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Eawag:
Swiss Federal Institute of Aquatic
Science and Technology

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Modelling Aquatic Ecosystems
Course 701-0426-00

Nele Schuwirth

ETH Zürich, Department of Environmental Systems Sciences
Eawag, Swiss Federal Institute of Aquatic Science and Technology

Lecturer

Nele Schuwirth (nele.Schuwirth@eawag.ch)
PhD in Geology,
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Privatdozentin ETHZ

Guest lectures

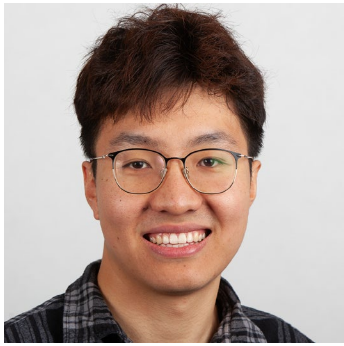
Andreas Scheidegger (andreas.scheidegger@eawag.ch)
MSc Applied Statistics, University Canberra
Statistician & Scientist at Eawag
Modelling, Systems Analysis, Data Science

Tribute to Peter Reichert

Peter Reichert (peter.reichert@eawag.ch)
PhD in Theoretical Physics
Head of Department Systems Analysis, Integrated Assessment and Modelling
Adjunct Professor at ETHZ

Retired since 2022

Course assistants



Chuxinyao (Nick) Wang (chuxinyao.wang@eawag.ch)

BSc Environmental Sciences

MSc in Computational methods in Ecology and Evolution

PhD student at ETHZ/Eawag

Mechanistic Modelling of Aquatic Mesocosms

Emma Chollet Ramampiandra (emma.chollet@eawag.ch)

MSc Mathematics, University of Neuchatel

PhD at ETHZ/Eawag

Postdoc at ETHZ/Eawag

Statistical and mechanistic modelling and machine learning

Goals of the Course

The students (you!) are able to

- **build** mathematical **models** of aquatic ecosystems that consider the most important biological, biogeochemical, and physical **processes**;
- **explain** the **interactions** between these processes and the **behavior** of the **system** that results from these interacting processes;
- **implement** and **apply** these ecological models;
- learn the key concepts of **model calibration** and the consideration of **stochasticity** and **uncertainty**.

Emphasis is on **integrating knowledge** in the form of models, on their use for **improving** the **understanding** and **management** of aquatic ecosystems and on their **limitations**.

Goals of the Exercises

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- **Hands-on experience** with
  model **implementation**, **simulation**, **sensitivity analysis**,
  and discussion of the behavior of a series of ecosystem models
  of increasing complexity
  to deepen and extend the knowledge gained in the lectures
- Gain some **experience with R**
  (also useful for statistical data analysis in future projects)

Emphasis is on **improving** the **understanding** of the behavior of the models and the aquatic ecosystems, not on programming.

Prerequisites and Time investment

Basic knowledge about structure and functioning of **aquatic ecosystems** as well as about **analysis**, **differential equations**, **linear algebra** and **probability**.

The time for the exercises will be provided during the course.
This decreases the time for lectures and makes them quite intensive.
You will need time between the course hours to read the manuscript.

Approximate time budget (3 credit points = 75-90 hours study time):

25-30 hours: Course attendance including supervised exercise time

25-30 hours: Reading the manuscript and preparing exercises

25-30 hours: Preparation of your own model and the oral exam.

Administrative Aspects

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Course and exercises will take place Wednesday 10:15 - 12:00 in LFW B2

Please **install before the exercise**:

A current version of R (http://www.r-project.org),

the editor R-Studio (http://www.rstudio.org),

and the R-package ecosim: `install.packages(c("ecosim"))`

Introduction to R programming:

https://cran.r-project.org/doc/contrib/Torfs+Brauer-Short-R-Intro.pdf

Program, manuscript, exercises etc. can be downloaded from:

`http://www.eawag.ch/forschung/siam/lehre/modaqecosys`

Administrative Aspects

There will be an **oral exam in the two weeks** after the semester **02.-13.06.25**

During the semester you will develop and implement your own model (in groups of two), interpret simulation results and perform a sensitivity analysis.

We will assign topics on 02.04.25.

Deadline for initial code submission: 08.05.25
Deadline for submission of R-files, results and interpretation: 23.05.25

This is mandatory for being admitted to the exam! In the oral exam we will start with questions about your model before moving on to other topics.

Use the time in the exercises to ask questions and get help!
Don’t do it last minute.

Structure of the Manuscript

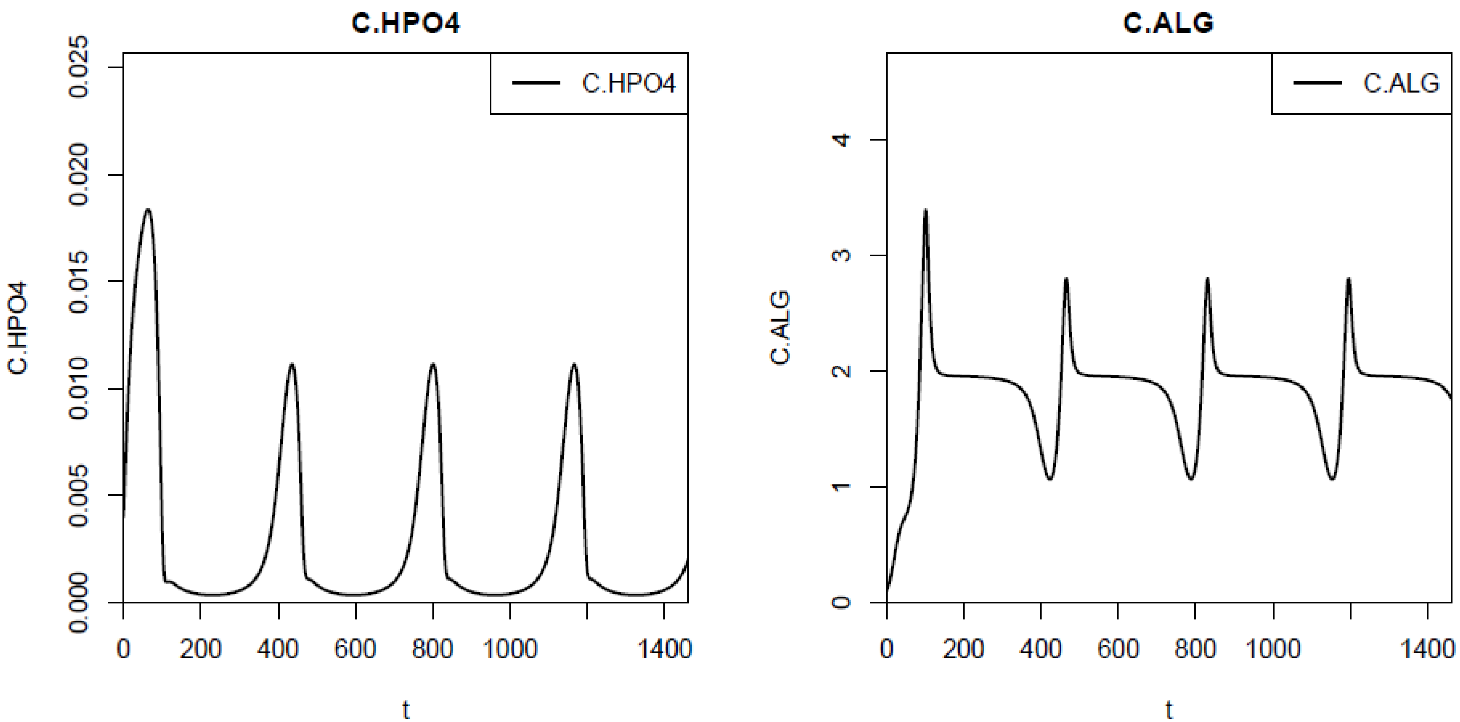
Structure of the Course

1. Introduction, principles of modelling environmental systems, mass balance in a mixed reactor, process table notation, simple lake plankton model
   Exercise: R, `ecosim`-package, simple lake plankton model
   Exercise: lake phytoplankton-zooplankton model
2. Process stoichiometry   Exercises: analytical solution, calculation with `stoichcalc`
3. Biological processes in lakes
4. Physical processes in lakes, mass balance in multi-box and continuous systems   Exercise: structured, biogeochemical-ecological lake model
   Assignments: build your own model by implementing model extensions
5. Physical processes in in rivers, bacterial growth, river model for benthic populations   Exercise: river model for benthic populations, nutrients and oxygen
6. Uncertainty, Parameter estimation, Stochasticity
   Exercise: parameter estimation
   Exercise: stochasticity, uncertainty
7. Existing models and applications in research and practice, examples and case studies, preparation of the oral exam, feedback

Questions?

Lecture 1: Goals

- Acquire basic knowledge of the formulation of transport and transformation processes to formulate a simple lake plankton model.
- Become familiar with the process table notation and rate formulation that will be the basis of the more complex models.



Motivation for ecosystem modelling?

What's your motivation to learn ecosystem modelling?

Motivation for ecosystem modelling?

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chapter 1

1. **Improving understanding of ecosystem function**:
   Test of quantitatively formulated hypotheses about system mechanisms. Estimation of fluxes and conversion rates. Stimulation of thinking about the function of an ecosystem.
2. **Summarizing and communicating knowledge**:
   Ecosystem models are perfect communication tools for exchanging quantitatively formulated knowledge of the processes in the ecosystem. A systematic notation facilitates the use of models for this purpose significantly.
3. **Supporting ecosystem management**:
   Prediction of the consequences of suggested measures. Estimation and consideration of prediction uncertainty is essential for this purpose of ecosystem modelling.

Zonation of aquatic ecosystems

Pelagic zone:

Water body not close to sediment and shore or bank.

Litoral zone:

Water body close to the shore or bank and the adjacent periodically inundated area.

Benthic zone:

Water body above the sediment and the top sediment layers.

