and we use it several times in this book, so that it is worthwhile to explain it in more detail.

Clearly, N is the compartment performing the work (growing), r is the maximal rate, whilst the term $\left[1 - \frac{N}{K} \right]$ is the rate limiting term.

- At very low densities ($N \ll K$), the limitation term $\left[1 - \frac{N}{K} \right]$ will be ≈ 1 and the population grows exponentially.
- In the neighborhood of the carrying capacity K , the limitation term approaches 0, the rate of change becomes very small and density will remain quasi-constant.
- At densities much higher than the carrying capacity, the limitation term $\left[1 - \frac{N}{K} \right]$ will be negative, and the population density will decrease quasi-exponentially towards K .

The carrying capacity model leads to asymptotic behaviour in time (Fig. 2.15 B). For starting values of population density much smaller than the carrying capacity, the trajectory of population density versus time is a sigmoid relationship (S-shaped curve, solid line). When initiated at very high values, population density will decline quasi-exponentially towards K (dashed line).

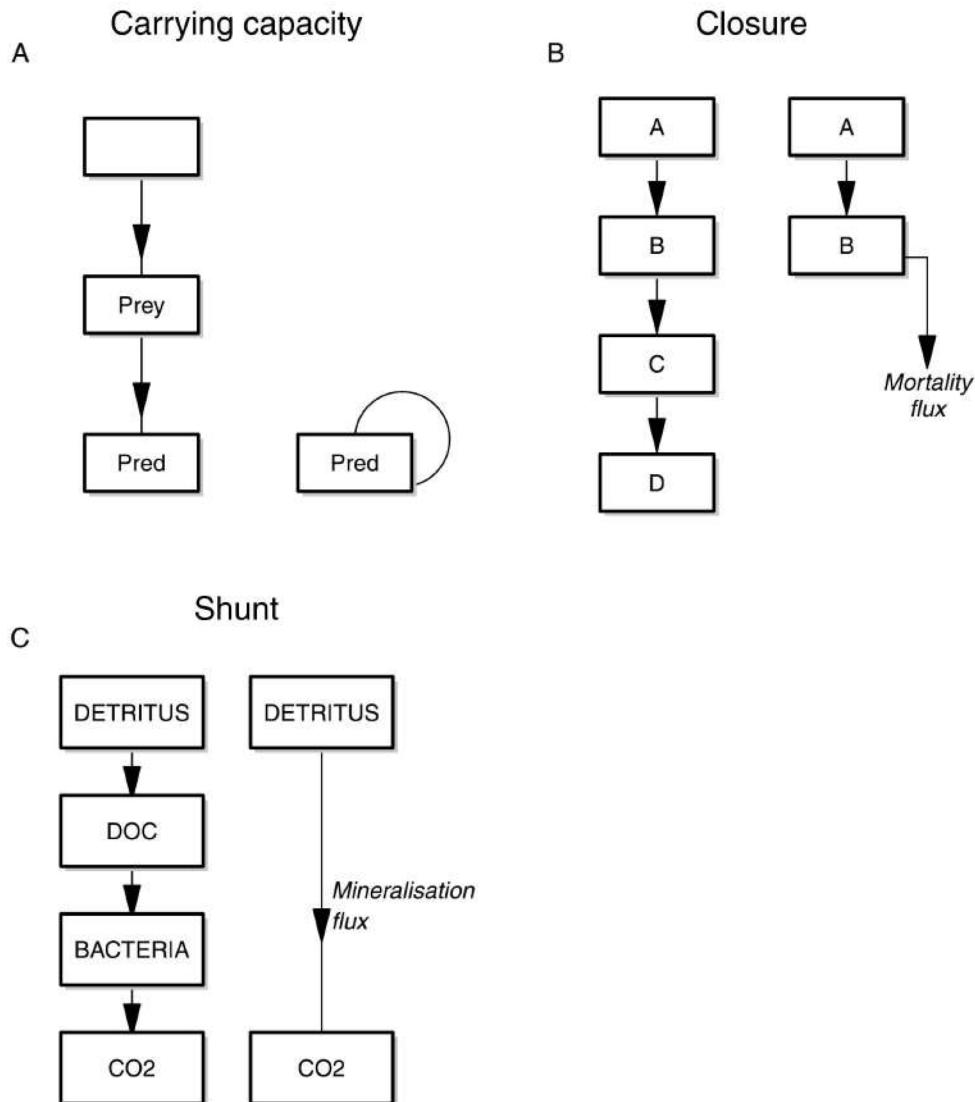


Fig. 2.15 Schematic representation of model simplifications. **A.** In simple models, the dependence of a predator on the dynamics of its prey is often not represented explicitly but mimicked by a function that only takes into account the value of the predator concentration; carrying capacity models are the most notorious examples of such simplifications. **B.** In food web models, the top-predators (here C, D) are often not represented; rather their effect on their prey (here B) is added as a mortality flux (the closure flux). **C.** If we are interested in the decay of detritus, and the eventual respiration, but not in the organisms performing the work (here bacteria), we simply model a direct flow between detritus and CO₂

In contrast to the models including functional responses, carrying capacity models do not need to include the dynamics of the limiting resource, so they are in a sense simpler. However, they are not as general as functional response models.

Gotelli (2001) clarifies how to derive the Verhulst model in a succinct way, which we find particularly informative:

We start with a very simple model that describes changes in population density (N) due to the difference between birth and death, which are both a function of density. Thus, we write the rate of change of density as:

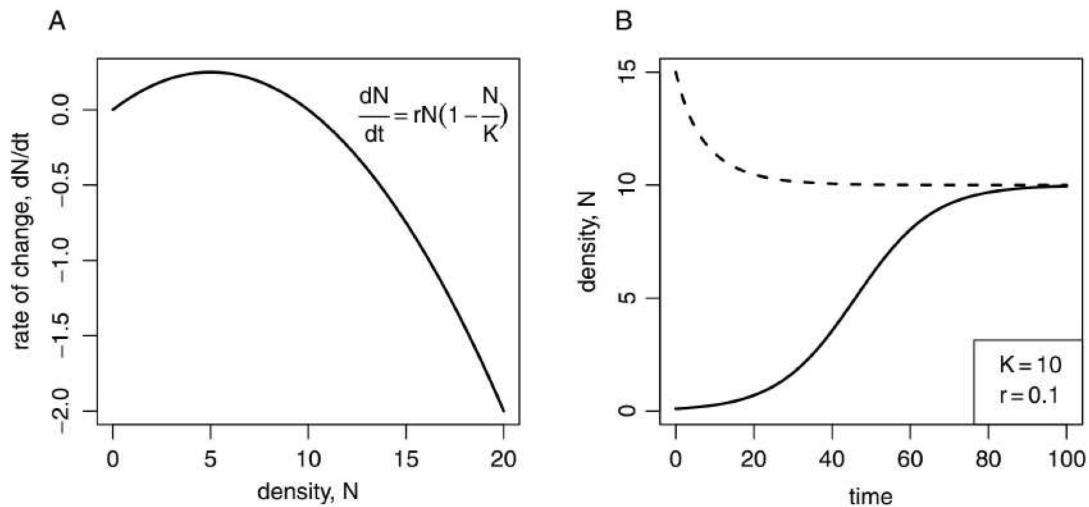


Fig. 2.16 The logistic equation. **A.** the rate of change as a function of density. **B.** Two solution curves, representing how density changes in time

$$\frac{dN}{dt} = [b(N) - d(N)] \cdot N \quad (2.57)$$

and where $b(N)$ and $d(N)$ are the per capita birth and death rate (units of time $^{-1}$) respectively.

As population density increases, less food will be available, space and shelter may fall short, predation pressure may be higher, or stress may increase due to too frequent contacts, or to reduction of a limiting substance (e.g. oxygen in schools of fish).

These phenomena will negatively affect the birth rate, and will increase mortality. The simplest way of expressing this in a model is by making the per capita birth rate ($b(N)$) a linearly decreasing and the death rate ($d(N)$) a linearly increasing function of density. With

$$b(N) = b_0 - b_1 \cdot N \quad (2.58)$$

and a similar description for death rate, we obtain:

$$\frac{dN}{dt} = [b_0 - b_1 \cdot N - (d_0 + d_1 \cdot N)] \cdot N \quad (2.59)$$

After rearranging and simplifying, we obtain the logistic growth equation:

$$\begin{aligned} \frac{dN}{dt} &= (b_0 - d_0) \cdot N \cdot \left[1 - \frac{b_1 + d_1}{b_0 - d_0} \cdot N \right] \\ \frac{dN}{dt} &= r \cdot N \cdot \left[1 - \frac{N}{K} \right] \end{aligned} \quad (2.60)$$

2.7.2 Closure Terms at the Highest Trophic Level

Food webs form a cascade of trophic levels, where one level is being eaten by another, etc. . . until the highest trophic level.

Most mathematical models do NOT resolve all these trophic levels, but introduce an empirical approximation of consumption by all higher trophic levels (predators) that are not explicitly included in the model (Fig. 2.16 B).

This approximation is called the model's *closure term* and it has the advantage that predator dynamics need not be modelled.

It is not always clear when to use closure terms (e.g. at what trophic level) and which kind of functionality to give the closure terms in a model. Often the approach may seem ad hoc, and it is therefore a continuous source of debate among modellers. Even more so because these arbitrarily chosen closure terms can have considerable influence on model behaviour. Especially model stability characteristics are fundamentally influenced by closure terms. Therefore they cannot be used carelessly.

As the predator in our example is not modelled, the mortality of the prey, induced by this level is a function of the prey concentration rather than the predator concentration. Most often used is a linear mortality or a quadratic mortality term:

$$\begin{aligned} \text{Mortality} &= k \cdot \text{PREY} \\ \text{Mortality} &= c \cdot \text{PREY} \cdot \text{PREY} \end{aligned} \quad (2.61)$$

In the first equation, the closure is linear, and parameter k has units of time $^{-1}$. Here it is effectively assumed that predation pressure (k) remains constant. In the second equation, the closure term is quadratic, units of c are conc $^{-1}$ time $^{-1}$ where 'conc' are the units of Prey. This equation assumes that the predatory rate ($c \cdot \text{PREY}$) fluctuates proportionally with the prey biomass.

Quadratic closure tends to stabilize food web models to a considerable degree, and its parameters also influence the steady state results of the models substantially. This may or may not be a desirable property. If the model aims to simulate real observations, enhanced stability may help to find 'good' solutions. However, if the model study aims at investigating the stability properties of different interaction terms, artificial stabilization by a quadratic closure may clutter the argument.

2.7.3 Simplification by Deletion of Intermediate Levels

In biogeochemical models, the processes associated with the mineralization (respiration) of organic matter are often of interest. Whereas mineralization is performed by bacteria and higher organisms, their dynamics is usually not relevant.

By assuming that organic matter decay proceeds at a first-order rate, the necessity to model explicitly the organisms that are performing the work, is avoided.

$$\text{OrganicMatterRespiration} = k \cdot \text{ORGANICMATTER} \quad (2.62)$$

This effectively assumes that, whatever organism is metabolizing, the rate of decomposition is controlled by the amount and reactivity (palatability) of the organic matter, and not by organism biomass. It is a closure term because it closes off the model formulation for the flux to CO₂, without considering all factors, other than organic matter concentration, influencing this flux. (Fig. 2.16 C).

2.8 Impact of Physical Conditions

Many physical quantities, such as temperature, light, water flow, and wind have an effect on ecosystems. These physical factors are either computed by physical models that are coupled to the biological descriptions or, more likely, they are imposed as forcing functions.

2.8.1 Temperature

Many rates are modulated by temperature. This applies as much to physical processes (e.g. molecular diffusion), as to chemical (reaction) rates, and physiological rates (growth, respiration, feeding, excretion,...). In aqueous environments, temperature also affects the solubility of many substances and therefore its exchange across the air-water interface.

The response of individual *organisms* to temperature is one where rates gradually increase towards a clearly defined temperature optimum, above which rates decline. This response of individual organisms should not be confused with the *ecosystem* response. Throughout the different seasons, ecosystems are characterised by a succession of species that are acclimated to different thermal conditions. As a result rates scale more or less exponentially to temperature, without the presence of a clear optimum, when viewed at the ecosystem level (Fig. 2.17). Typically, biological processes will more or less double in rate for a temperature increase of 10°C, as long as temperature is within acceptable ranges. Below and above, rates will drop strongly and organisms may die because essential enzymes denaturalise.

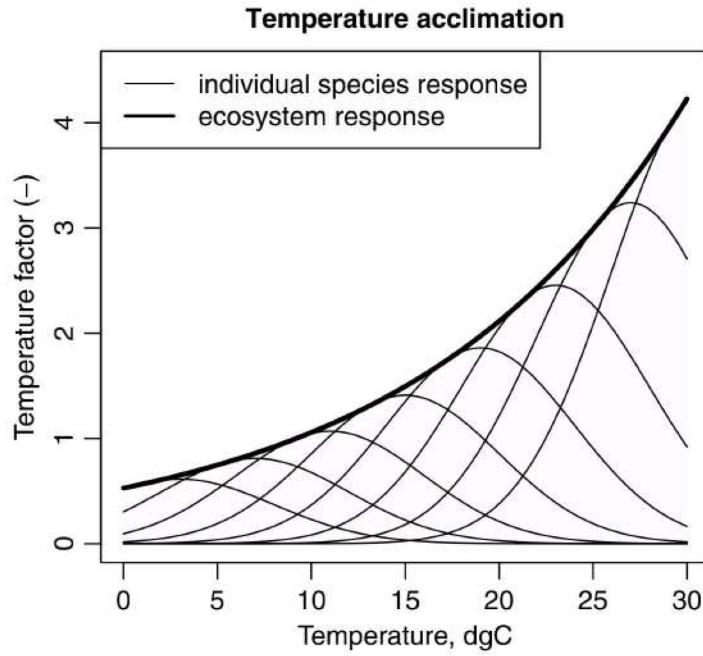
Thus, for *multispecies* assemblages, an exponential increase with temperature is most often used.

The formulation for multispecies assemblages comes in many different shapes, the most well-known is the *Q10* formulation:

$$\text{TempFactor} = \exp\left(\frac{T - T_{ref}}{10} \log_e(q10)\right) \quad (2.63)$$

where *Tref* = reference temperature at which TempFactor = 1. This is the temperature at which the rate parameters are expressed. Parameter *q10* is the factor of increase for every increase of the temperature with 10°C. A typical value for *q10* is 2.

Fig. 2.17 Response to temperature for individual species (thin lines) and for the ecosystem (thick line)



For instance, with R_{20} the rate at 20°C and a q_{10} of 2, the value of the rate at 10°C will be:

$$R_{10} = R_{20} \cdot \exp\left(\frac{10 - 20}{10} \log_e(2)\right) = R_{20} \cdot 0.5 \quad (2.64)$$

or a halving of the rate.

Another description of the same exponential dependence is given by:

$$\text{TempFactor} = \exp(Tcoeff \cdot T) \quad (2.65)$$

where the rate parameters must now be defined at 0°C. A value for $Tcoeff = \log_e(2)/10 = 0.069$ corresponds to a q_{10} of 2.

In most models, temperature is imposed as a forcing function, although, in aquatic environments it can be dynamically described by physical models that are driven by atmospheric conditions (wind, air temperature, air humidity, solar radiation).

2.8.2 Light

Being the energy source of photosynthesis, the availability of light in the photosynthetically active range (PAR=photosynthetically active radiation) drives most ecological systems. In addition to its functioning as an energy source, solar radiation heats up the water and exposed sediments.

Within water masses, the decline of solar radiation with depth (Fig. 2.18B) effectively divides the water column into an autotrophic and a heterotrophic part. This is essential for understanding the vertical distribution of the biotic (algae, zooplankton) and abiotic components (nutrients) in the water column. In summer, when oceanic water columns are stratified, the upper water layer is typically depleted in nutrients, whereas the deeper layers are rich in nutrients but too dark for algal growth. As algae need both light and nutrients for growth, a chlorophyll maximum often develops at intermediate depth, where some light is available and moreover some nutrients are mixed in from below (Fig. 2.18D).

Similarly the light intensity declines as light penetrates in a dense plant canopy.