Interstitial zone:

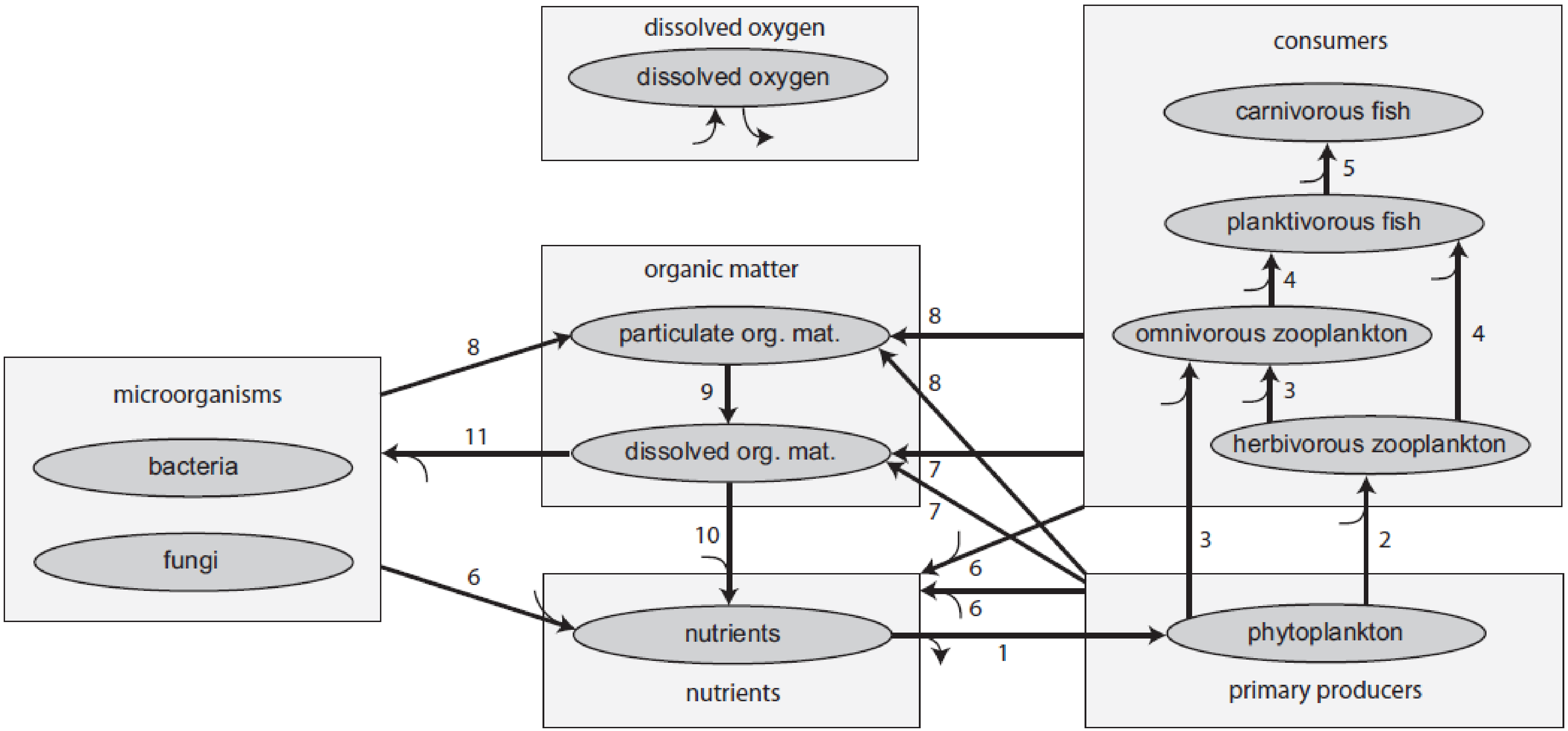
Pore space in the sediment below the benthic zone.

Pelagic / Benthic Food Webs

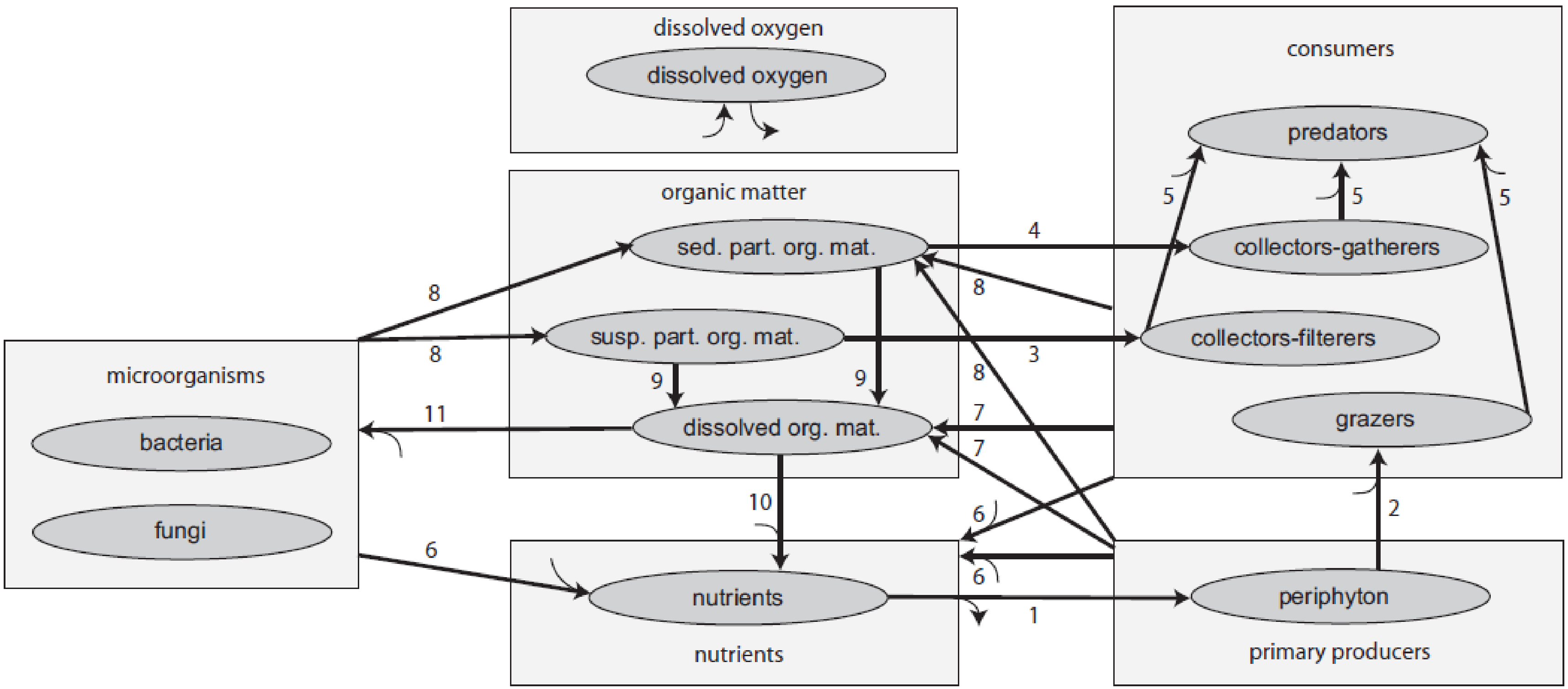
Imagine your favorite lake or stream...

To draw the food-web of this system, what are important organism groups to consider and what do they feed on?