The decline of light (I) with depth (z) can be described as a simple differential equation, expressing the rate of change of light with depth (dI/dz). Light intensity is lost in constant proportion to the available light, and the proportionality coefficient is the extinction coefficient, k (units of m^{-1}):

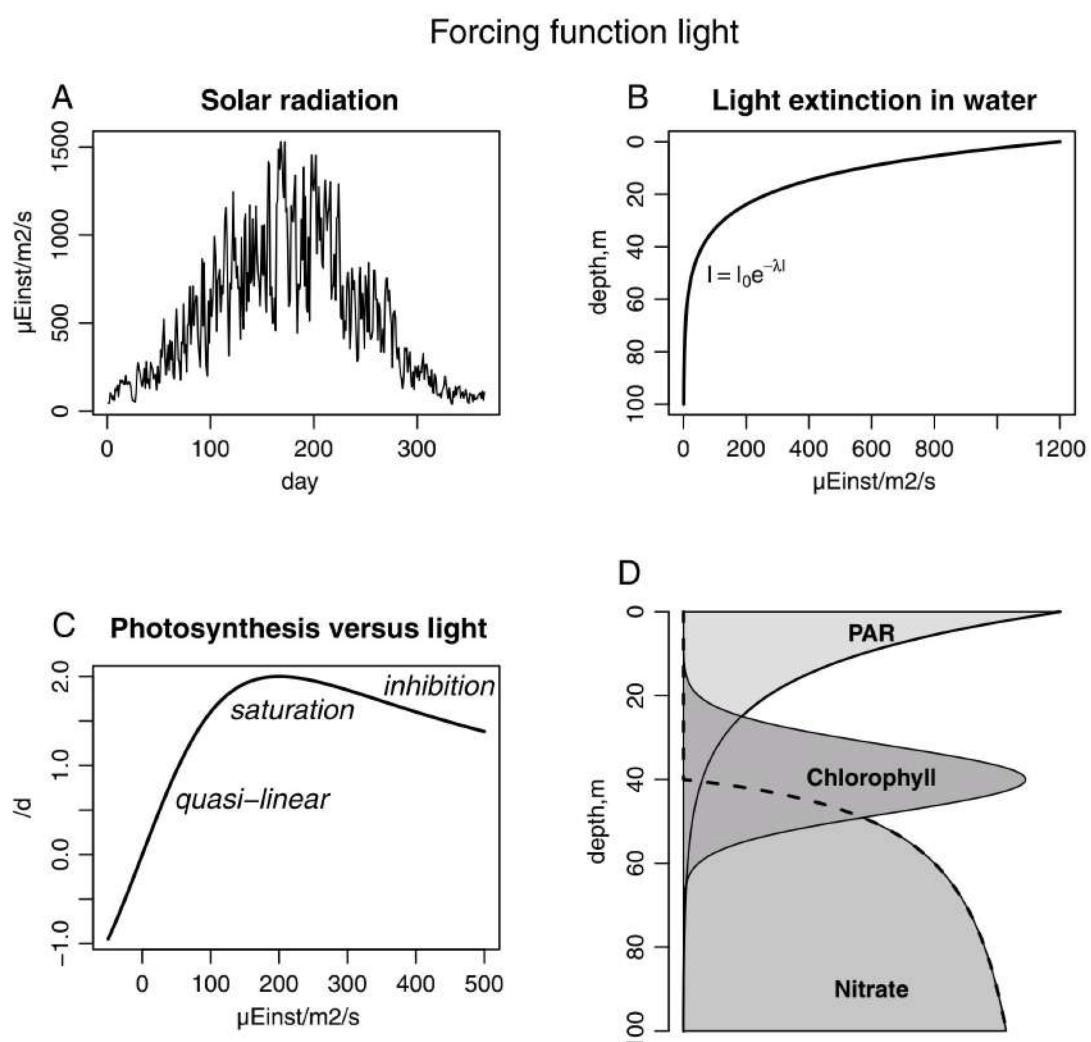


Fig. 2.18 Light forcing function. **A.** Typical time series with daily solar radiation, representative for temperate areas. **B.** Light intensity declines as a function of water depth. **C.** Typical photosynthetic response to light. **D.** The decrease of light with water depth divides the water column into distinct functional zones. See text for explanation

$$\frac{dI}{dz} = -k \cdot I \quad ; \quad I|_{z=0} = I_0 \quad (2.66)$$

With I_0 the light intensity at the upper (e.g. air-water) interface ($z=0$), it is possible to calculate the light intensity at any depth. The solution to this differential equation (see Chapter 5) is the Lambert-Beer relationship:

$$I|_z = I_0 \cdot \exp(-kz) \quad (2.67)$$

Light is always imposed as a forcing function, either using actual measurements (from the meteorological office) or using special algorithms that approximate light intensity as a function of latitude and season. Depending on the type and scale of the model, seasonal, diurnal and within-day variations in light intensity may be of importance, and these require different algorithms.

2.8.2.1 Light Limitation Functions

The response of photosynthesis to light (Fig. 2.18 C) is a well-known process, both from a biochemical and a physiological perspective. The typical response is a saturation curve, where saturation is reached above a certain photon flux and with a quasi-linear response at low light level. This reflects the properties of the photosynthetic system, which is light-limited at low levels and limited by the functioning of the enzyme system at high light levels. Above a certain threshold, this may even lead to light inhibition, with lower rates of photosynthesis than at the optimal light intensity.

There are several mathematical formulations to describe this functional form, involving either one or two parameters. Some include light inhibition; others do not take this into account.

Some of the most often used *1-parameter functions* are:

Steele's model, (Fig. 2.19 A)	$\text{LightLim} = \frac{I}{I_{opt}} \cdot \exp\left(1 - \frac{I}{I_{opt}}\right)$	(2.68)
Monod model, (Fig. 2.19 B)	$\text{LightLim} = \frac{I}{I + ksI}$	
Evan's model (Fig. 2.19 B)	$\text{LightLim} = \frac{I}{\sqrt{I_{opt}^2 + I^2}}$	

Note that only Steele's model, although only requiring 1 parameter, does include light inhibition.

For marine algae, typical values for I_{opt} are $50\text{-}300 \mu\text{Einst m}^{-2} \text{s}^{-1}$; ks is typically in the range of $50\text{-}150 \mu\text{Einst m}^{-2} \text{s}^{-1}$.

2-parameter functions (Fig. 2.19 C) are significantly more complex:

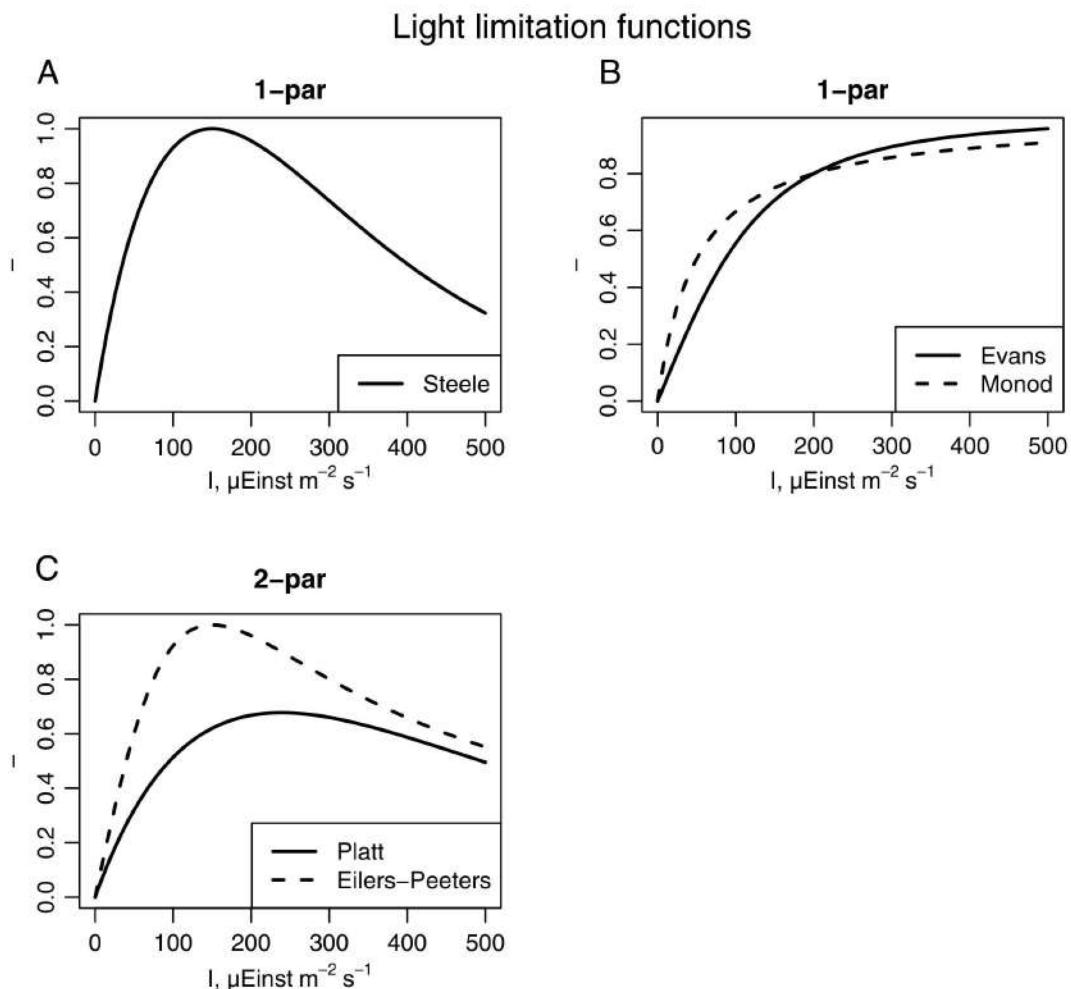


Fig. 2.19 Examples of light-limitation functions. **A–B**: one-parameter functions, **C**: two-parameter functions. See text for more details

The Platt model:	$\text{LightLim} = \left(1 - \exp\left(\frac{-\alpha \cdot I}{pMax}\right)\right) \cdot \exp\left(\frac{-\beta \cdot I}{pMax}\right)$
Eilers-Peeters model	$\text{LightLim} = \frac{2 \cdot (1 + \beta) \cdot I/I_{opt}}{(I/I_{opt})^2 + 2 \cdot \beta \cdot I/I_{opt} + 1}$

With $pMax$ the maximal photosynthesis rate (d^{-1}). Typical values for α and β are $0.005\text{--}0.01 (\mu\text{Einst m}^{-2} \text{s}^{-1})^{-1} \text{ d}^{-1}$. (Note: in the Platt model, α and β do not occur independently from $pMax$, so there are effectively only 2 independent parameters).

2.8.3 Other Physical Impacts

Currents and turbulence obviously have a large impact on pelagic animals with limited swimming capacity. However, they also affect sediment-inhabiting (benthic) animals in various ways. Many benthic animals have pelagic larvae that are

transported with the water movement; filter feeders require sufficient water motion to supply their food and remove their waste, deposit-feeding animals (feeding from organic matter in and on top of the sediment) rely on settlement of organic matter and low-flow conditions. In return, large beds of benthic (sediment-dwelling) organisms such as bivalves may change the hydrodynamics due to their impact on the roughness of the bottom, as induced by their structure (shells).

Current fields and turbulence are often imposed as a forcing function, although they can also be generated by so-called hydrodynamic models, which consist, just as ecological models, of a set of coupled differential equations. Most typically these models describe the flow velocity in 2 or 3 directions (vertical, N-S and E-W) and discriminate between horizontal and vertical turbulence.

Wind impacts the currents and turbulence in water, but also the exchange of gaseous substances at the air-water interface, by creating local turbulence. This atmospheric variable is almost always imposed as a forcing function. Rare exceptions are the coupled atmospheric-ocean circulation models.

2.9 Examples

2.9.1 NPZD, a Simple Ecosystem Model for Aquatic Environments

NPZD is an acronym that stands for Nutrient, Phytoplankton, Zooplankton and Detritus. It is an often-used type of model in the marine and freshwater system and describes only four state variables. In the marine environment, the nutrient is generally dissolved inorganic nitrogen and the model currency is in nitrogen units; freshwater models generally deal with phosphorus.

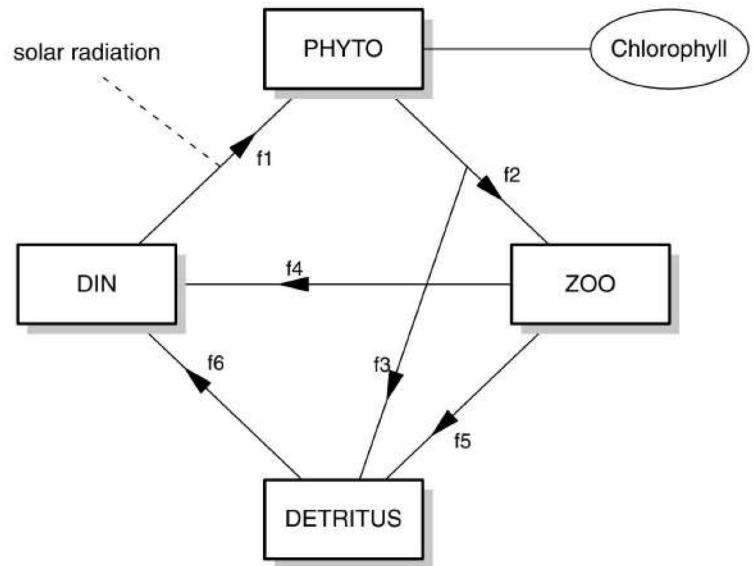
2.9.1.1 Step 1. Flowchart

To create an NPZD model, we start by drawing the flowchart, comprising the state variables (square boxes), the flows (arrows connecting the state variables), the forcing functions and the ordinary variables. The flowchart of an NPZD model is given in Fig. 2.20, where:

- f1 = net nitrogen uptake of algae
- f2 = zooplankton grazing
- f3 = zooplankton faeces production
- f4 = zooplankton excretion
- f5 = zooplankton mortality
- f6 = detritus mineralization

All four state variables are expressed in mmolN.m^{-3} , solar radiation is a forcing function and Chlorophyll is an output variable.

Fig. 2.20 Flowchart of the NPZD (nutrient, phytoplankton, zooplankton, detritus) model



2.9.1.2 Step 2. Conceptual Model

Next, we write the conceptual model, which specifies the rate of change of the four state variables as the sum of all inflows (arrows directed into the boxes) minus all outflows,

For the NPZD model the conceptual model is:

$$\begin{aligned}
 \frac{d \text{ PHYTO}}{dt} &= f_1 - f_2 \\
 \frac{d \text{ ZOO}}{dt} &= f_2 - f_3 - f_4 - f_5 \\
 \frac{d \text{ DETRITUS}}{dt} &= f_3 + f_5 - f_6 \\
 \frac{d \text{ DIN}}{dt} &= f_4 + f_6 - f_1
 \end{aligned} \tag{2.69}$$

2.9.1.3 Step 3. Mathematical Formulations

Thirdly, we create a mathematical expression for all the flows. We distinguish between:

- Flows that express ecological interactions between two components. These flows are modelled as: `maxRate*WORKER*RateLimitingTerms`.

Net nitrogen uptake (f_1 , units of $\text{mmol N m}^{-3} \text{ d}^{-1}$):

- The phytoplankton (PHYTO) performs the work and sets the maximal rate (parameter maxUptake).
- Nitrogen uptake is limited by light availability, expressed as a Monod function (parameter k_{SPAR} , units $\mu\text{Einst m}^{-2} \text{ s}^{-1}$)

- Nutrient uptake is also limited by availability of DIN, also expressed by a Monod formulation (parameter ks_{DIN} , units mmol N m^{-3}).
- Liebig's law of the minimum is used for total limitation:

$$\text{N_Uptake} = \text{maxUptake} \cdot \text{MIN}\left(\frac{\text{PAR}}{\text{PAR} + ks_{PAR}}, \frac{\text{DIN}}{\text{DIN} + ks_{DIN}}\right) \cdot \text{PHYTO} \quad (2.70)$$

where PAR is the photosynthetically active radiation, a forcing function ($\mu\text{Einst m}^{-2}\text{s}^{-1}$).

Zooplankton grazing (f2, units of $\text{mmol N m}^{-3} \text{d}^{-1}$):

- Is first-order to zooplankton biomass, the component performing the work (parameter maxGrazing)
- We use a Monod formulation for grazing limitation by the phytoplankton concentration (parameter ks_{PHYTO})

$$\text{Grazing} = \text{maxGrazing} \cdot \frac{\text{PHYTO}}{\text{PHYTO} + ks_{PHYTO}} \cdot \text{ZOO} \quad (2.71)$$

2. Flows that are expressed as a function of another flow.

Zooplankton faeces production, f3:

- This is expressed as a constant fraction of total grazing (parameter $pFaeces$ (<1)):

$$\text{FaecesProduction} = \text{Grazing} \cdot pFaeces \quad (2.72)$$

3. Flows which are simply first-order to the source compartment.

Zooplankton excretion, f4; this flow is first-order to zooplankton biomass:

$$\text{Excretion} = \text{excretionRate} \cdot \text{ZOO} \quad (2.73)$$

4. Closure terms, which take into account the action of components that are not explicitly modelled. Here there are two closures:

- *Zooplankton mortality*, f5, caused by predators that are not explicitly modelled. We can describe that as second-order to zooplankton biomass:

$$\text{Mortality} = \text{mortalityRate} \cdot \text{ZOO}^2 \quad (2.74)$$
- *Detritus mineralization*, f6, performed by bacteria that are not part of the model; this is described as first-order to detritus concentration:

$$\text{Mineralization} = \text{mineralizationRate} \cdot \text{DETRITUS} \quad (2.75)$$