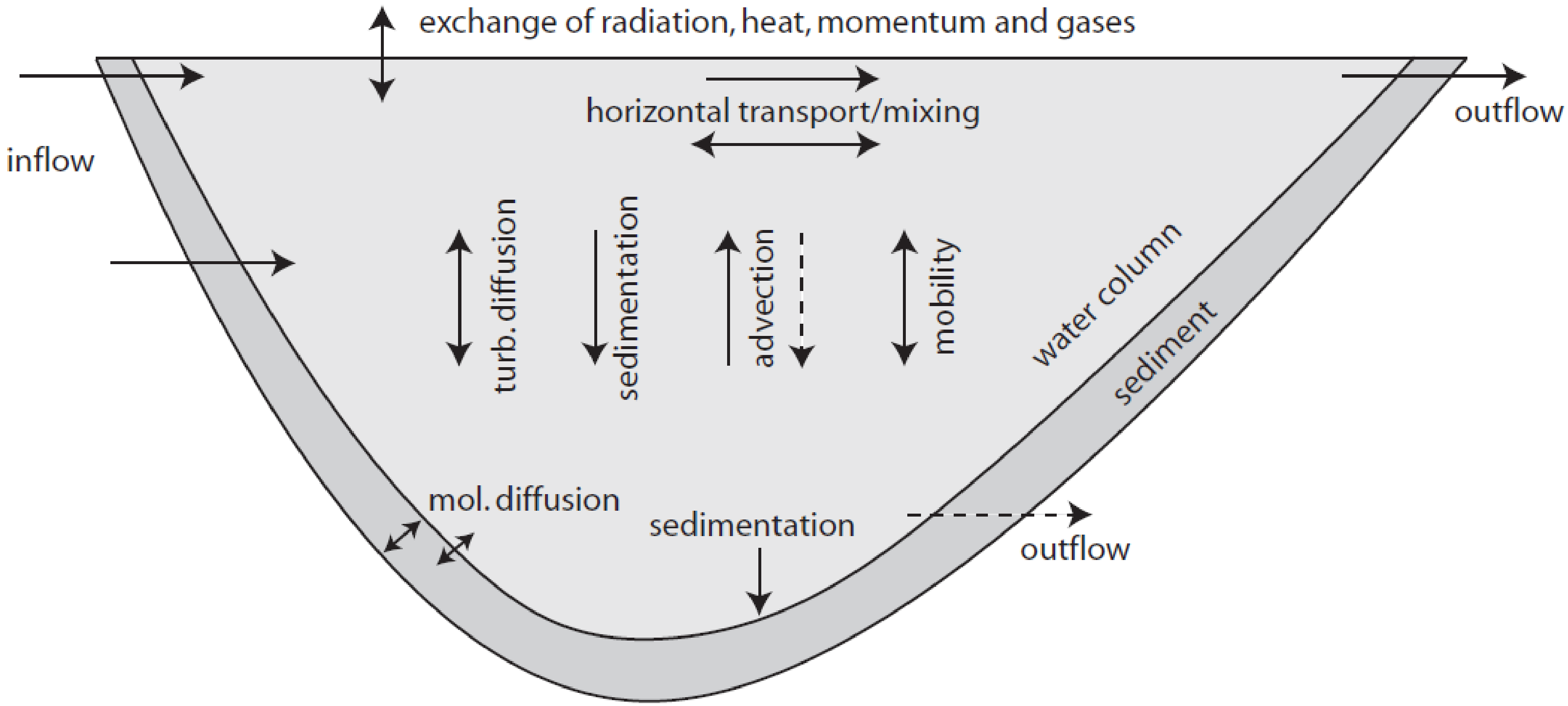
Pelagic Food Web



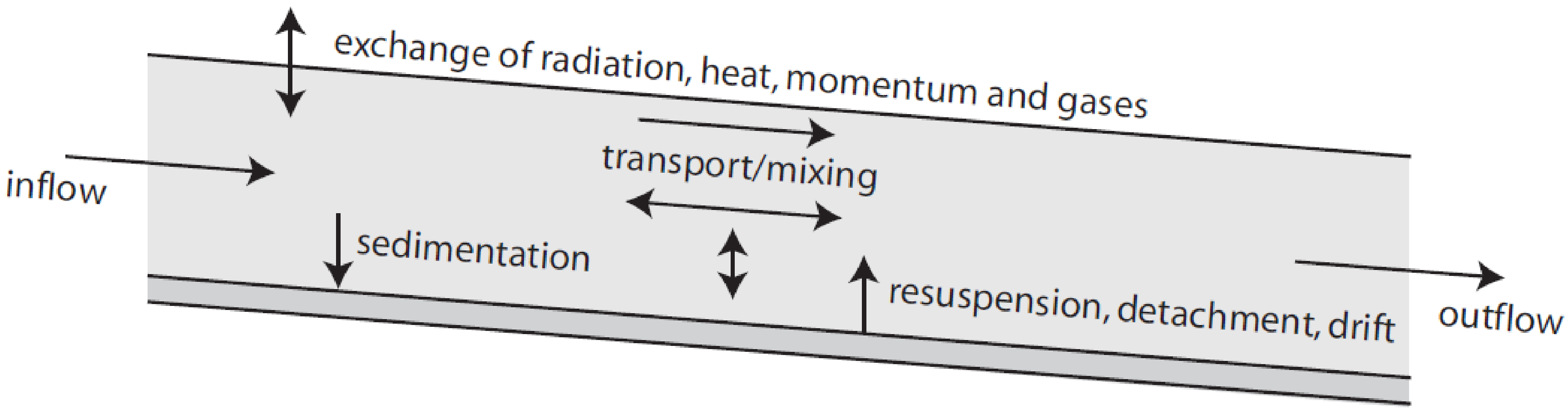
Benthic Food Web



Transport Processes in a Lake

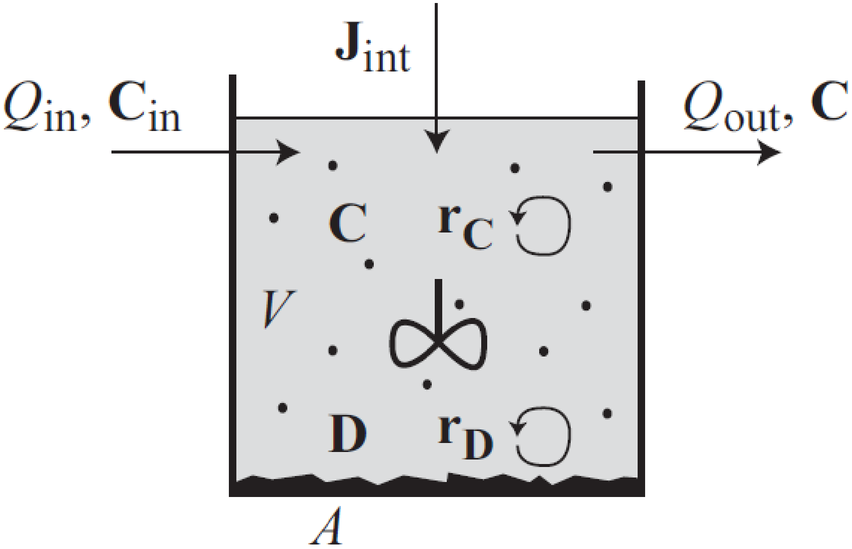


Transport Processes in a River



Principles of Modelling

chapter 2



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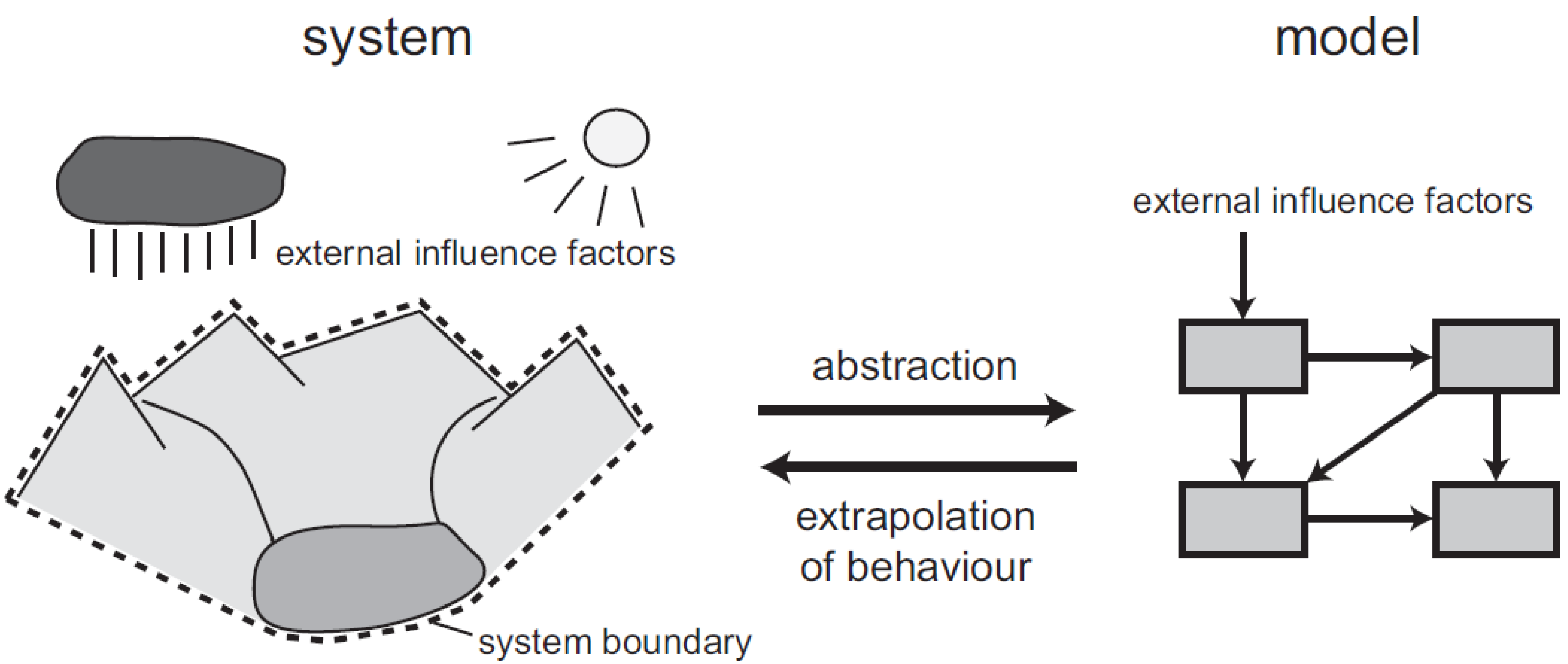
Meaning of models



→ many (rather arbitrary) choices and assumptions!
→ model has to fit the purpose!

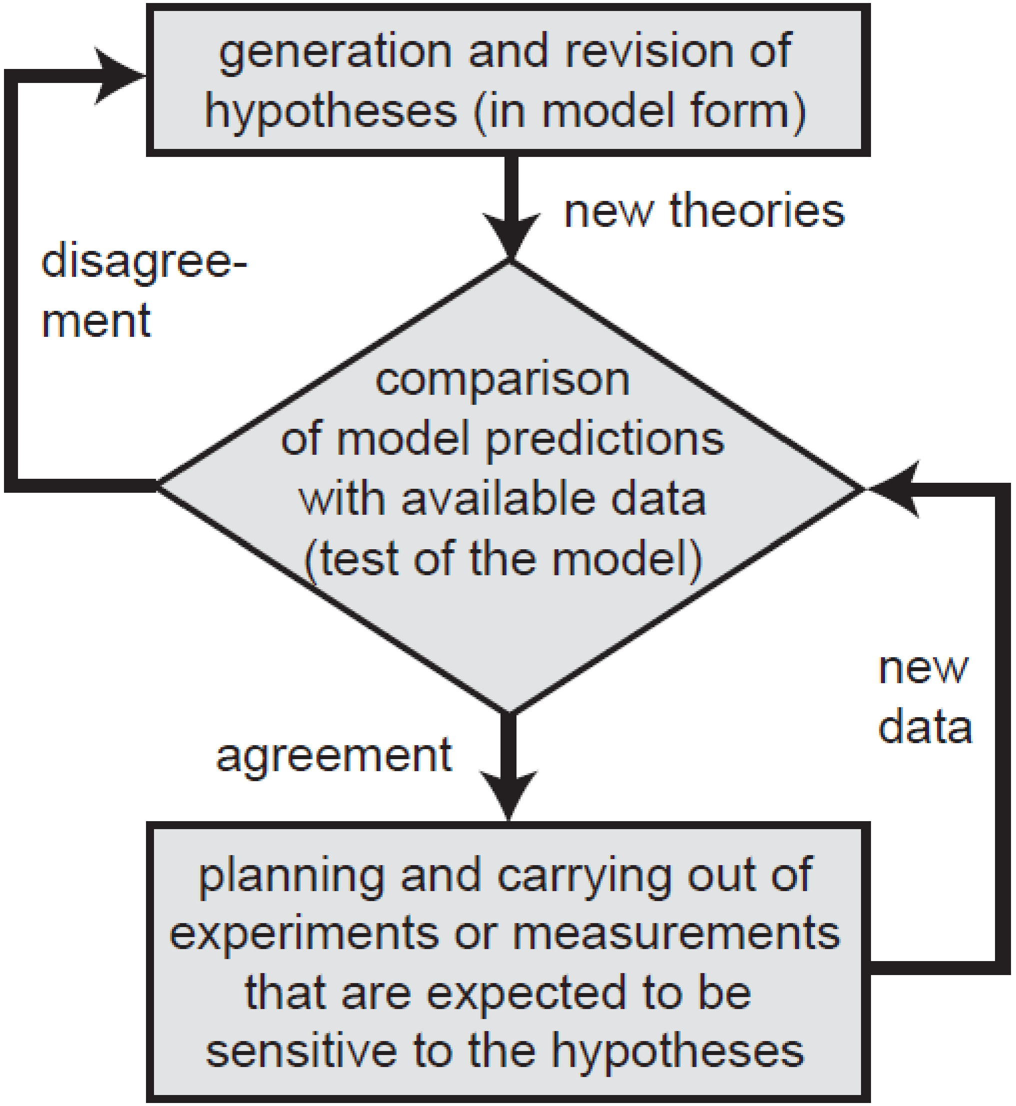
Formulation of ecosystem models

Essential techniques: Empirical relationships and mass-balance equations.

Typical form of an environmental model:

Mechanistic description of mass conservation - use of empirical expressions for the formulation of transformation and transfer processes.

Learning with models



Clarification of terms

Mathematical Model: Simplified mathematical description of a (real) system — $y = ax + b$; $dy/dt = a*x(t)*y - b*y$

Input variable: External influence factor, predictor / explanatory / independent variable — x

Output variable: State / response / dependent variable — y

Parameter: (Unknown) variable needed to relate input to output — a, b

Model types

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Mechanistic models (aka process-based, causal models)

- are *knowledge/theory* driven,
  explicitly describe mechanisms/processes to relate input and output
- parameters have a (physical, biological) meaning, are not necessarily calibrated

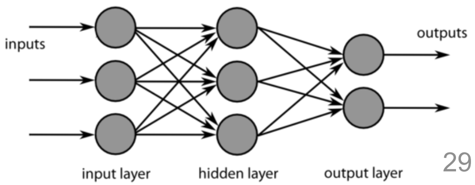
e.g.: individual based models, population / predator-prey / food web / community models based on ordinary differential equations, meta-community models, ecosystem models

Empirical models

- are *data* driven, based on empirical relationship between input and output

a) **Statistical models**: parameters are calibrated, do not have a (physical, biological) meaning, still interpretable, make statistical assumptions that can be tested
e.g. multivariate regression models, autoregressive time series models