Finally, we convert from phytoplankton biomass (in mmol N m^{-3}) to chlorophyll (mg Chl m^{-3}) by assuming a constant proportionality factor, *Chl Nratio* (units of $\text{mgChl} (\text{mmol N})^{-1}$):

$$\text{Chlorophyll} = \text{Chl_Nratio} \cdot \text{PHYTO} \quad (2.76)$$

The following table lists typical parameters values:

Parameter	Value	Units
maxUptake	1.0	Day ⁻¹
ksPAR	120	$\mu\text{Einst m}^{-2} \text{s}^{-1}$
ksDIN	0.5	mmol m ⁻³
maxGrazing	1.0	Day ⁻¹
ksPHYTO	1	mmol N m ⁻³
pFaeces	0.3	—
mortalityRate	0.4	(mmolN m ⁻³) ⁻¹ day ⁻¹
excretionRate	0.1	Day ⁻¹
mineralizationRate	0.1	Day ⁻¹
Chl_N_ratio	1	mg chl (mmolN) ⁻¹

2.9.1.4 Step 4. Testing the Correctness of the Equations

We first test the consistency of units. We restrict ourselves to one equation, the grazing of the zooplankton:

$$\text{Grazing} = \text{maxGrazing} \cdot \frac{\text{PHYTO}}{\text{PHYTO} + k_{\text{PHYTO}}} \cdot \text{ZOO} \quad (2.77)$$

With ZOO in mmolN m^{-3} , and the model time unit in days, the grazing is expressed in $\text{mmol N m}^{-3} \text{d}^{-1}$.

The dimensions relate as follows:

$$\text{mmolN} \cdot \text{m}^{-3} \cdot \text{d}^{-1} = \text{d}^{-1} \cdot \frac{\text{mmolN} \cdot \text{m}^{-3}}{\text{mmolN} \cdot \text{m}^{-3} + \text{mmolN} \cdot \text{m}^{-3}} \cdot \text{mmolN} \cdot \text{m}^{-3} \quad (2.78)$$

which is dimensionally consistent.

We then test for mass conservation. As there are no external sinks nor sources, total nitrogen concentration should be constant. In other words: the rate of change of total nitrogen should be 0. Total nitrogen is the sum of phytoplankton, zooplankton, DIN and detritus, and the rate of change of total nitrogen is just the sum of the rates of changes of these state variables:

$$\begin{aligned} \text{dtotalN/dt} &= \text{dPHYTO/dt} + \text{dZOO/dt} + \text{dDETTRITUS/dt} + \text{dDIN/dt} \\ \text{dtotalN/dt} &= f_1 - f_2 + f_2 - f_3 - f_4 - f_5 + f_3 + f_5 - f_6 + f_4 + f_6 - f_1 = 0 \end{aligned}$$

2.9.1.5 Step 5. Solving the Model

We will learn how to solve such models in next chapters. With a light intensity that varies as a sine-wave with the season, the output in Fig. 2.21 is obtained:

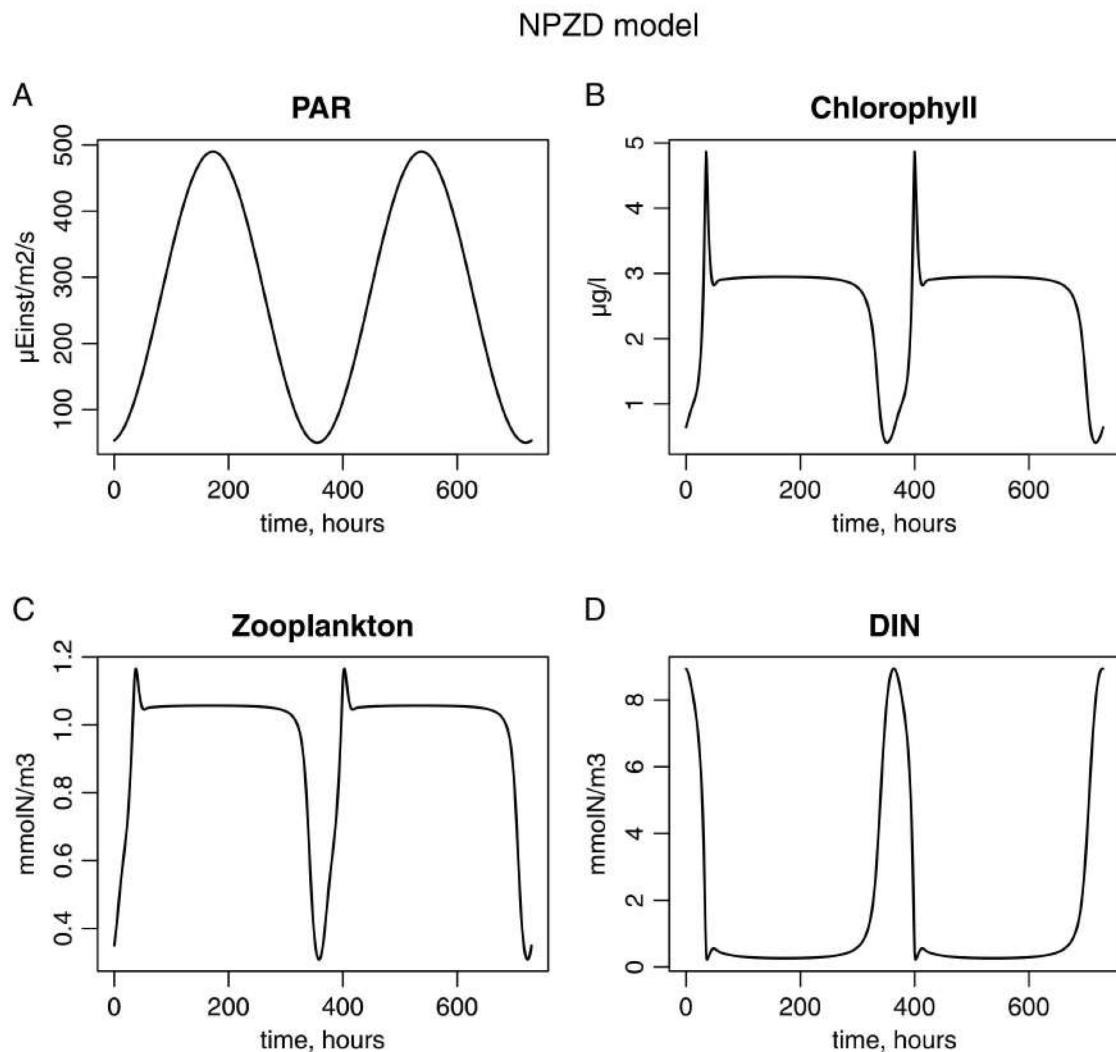


Fig. 2.21 Solution of the NPZD model, obtained after 3 years of simulation. Only the last two years are depicted. **A.** The photosynthetically active radiation (forcing function). **B.** Chlorophyll, **C.** Zooplankton and **D.** Dissolved Inorganic Nitrogen concentration

2.9.2 AQUAPHY, a Physiological Model of Unbalanced Algal Growth (**)

AQUAPHY (Lancelot et al., 1991) is a complex, physiological model that describes the growth of algae in response to nutrients and light.

Algae need carbon (CO_2), light energy and elements such as nitrogen and phosphorus for growth. Carbon is assimilated through the process of photosynthesis where CO_2 is incorporated into organic form (carbohydrates of low molecular weight), using light as an energy source. Nitrogen is taken up in inorganic form, usually as ammonium or nitrate, and built into complex molecules such as proteins, that form the biosynthetic and photosynthetic apparatus of the algae. Carbohydrates are also essential for synthesising these proteins, as they act both as a carbon source and as an energy source (through respiration). The surplus of low molecular weight carbohydrates that is not channelled into protein production is converted into storage

molecules (such as starch), that serve as a source of carbon and energy during times when photosynthesis stops (night).

Thus carbon assimilation is limited by light intensity (CO_2 is almost never limiting in the water column), whereas nitrogen assimilation is limited both by the availability of nutrients and of carbohydrates.

The conditions for carbon and nitrogen assimilation may not be simultaneously fulfilled. For instance, during night, photosynthesis will stop (due to lack of light energy), but nitrogen assimilation may continue as long as both nutrients and carbohydrates are available.

Due to this uncoupling of carbon and nitrogen assimilation, algae have, to a certain degree, a variable stoichiometry: their carbon to nitrogen (C:N) ratio is higher under high light or low nutrient conditions (high light will favour photosynthesis, low nutrients will reduce nitrogen assimilation). However, algae also try to keep their C:N ratio within certain physiologically tolerable limits. Thus, if there is excess carbon, the acquisition of new carbon through photosynthesis will be downgraded, whilst under carbon shortage, photosynthesis will be performed at maximal rates, as set by the prevailing light conditions.

Models that describe this uncoupling between carbon and nitrogen assimilation are called *unbalanced growth* models. They differ from the more often used *balanced growth* models, where nitrogen and carbon assimilation occurs simultaneously and where algae have fixed stoichiometry.

In AQUAPHY, algal biomass is described via 3 different state variables: low molecular weight carbohydrates (**LMW**) that are the product of photosynthesis, storage molecules (**RESERVE**) and the biosynthetic and photosynthetic apparatus (**PROTEINS**). All state variables are expressed in mmol C m^{-3} .

Only proteins contain nitrogen and chlorophyll, at a fixed amount (i.e. using a fixed stoichiometric ratio). As the relative amount of proteins changes in the algae, so does the N:C and the Chl:C ratio.

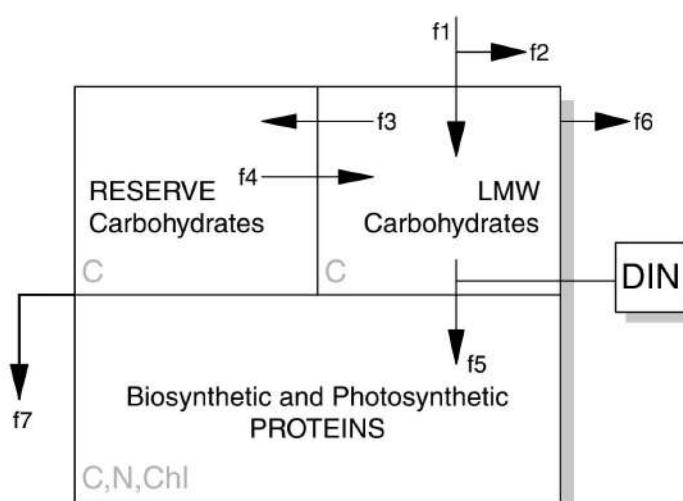


Fig. 2.22 Flowchart of the AQUAPHY model

An additional state variable, dissolved inorganic nitrogen (**DIN**) has units of mmol N m⁻³.

The model formulation proceeds, in three steps.

Step 1. The *flowchart* is depicted in Fig. 2.22. Fluxes are:

Where: f1=Photosynthesis, f2=Exudation, f3=Storage, f4=Catabolism, f5=Protein Synthesis, f6=Respiration, f7=Loss due to mortality

Step 2. The *conceptual model equations* are:

$$\begin{aligned} \frac{dLMW}{dt} &= \text{Photosynthesis+Catabolism} \\ &\quad -\text{Exudation-Storage-Respiration-ProteinSynthesis-LMWMortality} \\ \frac{dRESERVE}{dt} &= \text{Storage-Catabolism-ReserveMortality} \\ \frac{dPROTEIN}{dt} &= \text{ProteinSynthesis-ProteinMortality} \\ \frac{dDIN}{dt} &= -\text{ProteinSynthesis} \cdot NCratio_Protein \end{aligned} \tag{2.79}$$

Step 3. To write the actual *mathematical equations*, we specify each of the constitutive processes, as a function of the state variables, and the forcing function (light). Proteins are performing most of the work, thus many rates are first-order with respect to the protein concentration.

The following functional dependencies apply:

- Photosynthesis (flow 1) is described using the Platt equation; there is no light inhibition.

$$\text{Photosynthesis} = maxPhotoSynt \cdot (1 - \exp^{\frac{\alpha \cdot IPAR}{maxPhotoSynt}}) \cdot PROTEIN \tag{2.80}$$

- Exudation (flow 2) is a fixed fraction of photosynthesis

$$\text{Exudation} = pExudation \cdot \text{Photosynthesis} \tag{2.81}$$

- Protein synthesis (flow 5) is limited by the relative availability of low molecular weight carbohydrates (LMW), and by the availability of dissolved inorganic nitrogen (DIN). There is a minimal ratio of LMW over PROTEIN at which the protein synthesis stops (*minQuota*).

$$\begin{aligned} \text{ProteinSynthesis} &= maxSynt \cdot \frac{\gamma}{\gamma + ks\gamma} \cdot \frac{\text{DIN}}{\text{DIN} + ksDIN} \cdot \text{PROTEIN} \\ \gamma &= \frac{\text{LMW}}{\text{PROTEIN}} - minQuota \end{aligned} \tag{2.82}$$

- Reserve production, or storage, (flow 3) is limited by the relative availability of LMW molecules (γ), where (γ) is defined as above:

$$\text{Storage} = \text{maxStorage} \cdot \frac{\gamma}{\gamma + ks_\gamma} \cdot \text{PROTEIN} \quad (2.83)$$

- Respiration (flow 6) includes basal respiration (1st term) and growth respiration (2nd term), the latter a fraction of protein synthesis.

$$\text{Respiration} = \text{respRate} \cdot \text{LMW} + p \cdot \text{ProteinSynthesis} \quad (2.84)$$

- Catabolism (flow 4) follows first-order kinetics with respect to reserve molecules

$$\text{Catabolism} = \text{catabolismRate} \cdot \text{RESERVE} \quad (2.85)$$

- Finally, mortality impacts all algal state variables similarly:

$$\begin{aligned} \text{LMWMortality} &= \text{mortRate} \cdot \text{LMW} \\ \text{ReserveMortality} &= \text{mortRate} \cdot \text{RESERVE} \\ \text{ProteinMortality} &= \text{mortRate} \cdot \text{PROTEIN} \end{aligned} \quad (2.86)$$

Step 4. We will check the *consistency of units* of the photosynthesis equation only (and leave it as an exercise to the reader for the other equations):

$$\begin{aligned} \text{Photosynthesis} &= \text{max PhotoSynt} \cdot (1 - e^{\frac{\alpha \cdot \text{IPAR}}{\text{max PhotoSynt}}}) \cdot \text{PROTEIN} \\ &\text{mmolC} \cdot \text{m}^{-3} \cdot \text{d}^{-1} = \text{d}^{-1} \cdot (-) \cdot \text{mmolC} \cdot \text{m}^{-3} \end{aligned} \quad (2.87)$$

Moreover, as the exponent $\alpha \cdot \text{IPAR}/\text{max PhotoSynt}$ should yield a dimensionless quantity, and with Ipar in $\mu \text{Einst m}^{-2} \text{s}^{-1}$, max PhotoSynt in d^{-1} , it follows that the units of α should be $\text{d}^{-1}(\mu \text{Einst m}^{-2} \text{s}^{-1})^{-1}$

We also check the *mass balance*.

There are a number of external carbon flows (f_1, f_2, f_6 and f_7) such that the total load will not be constant:

$$\frac{d \text{TotalC}}{dt} = \frac{d \text{LMW}}{dt} + \frac{d \text{PROTEIN}}{dt} + \frac{d \text{RESERVE}}{dt} = f_1 - f_2 - f_6 - f_7 \quad (2.88)$$

We also check consistency for nitrogen. Within the algal cells, only proteins contain nitrogen:

$$\frac{d \text{TotalN}}{dt} = \frac{d \text{PROTEIN}}{dt} \cdot N \text{Cratio_protein} + \frac{d \text{DIN}}{dt} = -\text{ProteinMortality} \quad (2.89)$$

Thus, the rate of change of total nitrogen = net export of total nitrogen, and the rate of change of total carbon = net carbon production, and mass is conserved.

Step 5. To *solve* the model, rather complicated techniques are necessary, and the model is implemented as a computer programme (see later chapters).