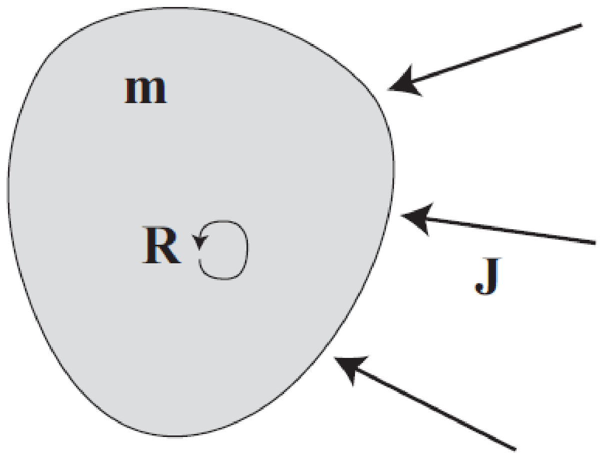
b) **Machine learning algorithms**: parameters are (usually) not interpretable, do not make statistical assumptions, are typically perceived as "black box"
e.g. (deep) artificial neural networks, random forests, boosted regression



General Mass Balance

chapter 3.1

General Mass Balance



m "masses" [m], **J** (net) inputs [m/T], **R** (net) production [m/T]

General Mass Balance

Integral form: calculate "mass" at t_{end} from "mass" at t_{ini} by adding net inputs and net production:

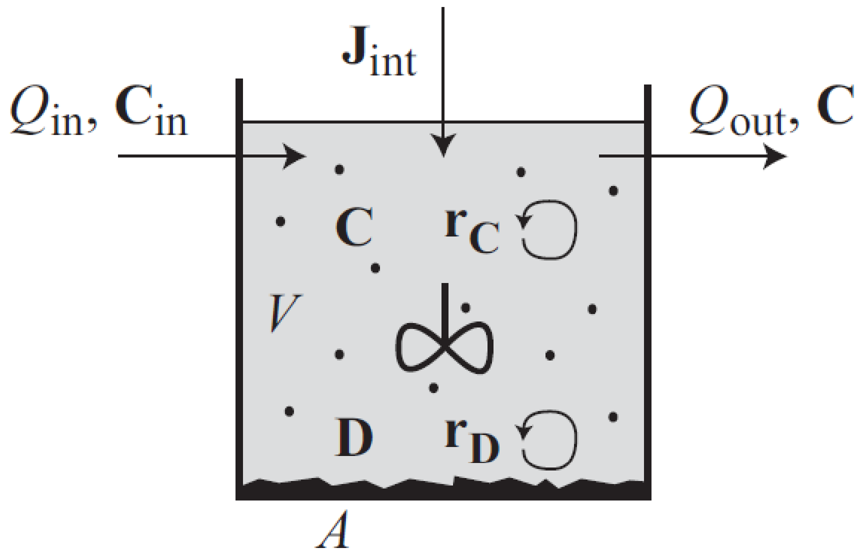
$$\mathbf{m}(t_{\mathrm{end}}) = \mathbf{m}(t_{\mathrm{ini}}) + \int_{t_{\mathrm{ini}}}^{t_{\mathrm{end}}} \mathbf{J}(t)\,\mathrm{d}t + \int_{t_{\mathrm{ini}}}^{t_{\mathrm{end}}} \mathbf{R}(t)\,\mathrm{d}t$$

Differential form: substitute t_{end} with t and differentiate:

$$\frac{\mathrm{d}\mathbf{m}}{\mathrm{d}t}(t) = \mathbf{J}(t) + \mathbf{R}(t)$$

Mass Balance in a Mixed Reactor

chapter 3.2



$\mathbf{C}$ concentration $[\mathrm{M}/\mathrm{L}^3]$
$\mathbf{D}$ surface density $[\mathrm{M}/\mathrm{L}^2]$
$Q_{\mathbf{in}}$ inflow, $Q_{\mathbf{out}}$ outflow $[\mathrm{L}^3/\mathrm{T}]$
$J_{\mathbf{int}}$ flux across the interface $[\mathrm{M}/\mathrm{T}]$

Mass Balance in a Mixed Reactor

$$\mathbf{m} = \begin{pmatrix} V \\ VC_1 \\ VC_2 \\ \vdots \\ VC_{n_v} \\ AD_1 \\ AD_2 \\ \vdots \\ AD_{n_a} \end{pmatrix}, \mathbf{J} = \begin{pmatrix} Q_{in} - Q_{out} \\ Q_{in}C_{in,1} - Q_{out}C_1 + J_{int,1} \\ Q_{in}C_{in,2} - Q_{out}C_2 + J_{int,2} \\ \vdots \\ Q_{in}C_{in,n_s} - Q_{out}C_{n_s} + J_{int,n_v} \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \mathbf{R} = \begin{pmatrix} 0 \\ Vr_{C_1} \\ Vr_{C_2} \\ \vdots \\ Vr_{C_{n_v}} \\ Ar_{D_1} \\ Ar_{D_2} \\ \vdots \\ Ar_{D_{n_a}} \end{pmatrix}$$

m "masses" [m], **J** (net) inputs [m/T], **R** (net) production [m/T]

Mass Balance in a Mixed Reactor

$$\mathbf{C} = \begin{pmatrix} C_1 \\ C_2 \\ \vdots \\ C_{n_\mathrm{v}} \end{pmatrix} \quad , \quad \mathbf{J}_\mathrm{int} = \begin{pmatrix} J_{\mathrm{int},1} \\ J_{\mathrm{int},2} \\ \vdots \\ J_{\mathrm{int},n_\mathrm{v}} \end{pmatrix} \quad , \quad \mathbf{r}_\mathbf{C} = \begin{pmatrix} r_{C_1} \\ r_{C_2} \\ \vdots \\ r_{C_{n_\mathrm{v}}} \end{pmatrix}$$

$$\mathbf{D} = \begin{pmatrix} D_1 \\ D_2 \\ \vdots \\ D_{n_\mathrm{a}} \end{pmatrix} \quad , \quad \mathbf{r}_\mathbf{D} = \begin{pmatrix} r_{D_1} \\ r_{D_2} \\ \vdots \\ r_{D_{n_\mathrm{a}}} \end{pmatrix}$$

Mass Balance in a Mixed Reactor

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$$\frac{\mathrm{d}V}{\mathrm{d}t} = Q_{\mathrm{in}} - Q_{\mathrm{out}}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(V\mathbf{C}\right) = Q_{\mathrm{in}}\mathbf{C}_{\mathrm{in}} - Q_{\mathrm{out}}\mathbf{C} + \mathbf{J}_{\mathrm{int}} + V\mathbf{r}_{\mathbf{C}}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(A\mathbf{D}\right) = A\mathbf{r}_{\mathbf{D}}$$

Mass Balance in a Mixed Reactor

$$\frac{\mathrm{d}V}{\mathrm{d}t} = Q_{\mathrm{in}} - Q_{\mathrm{out}}$$

$$\frac{\mathrm{d}\mathbf{C}}{\mathrm{d}t} = \frac{Q_{\mathrm{in}}}{V}\left(\mathbf{C}_{\mathrm{in}} - \mathbf{C}\right) + \frac{\mathbf{J}_{\mathrm{int}}}{V} + \mathbf{r}_{\mathbf{C}}$$

$$\frac{\mathrm{d}\mathbf{D}}{\mathrm{d}t} = \mathbf{r}_{\mathbf{D}}$$

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Example 11.1

Differential Equations

net input via in/outflow

consumption by algae

$$\frac{dC_{\mathrm{HPO4}}}{dt} = \frac{Q_{\mathrm{in}}}{V}\left(C_{\mathrm{HPO4,in}} - C_{\mathrm{HPO4}}\right) - \alpha_{\mathrm{P,ALG}} \cdot k_{\mathrm{gro,ALG}} \frac{C_{\mathrm{HPO4}}}{K_{\mathrm{HPO4}} + C_{\mathrm{HPO4}}} C_{\mathrm{ALG}}$$

loss via outflow

growth of algae

$$\frac{dC_{\mathrm{ALG}}}{dt} = -\frac{Q_{\mathrm{in}}}{V} C_{\mathrm{ALG}} + k_{\mathrm{gro,ALG}} \frac{C_{\mathrm{HPO4}}}{K_{\mathrm{HPO4}} + C_{\mathrm{HPO4}}} C_{\mathrm{ALG}} - k_{\mathrm{death,ALG}} C_{\mathrm{ALG}}$$

death of algae

Process Table Notation

chapter 4.1

Process	Substances					Rate
	s_1	s_2	s_3	$\cdots$	$\mathsf{s}_{n_\mathrm{s}}$	
p_1	ν_{11}	ν_{12}	ν_{13}	$\cdots$	ν_{1n_s}	ρ_1
p_2	ν_{21}	ν_{22}	ν_{23}	$\cdots$	ν_{2n_s}	ρ_2
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$
$\mathsf{p}_{n_\mathrm{p}}$	$\nu_{n_\mathrm{p}1}$	$\nu_{n_\mathrm{p}2}$	$\nu_{n_\mathrm{p}3}$	$\cdots$	$\nu_{n_\mathrm{p}n_\mathrm{s}}$	ρ_{n_p}

Substance transformation rate in homogeneous environment:

$$r_j = \sum_{i=1}^{n_\mathrm{p}} \nu_{ij}\ \rho_i$$

One of the (non-zero) stoichiometric coefficients, ν_{ij}, in each row can be selected to be plus or minus unity. This makes the corresponding process rate, ρ_j, to the (positive or negative) contribution of this process to the total transformation rate of the corresponding substance, s_i.

Process Table Notation

Typical Elements of Process Rates

chapter 4.2

Process rate with maximum/standard specific growth rate and non-dimensional modification factors that account for the influence of temperature, light intensity, nutrients, etc.

$$\rho_{\mathrm{gro,ALG}} = k_{\mathrm{gro,ALG},T_0} \cdot f_{\mathrm{temp}}(T) \cdot f_{\mathrm{rad}}(I) \cdot f_{\mathrm{lim}}(C_{\mathrm{HPO_4^{2-}}}, C_{\mathrm{NH_4^+}}, C_{\mathrm{NO_3^-}}) \cdot C_{\mathrm{ALG}}$$

$$\rho_{\mathrm{miner,anox,POM}} = k_{\mathrm{miner,anox,POM},T_0} \cdot f_{\mathrm{temp}}(T) \cdot f_{\mathrm{inh}}(C_{\mathrm{O_2}}) \cdot f_{\mathrm{lim}}(C_{\mathrm{NO_3^-}}) \cdot C_{\mathrm{POM}}$$