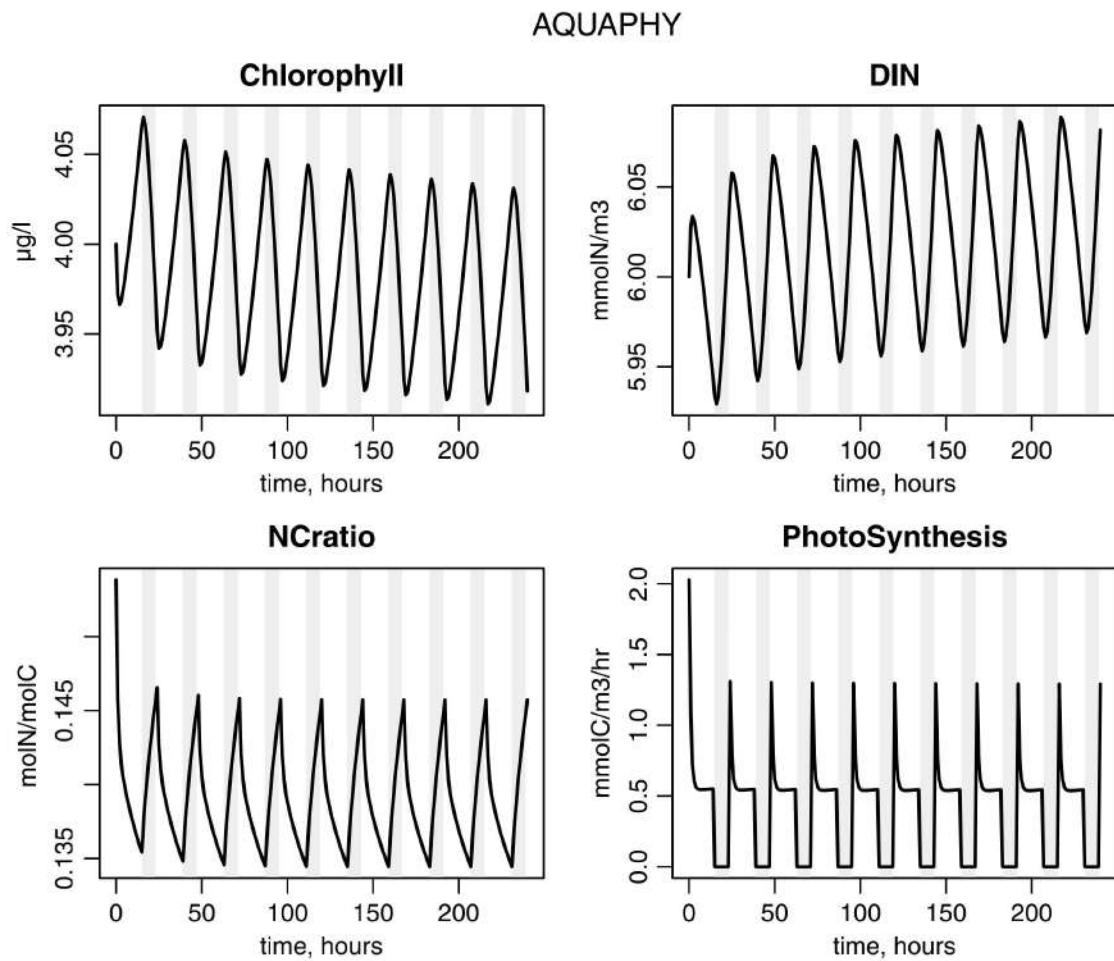
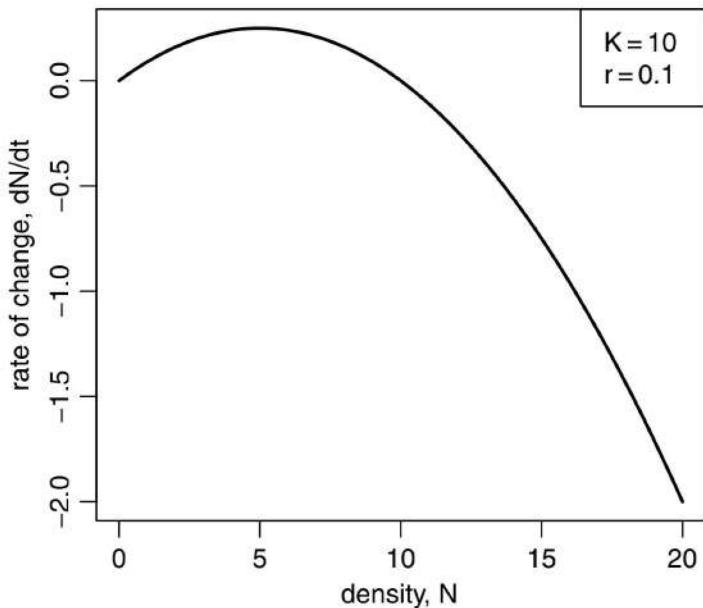


Fig. 2.23 Solution of the AQUAPHY model. The *light* and *dark* periods are denoted by *blank* and *shadowed* areas respectively. Note the daily variation in all depicted variables. See text for more explanation

In Fig. 2.23, the model has been run for 10 days under a 15 h light, 9 h darkness illumination regime; there is constant inflow of DIN and outflow of culture water (i.e. it is a dilution culture, see Chapter 3). The model output demonstrates the diurnal and long-term change of the algal chlorophyll concentration and DIN concentration. Also, the effect of the light-dark cycle on the algal stoichiometric N:C ratio is clear: the Nitrogen to Carbon ratio of the algae decreases during the day when carbon is assimilated, and increases during the night when the algae have stopped photosynthesising but continue to assimilate nitrogen. Finally, the photosynthesis process is triggered as soon as the light is switched on. Soon after that, the accumulation of low molecular weight carbohydrates inhibits photosynthesis and the rate declines. Photosynthesis stops during night.

This model has been used in a number of environmental model applications, e.g. to model the phytoplankton growth in the Weddell sea, Mediterranean, and North Sea.

Fig. 2.24 Rate of change as a function of density for the carrying-capacity formulation. R-code, see text



2.10 Case Studies in R

Even during the initial phase of the modelling process, before we even start to solve the models, we can make good use of the R software: R is extremely well suited for making graphs, and thus visualising the mathematical formulations.

2.10.1 Making Sense Out of Mathematical Formulations

The easiest way of understanding mathematical formulations is to make graphs. We will first do so for the carrying-capacity formulation.

$$\frac{dN}{dt} = r \cdot N \cdot \left[1 - \frac{N}{K} \right] \quad (2.90)$$

We make a graph, depicting the rate of change $\frac{dN}{dt}$ as a function of density (N , ind m^{-2}), and using the following parameter values: $r = 0.1 \text{ d}^{-1}$, $K = 10 \text{ ind m}^{-2}$.

R-code

We first assign a value to the parameters r and K :

```
r <- 0.1 # intrinsic rate of increase /day
K <- 10 # carrying capacity
```

Note that in R

- the left arrow '`<-`' is an assignment operator; i.e. if we write '`A <- 3`' then A obtains the value 3.
- the symbol '#' demarcates a comment, which lasts till the end of the line and which is ignored by R.

Before plotting, we open a new window, (the height and width are expressed in inches). Note that `windows()` only works in Microsoft windows ®. Instructions for other operating systems can be found in the R documentation.

```
windows(width=5,height=5)
```

To plot the rate of change as a function of density (x), we use R-function '`curve`' which is particularly handy to plot an expression (`expr`), i.e. a function of x. Parameters '`from`' and '`to`' set the x-axis limits, `lwd=2` sets the line width to double the default, `xlab` and `ylab` specify labels of the x- and y axes. A legend adds the parameter values to the graph. The result is depicted in Fig. 2.24:

```
curve(expr= r*x*(1-x/K), from=0, to=20, lwd=2,
       xlab="density, N", ylab="rate of change, dN/dt")
legend("topright", c("K=10", "r=0.1"))
```

2.10.2 One Formula, Several Parameter Values

To really demystify a mathematical formulation, it should be plotted with different parameter values.

Here is how to do this in R. We plot a type-II (Monod or Michaelis-Menten) rate limiting term for describing grazing of a consumer on its food. We plot the function for several values of the half-saturation constant *ks*.

We start by defining the values of *food* and the parameter values for which we want to depict the relationship. R's function `seq(0, 30, by=0.1)` creates a sequence, from 0 to 30 and with interval 0.1. Then we calculate the Monod function for every combination of the food and *ks* values. R's function `outer` does that; the results are stored in a matrix called `foodmat`. Next, all columns of `foodmat` are plotted using `matplot`. Note that the title (`main`) has been written as an expression. Also, we overrule the default colors (`col`). By default, `matplot` uses a different color for each column plotted; here we use black for all lines. We also set the line width to double the default (`lwd`). Finally a legend clarifies the plot.

```

food <- seq(0,30,by=0.1)
ks   <- seq (1,10, by=2)

foodmat <- outer(food,ks,function(x,y) x / (y +x))

matplot(x=food,foodmat,type="l",col="black",
        xlab="food",ylab="-",lwd=2,
        main= expression (frac(food , food+ks)))

legend ("bottomright", as.character(ks), title="ks=",
        lty=1:5,lwd=2)

```

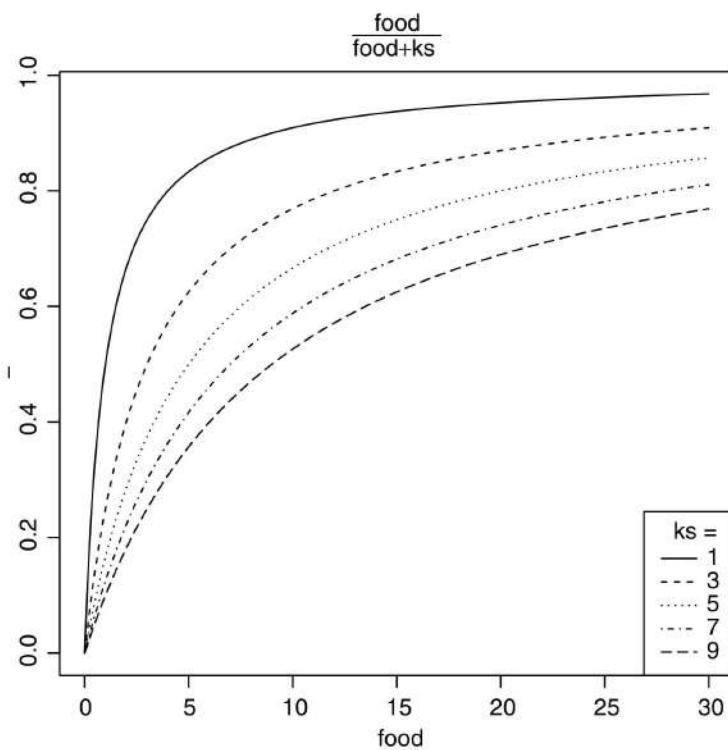


Fig. 2.25 Output generated by the R-code from example 2.10.2

2.11 Projects

2.11.1 Conceptual Model: Lake Eutrophication

Phosphorus is the nutrient that is generally limiting primary production in lakes. Increasing the input of phosphorus increases the concentration of phytoplankton, which may have a radical effect on water quality. Cladoceran grazers (zooplankton) are the main consumers of lake algae and may reduce algal biomass.

To overcome the negative impacts of eutrophication, the concept of biomanipulation was introduced in the seventies, which consisted of reducing the predation

pressure on these large cladocerans. When successful, this treatment resulted in a reduced phytoplankton biomass and a higher zooplankton biomass dominated by large organisms. However, several cases were reported where this manipulation failed to give the desired results. Close examination revealed that failure was most likely in lakes that received a phosphorus input above a certain critical level.

Tasks:

Make a conceptual model that serves to investigate the effect of biomanipulation on a lake ecosystem.

- Review the components that should be included in the model.
- What state variables will be in your model?
- What forcing functions?
- What types of relations?
- What will be the space and time scale of your model?

Start by drawing a conceptual diagram, consisting of boxes (the state variables), linked by arrows (fluxes). Also include input and output from and to the external world. Give sensible names to each of the fluxes.

Then, for each state variable, express their rate of change as a function of the source and sink fluxes.

How would you investigate the effect of biomanipulation?

2.11.2 Model Formulation: Nutrient-Limited Batch Culture

Phytoplankton is grown in a well-mixed closed culture vessel (a so-called batch culture). Algal growth is limited by dissolved inorganic nitrogen (DIN) only, other nutrients and light are never limiting (Fig. 2.26).

Assume:

1. The maximum DIN uptake rate of the algae is set by the prevailing light conditions, and given by the parameter $p_{max} = 1.0 \text{ d}^{-1}$.
2. Actual nitrogen uptake is governed by Monod kinetics with parameter $k_s = 1.0 \mu\text{mol N.dm}^{-3}$.

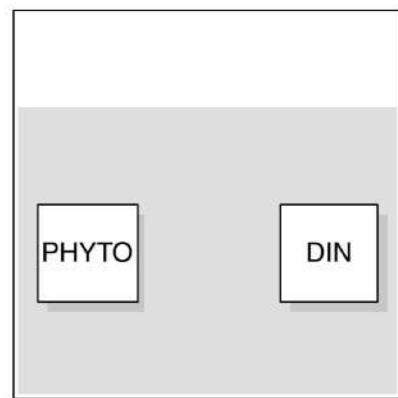
Task:

1. Write the mathematical formula that describes uptake of DIN by the algae. Give the units of the parameters and state variables
2. Make a model that describes the interaction of algae and DIN.

Start with a conceptual model.

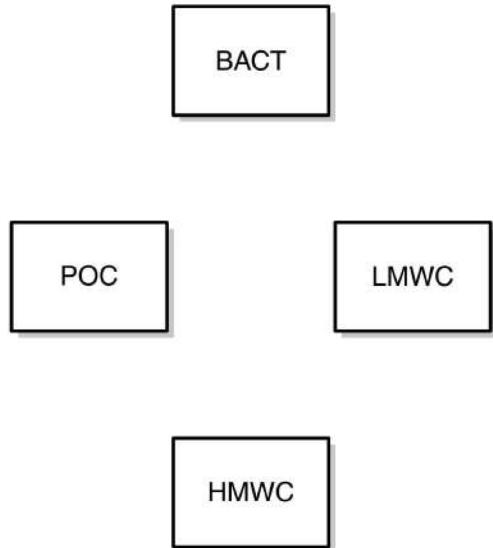
- What are the state variables in this model?
- Which are the flows? Draw the flow chart.
- Write the rate of change of the state variables as the sum of influxes – effluxes.
- Write the mathematical equations for the fluxes.
- Check the mass balance of the model. Is mass conserved by the equations?

Fig. 2.26 Components of the batch culture model



2.11.3 Model Formulation: Detritus Degradation

Fig. 2.27 State variables in the detritus degradation model



Detritus is degraded by the action of heterotrophic bacteria. This is not a one-step process: bacteria cannot ‘eat’ detritus!

A model that is closer to the reality of the process considers that particulate detritus (POC) is first degraded by the action of bacterial exoenzymes to high-molecular-weight dissolved organic carbon (HMWC). This in turn is attacked by enzymes to yield low-molecular-weight dissolved organic carbon (LMWC), which can then be taken up by the bacteria (BACT) which grow on it.

Assumptions:

- We will not model the exoenzyme concentration explicitly in the model. Instead, we assume that the maximal rate of hydrolysis (degradation) of POC and of HMWC is proportional to bacterial biomass [note: it are the bacteria that perform the work, they set the maximal rate]. We will use the parameters K_{maxPOC} and

$K_{maxHMWC}$ as maximal specific rates for the hydrolysis of POC and HMWC respectively.

- The hydrolysis of POC and HMWC is limited by the concentration of the resource. We will use Monod kinetics for both limitations, with half-saturation constants ks_{POC} and ks_{HMWC} respectively.
- POC is produced by algae which are external to our model. We impose a constant influx of POC into the model system as FluxPOC. POC is consumed by hydrolysis to HMWC.
- HMWC is produced by the hydrolysis of POC, and lost by hydrolysis to LMWC.
- LMWC is produced by the hydrolysis of HMWC, and lost by the uptake by bacteria. Again we assume that maximum uptake is directly proportional to bacterial biomass, with rate parameter $upMax$, and limited by substrate availability: Monod kinetics with parameter ks_{UP} .
- Bacteria grow by uptake of LMWC, but loose carbon by basal respiration ($rBas$) and by activity respiration: they respire a fraction $pLoss$ of the uptake. Moreover, bacteria are subject to predation, and this is modelled as a quadratic closure term, with parameter $rClos$.

Tasks :

Make a coupled model of this process.

Use four state variables as depicted in Fig. 2.27.

For each state variable sketch the influxes and effluxes in a flow chart.

Assemble the rate of change of the state variables as the sums of these positive and negative fluxes.

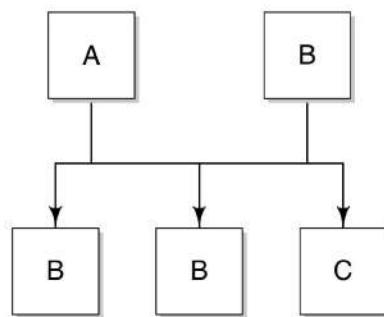
Write the formulations for each of these fluxes. Remember the two basic rules:

1. The compartment that is doing the work sets the maximal flux: maxflux =maxrate*WORKER
2. The effect of the resource that is limiting is expressed as a functional response. Use Monod kinetics.

Check the dimensionality of your model.

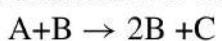
What are the units of $rClos$, $rBas$ and $pLoss$?

Fig. 2.28 Schematic representation of an autocatalytic reaction



2.11.4 Model Formulation: An Autocatalytic Reaction

An autocatalytic reaction is one where the reaction product is itself the catalyst for the reaction. For instance:



Write the rate of change of the concentrations [A], [B] and [C] (Fig. 2.28).