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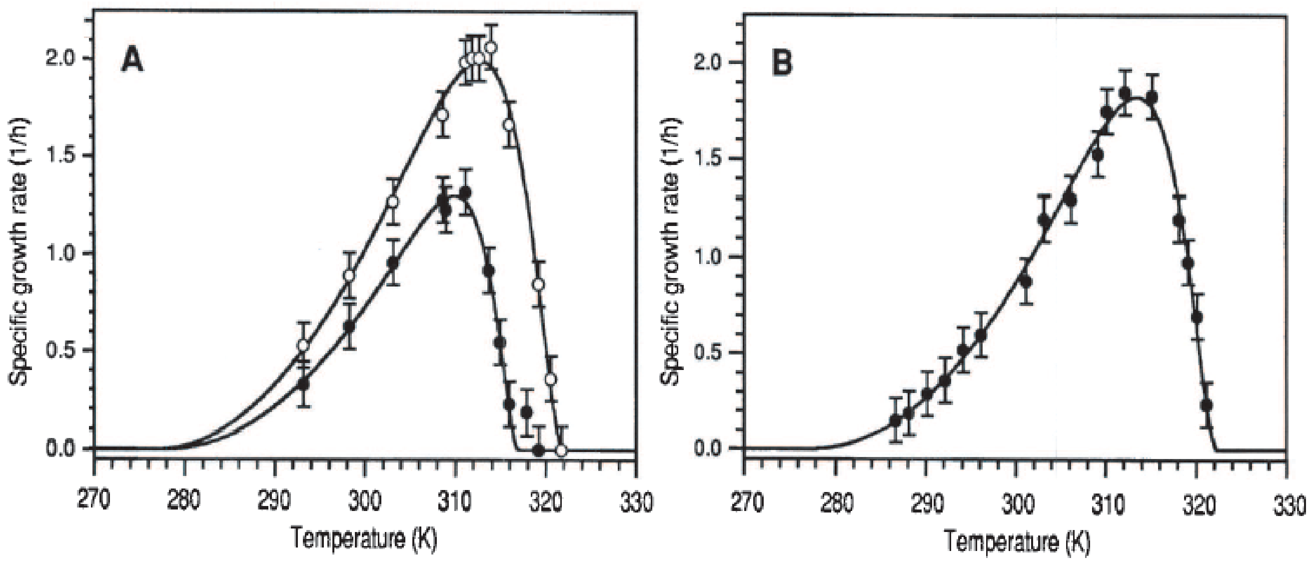
Temperature dependence factor

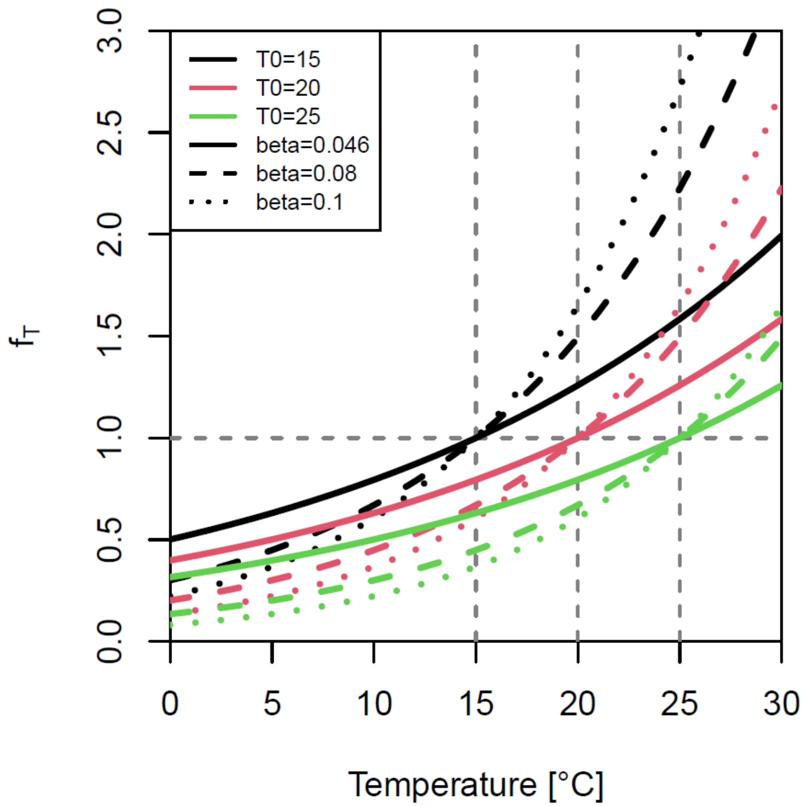


Exponential:

$$f_{\mathrm{temp}}^{\mathrm{exp}}(T) = \exp\Big(\beta(T - T_0)\Big)$$

Typical Elements of Process Rates

Temperature dependence factor



Exponential:

$$f_{\text{temp}}^{\text{exp}}(T) = \exp\Big(\beta(T - T_0)\Big)$$

Typical Elements of Process Rates

Limitation by substance concentrations

Monod:

$$f_{\lim}^{\text{Monod}}(C) = \frac{C}{K + C}$$

Exponential:

$$f_{\lim}^{\exp}(C) = 1 - \exp\left(-\frac{C}{K}\right)$$

Blackman:

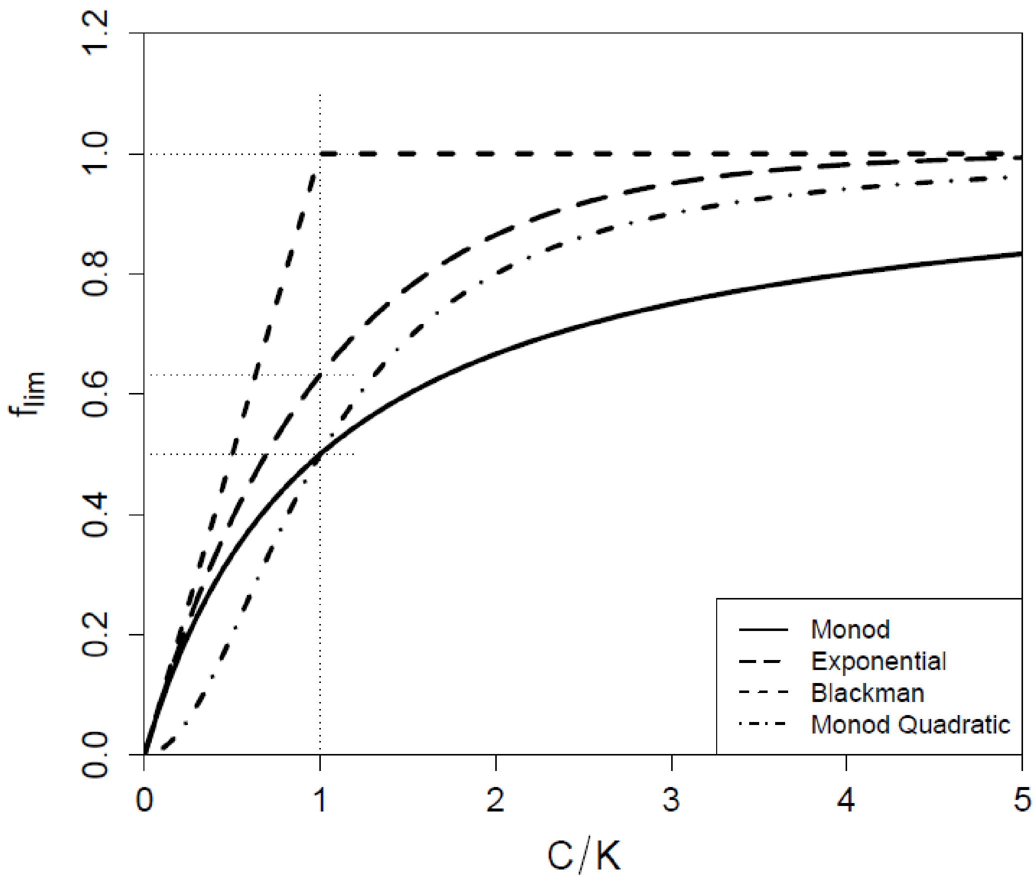
$$f_{\lim}^{\text{Blackman}}(C) = \begin{cases} \dfrac{C}{K} & \text{for } C < K \\ 1 & \text{for } C \geq K \end{cases}$$

Monod Quadratic:

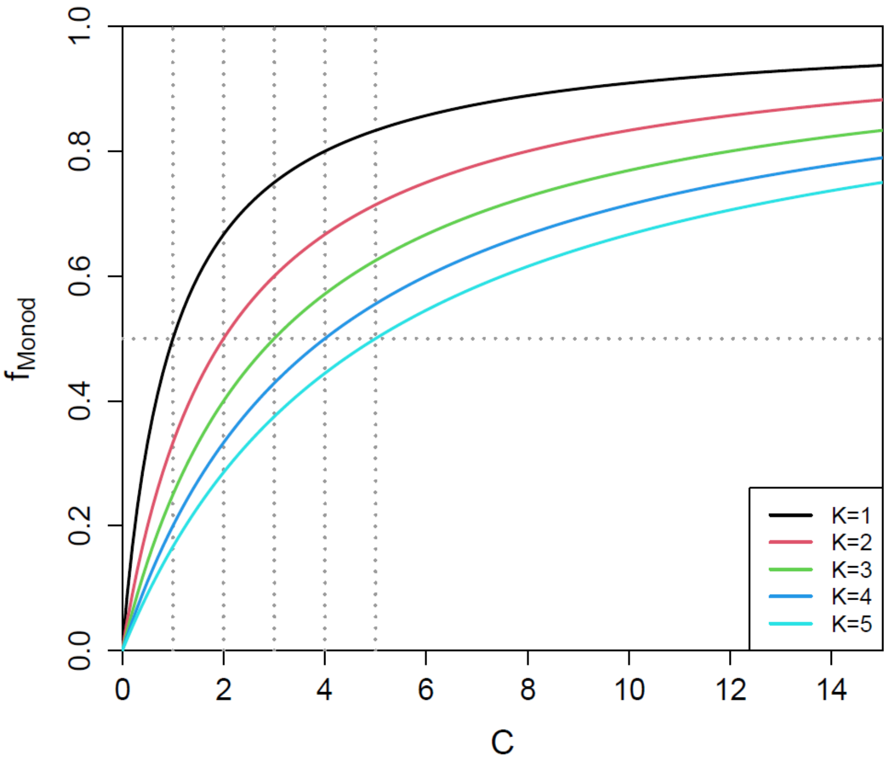
$$f_{\lim}^{\text{Monodquad}}(C) = \frac{C^2}{K^2 + C^2}$$

Typical Elements of Process Rates

Limitation by substance concentrations



Limitation by substance concentrations



$$f_{\text{lim}}^{\text{Monod}}(C) = \frac{C}{K+C}$$

Typical Elements of Process Rates

Limitation by multiple substances

Product:

$$f_N(C_{\mathrm{HPO4}}, C_{\mathrm{NH4}}, C_{\mathrm{NO3}}) = \frac{C_{\mathrm{HPO4}}}{K_{\mathrm{HPO4}} + C_{\mathrm{HPO4}}} \cdot \frac{C_{\mathrm{NH4}} + C_{\mathrm{NO3}}}{K_{\mathrm{N}} + C_{\mathrm{NH4}} + C_{\mathrm{NO3}}}$$

Minimum (Liebig's Law):

$$f_N(C_{\mathrm{HPO4}}, C_{\mathrm{NH4}}, C_{\mathrm{NO3}}) = \min\left(\frac{C_{\mathrm{HPO4}}}{K_{\mathrm{HPO4}} + C_{\mathrm{HPO4}}}, \frac{C_{\mathrm{NH4}} + C_{\mathrm{NO3}}}{K_{\mathrm{N}} + C_{\mathrm{NH4}} + C_{\mathrm{NO3}}}\right)$$

Typical Elements of Process Rates

Inhibition by substance concentrations

Monod:

$$f_{\text{inh}}^{\text{Monod}}(C) = \frac{K}{K + C}$$

Exponential:

$$f_{\text{inh}}^{\text{exp}}(C) = \exp\left(-\frac{C}{K}\right)$$

Blackman:

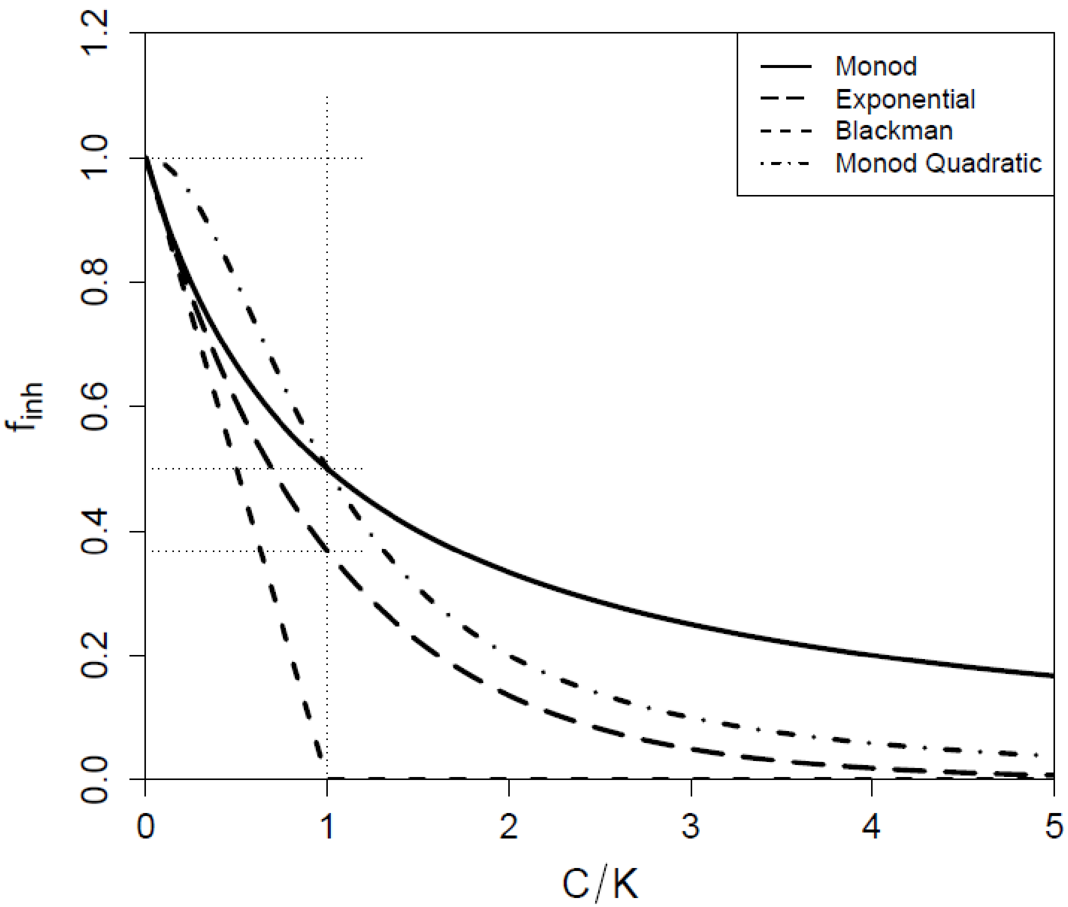
$$f_{\text{inh}}^{\text{Blackman}}(C) = \begin{cases} 1 - \dfrac{C}{K} & \text{for } C < K \\ 0 & \text{for } C \geq K \end{cases}$$

Monod Quadratic:

$$f_{\text{inh}}^{\text{Monodquad}}(C) = \frac{K^2}{K^2 + C^2}$$

Typical Elements of Process Rates

Inhibition by substance concentrations



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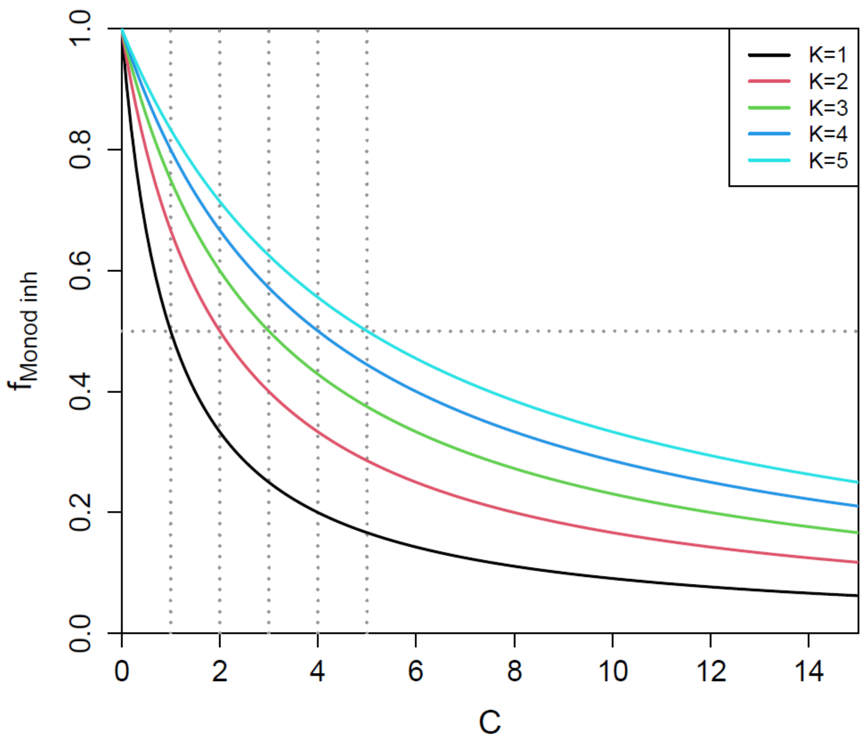
Inhibition by substance concentrations



$$f_{\text{inh}}^{\text{Monod}}(C) = \frac{K}{K+C}$$

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Light dependence factor

Monod:

$$f_{\text{rad}}^{\text{Monod}}(I) = \frac{I}{K_I + I}$$

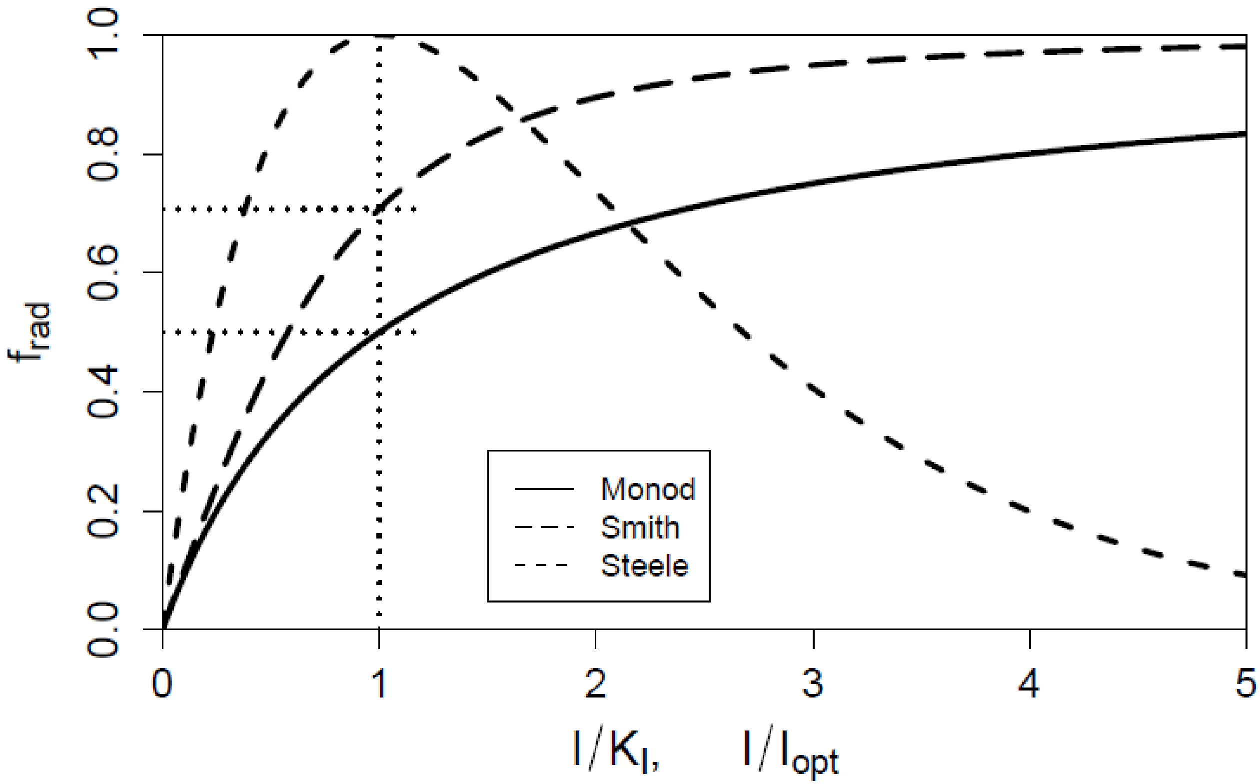
Smith:

$$f_{\text{rad}}^{\text{Smith}}(I) = \frac{I}{\sqrt{K_I^2 + I^2}}$$

Steele:

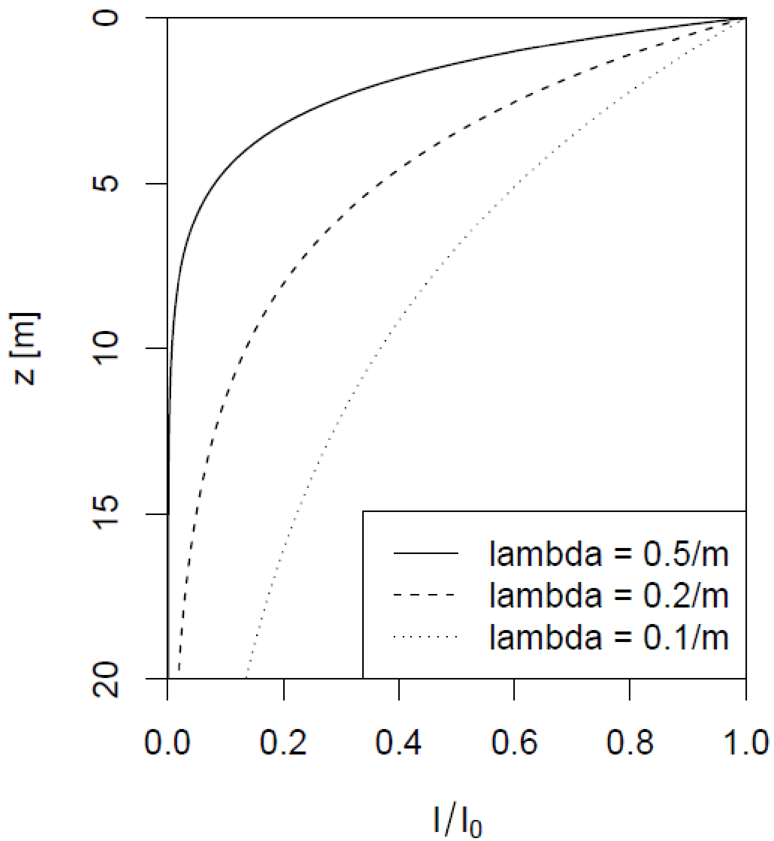
$$f_{\text{rad}}^{\text{Steele}}(I) = \frac{I}{I_{\text{opt}}} \exp\left(1 - \frac{I}{I_{\text{opt}}}\right)$$

Light dependence factors



Light attenuation:

$$I(z) = I_0 \exp(-\lambda z);$$



Light attenuation

For a model with a mixed reactor, the light dependence factor (and not the light itself!) has to be averaged across depth.

Average light dependence factor:

$$\bar{f}_{\mathrm{rad}}(I_0, \lambda, h) = \frac{1}{h} \int_0^h f_{\mathrm{rad}}\Big(I_0 \exp(-\lambda z)\Big) \mathrm{d}z$$

Average light dependence factors

Monod:

$$\bar{f}_{\mathrm{rad}}^{\mathrm{Monod}}(I_0,\lambda,h) = \frac{1}{\lambda h}\log\left(\frac{K_I + I_0}{K_I + I_0\exp(-\lambda h)}\right)$$

Smith:

$$\bar{f}_{\mathrm{rad}}^{\mathrm{Smith}}(I_0,\lambda,h) = \frac{1}{\lambda h}\log\left(\frac{\frac{I_0}{K_I} + \sqrt{1 + \left(\frac{I_0}{K_I}\right)^2}}{\frac{I_0\exp(-\lambda h)}{K_I} + \sqrt{1 + \left(\frac{I_0\exp(-\lambda h)}{K_I}\right)^2}}\right)$$

Steele:

$$\bar{f}_{\mathrm{rad}}^{\mathrm{Steele}}(I_0,\lambda,h) = \frac{\mathrm{e}}{\lambda h}\left[\exp\left(-\frac{I_0\exp(-\lambda h)}{I_{\mathrm{opt}}}\right) - \exp\left(-\frac{I_0}{I_{\mathrm{opt}}}\right)\right]$$

Typical Elements of Process Rates

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Preference Among Different Food Sources

Many organisms can grow on different food sources.

As the stoichiometry and kinetics of growth on one food source may be different from that on another, it is best to represent growth on different food sources by different processes.

The process rates of these processes can still have many terms in common. But they also need a preference factor that depends on the concentrations of all food sources.

Preference Among Different Food Sources

Simplest conceptually satisfying expression:

$$f^{i}_{\mathrm{pref}}(C_1, \ldots, C_n) = \frac{p_i C_i}{\sum\limits_{j=1}^{n} p_j C_j}$$

n: food sources with concentrations $C_1, \ldots, C_n$,
p_j: preference coefficient for food source j.

chapter 11.1

Process Table

Process	Substances / Organisms HPO4 $[gP/m^3]$	ALG $[gDM/m^3]$	Rate
Growth of algae	$-\alpha_{P,ALG}$	1	$\rho_{gro,ALG}$
Death of algae		-1	$\rho_{death,ALG}$

Process Rates

$$\rho_{\mathrm{gro,ALG}} = k_{\mathrm{gro,ALG}} \frac{C_{\mathrm{HPO4}}}{K_{\mathrm{HPO4}} + C_{\mathrm{HPO4}}} C_{\mathrm{ALG}}$$

$$\rho_{\mathrm{death,ALG}} = k_{\mathrm{death,ALG}} \, C_{\mathrm{ALG}}$$

Lake Phytoplankton Model

Transformation Rates

$$r_{\mathrm{HPO4}} = -\alpha_{\mathrm{P,ALG}} \cdot k_{\mathrm{gro,ALG}} \frac{C_{\mathrm{HPO4}}}{K_{\mathrm{HPO4}} + C_{\mathrm{HPO4}}} C_{\mathrm{ALG}}$$

$$r_{\mathrm{ALG}} = k_{\mathrm{gro,ALG}} \frac{C_{\mathrm{HPO4}}}{K_{\mathrm{HPO4}} + C_{\mathrm{HPO4}}} C_{\mathrm{ALG}} - k_{\mathrm{death,ALG}} C_{\mathrm{ALG}}$$

Mass Balance in Well-Mixed Epilimnion

$$\frac{\mathrm{d}\mathbf{C}}{\mathrm{d}t} = \frac{Q_{\mathrm{in}}}{V}\left(\mathbf{C}_{\mathrm{in}} - \mathbf{C}\right) + \frac{\mathbf{J}_{\mathrm{int}}}{V} + \mathbf{r}$$

$$\mathbf{C} = \begin{pmatrix} C_{\mathrm{HPO4}} \\ C_{\mathrm{ALG}} \end{pmatrix} \quad \mathbf{C}_{\mathrm{in}} = \begin{pmatrix} C_{\mathrm{HPO4,in}} \\ 0 \end{pmatrix} \quad \mathbf{J}_{\mathrm{int}} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

Lake Phytoplankton Model

Mass Balance in Well-Mixed Epilimnion

$$\frac{\mathrm{d}\mathbf{C}}{\mathrm{d}t} = \frac{Q_{\mathrm{in}}}{V}\left(\mathbf{C}_{\mathrm{in}} - \mathbf{C}\right) + \frac{\mathbf{J}_{\mathrm{int}}}{V} + \mathbf{r}$$

Differential Equations

$$\frac{\mathrm{d}C_{\mathrm{HPO4}}}{\mathrm{d}t} = \frac{Q_{\mathrm{in}}}{V}\left(C_{\mathrm{HPO4,in}} - C_{\mathrm{HPO4}}\right) + r_{\mathrm{HPO4}}$$

$$\frac{\mathrm{d}C_{\mathrm{ALG}}}{\mathrm{d}t} = -\frac{Q_{\mathrm{in}}}{V}C_{\mathrm{ALG}} + r_{\mathrm{ALG}}$$

Differential Equations

$$\frac{\mathrm{d}C_{\mathrm{HPO4}}}{\mathrm{d}t} = \frac{Q_{\mathrm{in}}}{V}\left(C_{\mathrm{HPO4,in}} - C_{\mathrm{HPO4}}\right) - \alpha_{\mathrm{P,ALG}} \cdot k_{\mathrm{gro,ALG}} \frac{C_{\mathrm{HPO4}}}{K_{\mathrm{HPO4}} + C_{\mathrm{HPO4}}} C_{\mathrm{ALG}}$$

$$\frac{\mathrm{d}C_{\mathrm{ALG}}}{\mathrm{d}t} = -\frac{Q_{\mathrm{in}}}{V} C_{\mathrm{ALG}} + k_{\mathrm{gro,ALG}} \frac{C_{\mathrm{HPO4}}}{K_{\mathrm{HPO4}} + C_{\mathrm{HPO4}}} C_{\mathrm{ALG}} - k_{\mathrm{death,ALG}} C_{\mathrm{ALG}}$$

Example 11.1

Differential Equations

$$\underbrace{\frac{\mathrm{d}C_{\mathrm{HPO4}}}{\mathrm{d}t} = \frac{Q_{\mathrm{in}}}{V}\left(C_{\mathrm{HPO4,in}} - C_{\mathrm{HPO4}}\right)}_{}$$

net input via in/outflow: $\frac{Q_{\mathrm{in}}}{V}\left(C_{\mathrm{HPO4,in}} - C_{\mathrm{HPO4}}\right)$

consumption by algae: $- \alpha_{\mathrm{P,ALG}} \cdot k_{\mathrm{gro,ALG}} \frac{C_{\mathrm{HPO4}}}{K_{\mathrm{HPO4}} + C_{\mathrm{HPO4}}} C_{\mathrm{ALG}}$

$$\frac{\mathrm{d}C_{\mathrm{HPO4}}}{\mathrm{d}t} = \frac{Q_{\mathrm{in}}}{V}\left(C_{\mathrm{HPO4,in}} - C_{\mathrm{HPO4}}\right) - \alpha_{\mathrm{P,ALG}} \cdot k_{\mathrm{gro,ALG}} \frac{C_{\mathrm{HPO4}}}{K_{\mathrm{HPO4}} + C_{\mathrm{HPO4}}} C_{\mathrm{ALG}}$$

loss via outflow: $- \frac{Q_{\mathrm{in}}}{V} C_{\mathrm{ALG}}$

growth of algae: $k_{\mathrm{gro,ALG}} \frac{C_{\mathrm{HPO4}}}{K_{\mathrm{HPO4}} + C_{\mathrm{HPO4}}} C_{\mathrm{ALG}}$

$$\frac{\mathrm{d}C_{\mathrm{ALG}}}{\mathrm{d}t} = - \frac{Q_{\mathrm{in}}}{V} C_{\mathrm{ALG}} + k_{\mathrm{gro,ALG}} \frac{C_{\mathrm{HPO4}}}{K_{\mathrm{HPO4}} + C_{\mathrm{HPO4}}} C_{\mathrm{ALG}} - k_{\mathrm{death,ALG}} C_{\mathrm{ALG}}$$

death of algae: $- k_{\mathrm{death,ALG}} C_{\mathrm{ALG}}$

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Extended Process Rates

Additional influence factors of algae growth rate to account for yearly cycles in temperature and light.

$$\rho_{\text{gro,ALG}} = k_{\text{gro,ALG}} \cdot \exp\Big(\beta_{\text{ALG}}(T - T_0)\Big) \cdot \frac{1}{\lambda h} \log\left(\frac{K_I + I_0}{K_I + I_0 \exp(-\lambda h)}\right) \cdot \frac{C_{\text{HPO4}}}{K_{\text{HPO4}} + C_{\text{HPO4}}} \cdot C_{\text{ALG}}$$

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Seasonally Varying Environmental Conditions

$$T(t) = \frac{T_{\mathrm{max}} + T_{\mathrm{min}}}{2} + \frac{T_{\mathrm{max}} - T_{\mathrm{min}}}{2} \cos\left(2\pi \frac{t - t_{\mathrm{max}}}{t_{\mathrm{per}}}\right)$$

$$I_0(t) = \frac{I_{0,\mathrm{max}} + I_{0,\mathrm{min}}}{2} + \frac{I_{0,\mathrm{max}} - I_{0,\mathrm{min}}}{2} \cos\left(2\pi \frac{t - t_{\mathrm{max}}}{t_{\mathrm{per}}}\right)$$

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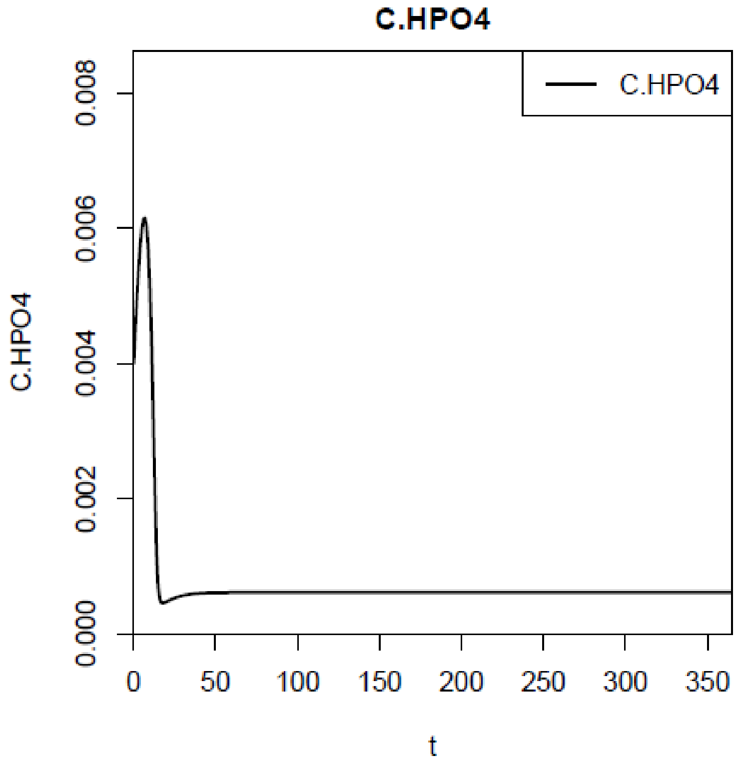
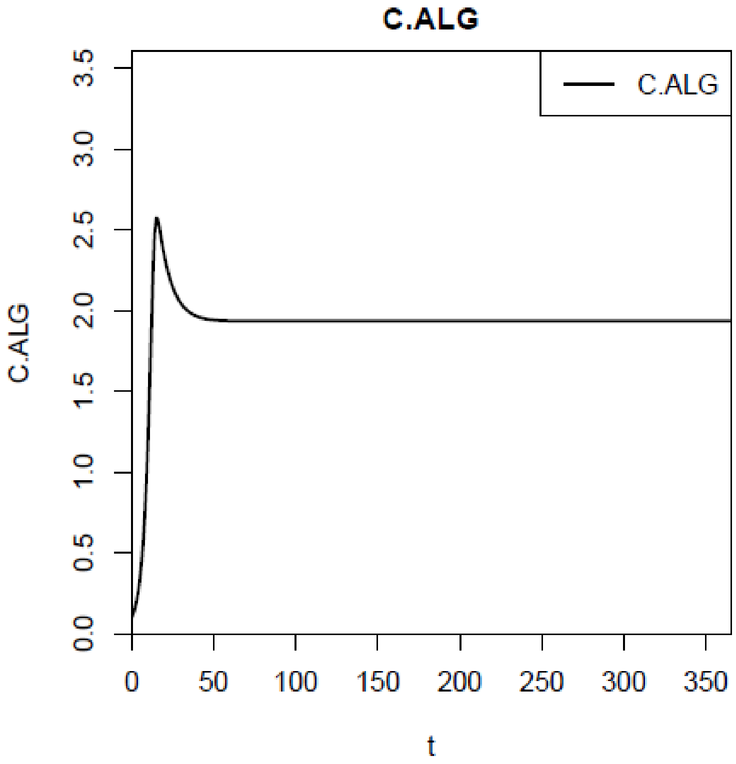
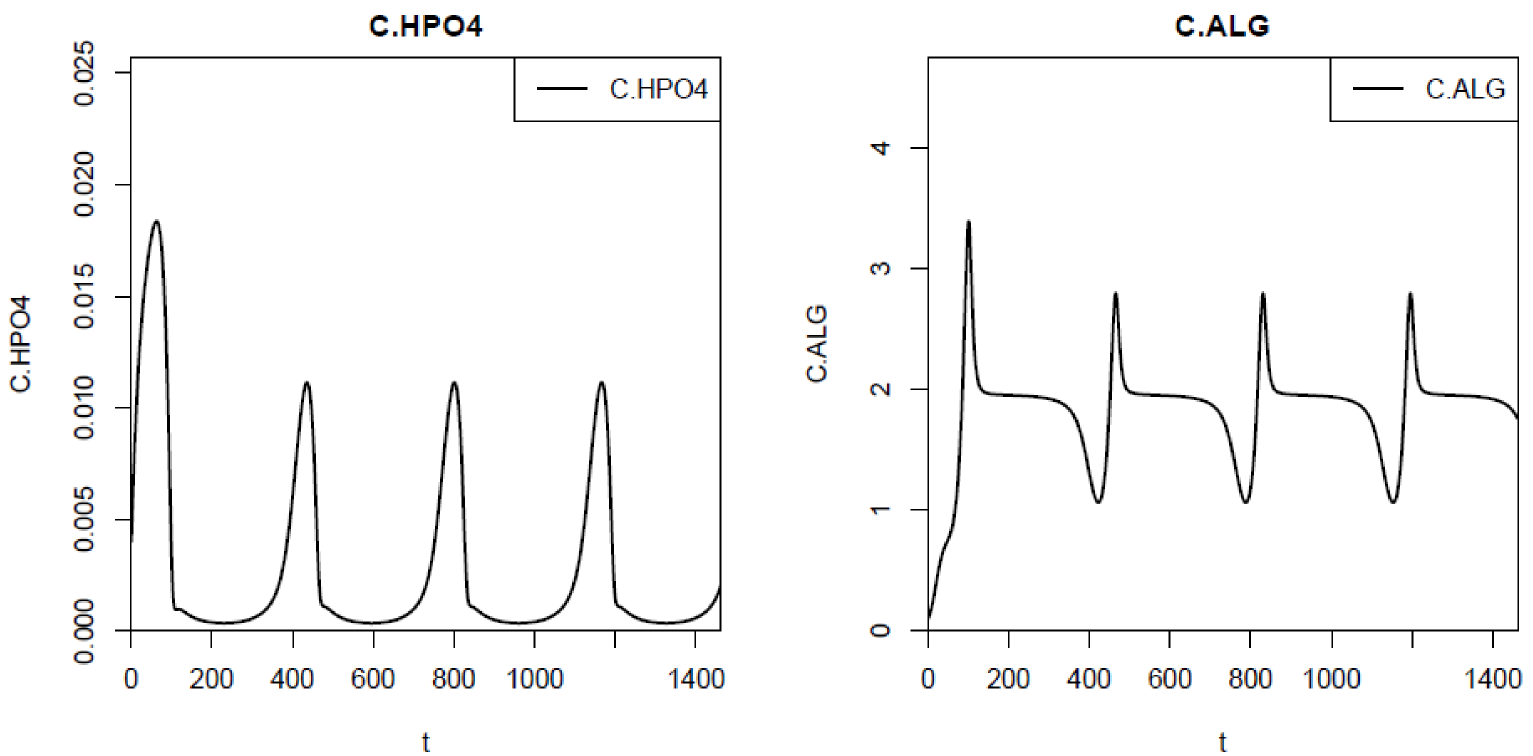
Results for constant environmental conditions





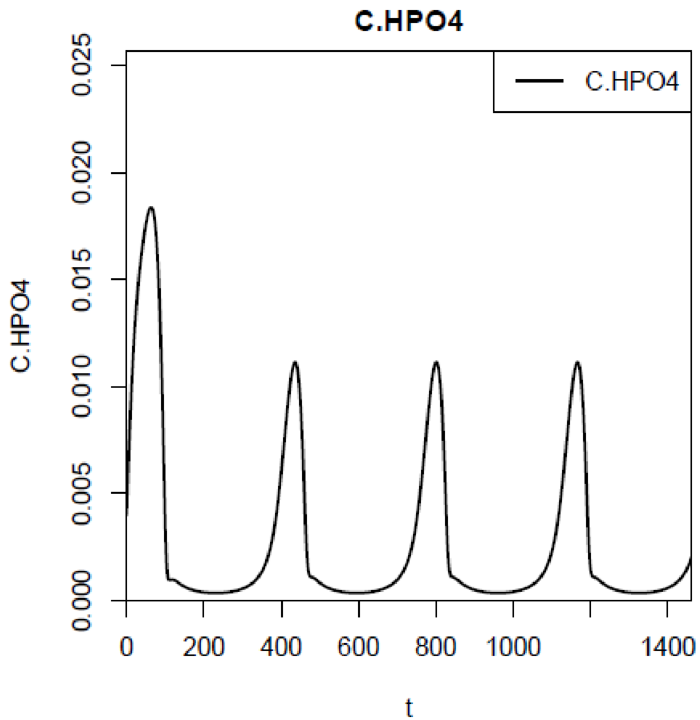
Lake Phytoplankton Model

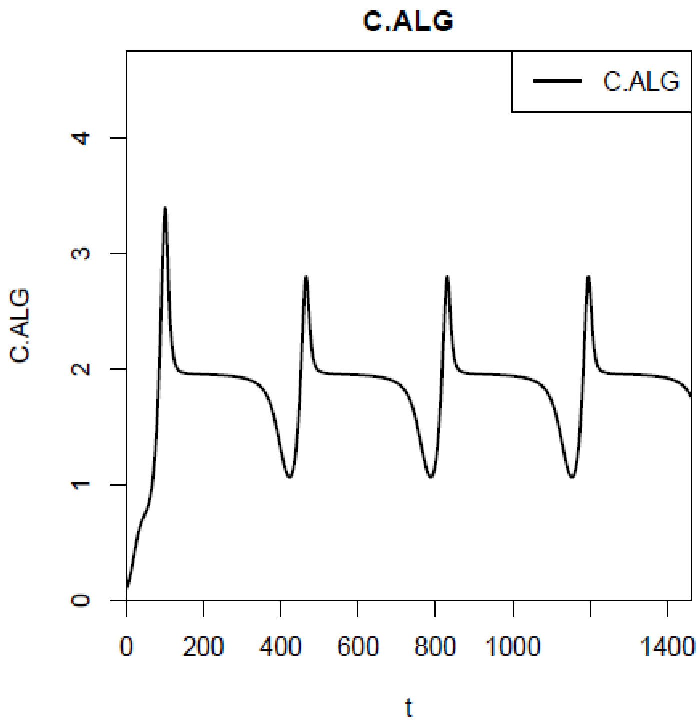
Results for periodic environmental conditions



Lecture 1: Goals

- Acquire basic knowledge of the formulation of transport and transformation processes to formulate a simple lake plankton model.
- Become familiar with the process table notation and rate formulation that will be the basis of the more complex models.





Outlook next week

1. Introduction, principles of modelling environmental systems, mass balance in a mixed reactor, process table notation, simple lake plankton model
   Exercise: R, `ecosim`-package, simple lake plankton model
   Exercise: lake phytoplankton-zooplankton model
2. Process stoichiometry Exercises: analytical solution, calculation with `stoichcalc`
3. Biological processes in lakes
4. Physical processes in lakes, mass balance in multi-box and continuous systems Exercise: structured, biogeochemical-ecological lake model
   Assignments: build your own model by implementing model extensions
5. Physical processes in in rivers, bacterial growth, river model for benthic populations Exercise: river model for benthic populations, nutrients and oxygen
6. Uncertainty, Parameter estimation, Stochasticity
   Exercise: parameter estimation
   Exercise: stochasticity, uncertainty
7. Existing models and applications in research and practice, examples and case studies, preparation of the oral exam, feedback

Preparation for next week

1. Install a current version of R and R-Studio and the `ecosim`-package on your notebook → see Program

2. If you are not very familiar with R, do the tutorial: https://cran.r-project.org/doc/contrib/Torfs+Brauer-Short-R-Intro.pdf

3. Read chapter 11.1 about the first didactical model

4. Read chapters 16.1 and 16.2 about the `ecosim`-package.

5. Think about your open questions to ask them next week!