Modelling Aquatic Ecosystems
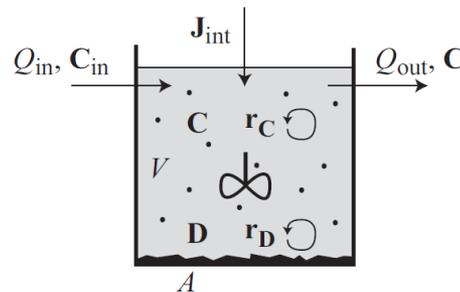# Course 701-0426-00

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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. Stochasticity, uncertainty, Parameter estimation
   Exercise: uncertainty, stochasticity

7. Existing models and applications in research and practice, examples and case studies, preparation of the oral exam, feedback

Goals of today

- Answer your questions about stoichiometry (or anything else)?

- Biological processes in lakes

- Practice for the oral exam

A real lake

A simplified box model

Process table for the model

Review Stoichiometry

Process	HPO$_4^{2-}$ gP	NH$_4^+$ gN	NO$_3^-$ gN	O$_2$ gO	ALG gDM	ZOO gDM	POMD gDM	POMI gDM	SPOMD gDM	SPOMI gDM	Rate
Growth of algae NO$_3^-$	−		−	+	1						$\rho_{\mathrm{gro,ALG,NO_3^-}}$
Growth of algae NH$_4^+$	−	−		+	1						$\rho_{\mathrm{gro,ALG,NH_4^+}}$
Respiration of algae	+	+		−	−1						$\rho_{\mathrm{resp,ALG}}$
Death of algae	0/+	0/+		0/+	−1		$(1-f_{\mathrm{I}})Y_{\mathrm{ALG,death}}$	$f_{\mathrm{I}}Y_{\mathrm{ALG,death}}$			$\rho_{\mathrm{death,ALG}}$
Growth of zooplankton	+	+		−	$\dfrac{-1}{Y_{\mathrm{ZOO}}}$	1	$\dfrac{(1-f_{\mathrm{I}})f_{\mathrm{e}}}{Y_{\mathrm{ZOO}}}$	$\dfrac{f_{\mathrm{I}}f_{\mathrm{e}}}{Y_{\mathrm{ZOO}}}$			$\rho_{\mathrm{gro,ZOO}}$
Respiration of zoopl.	+	+		−		−1					$\rho_{\mathrm{resp,ZOO}}$
Death of zooplankton	0/+	0/+		0/+		−1	$(1-f_{\mathrm{I}})Y_{\mathrm{ZOO,death}}$	$f_{\mathrm{I}}Y_{\mathrm{ZOO,death}}$			$\rho_{\mathrm{death,ZOO}}$
Nitrification		−1	+	−							ρ_{nitri}
Oxic mineral. of org. part.	+	+		−			−1				$\rho_{\mathrm{miner,ox,POMD}}$
Ox. min. of org. part. in sed.	+	+		−					−1		$\rho_{\mathrm{miner,ox,SPOMD}}$
Anox. min. of org. part. in sed.	+	+	−						−1		$\rho_{\mathrm{miner,anox,SPOMD}}$
Sed. of deg. org. part.							−1		1		$\rho_{\mathrm{sed,POMD}}$
Sed. of inert org. part.								−1		1	$\rho_{\mathrm{sed,POMI}}$

Substances / Organisms

Table 11.9: Process table of the model for biogeochemical cycles in a lake.

stoichiometric matrix ν:
relative amounts of ingredients and products

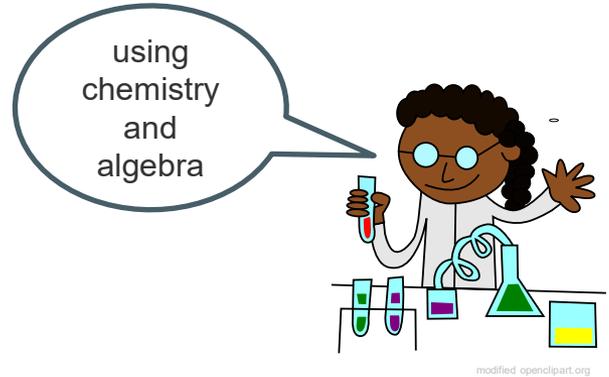process rates:
how fast are
the processes

Stoichiometry of a chocolate cake

process	Chocolate [g]	Egg [no.]	Butter [g]	Sugar [g]	Cake [no.]	rate [min^{-1}]
baking "the best" chocolate cake (SRF)	-300	-5	-100	-100	+1	1/25 (at 180 °C) + preparation and cleaning

https://tinyurl.com/Schoggikuchen

Review Stoichiometry

How to derive stoichiometric coefficients ν_{ij} ?

> using chemistry and algebra

- Chemical substance notation $\rightarrow$ solving algebraic equations

- Parameterized elemental mass fractions $\rightarrow$ solving more complicated algebraic equations

- General solution $\rightarrow$ implementation in R using package `stoichcalc`

At the model level:

1) Choose the substances/organisms to be considered in the model.

2) Choose the "elementary constituents" to be considered in the model.

3) Add substances needed for elemental mass balances (e.g. H_2O, ...) .

4) Construct the composition matrix (with fixed values or parameters)

At the process level (for each process):

1) Choose the substances involved in the process,
   and which one to normalize to +1 or -1

2) Identify the sign of each stoichiometric coefficient based on knowledge

3) Figure out, if you need additional constraints and specify them.

4) Calculate the stoichiometric coefficients

   a) manually solving mass balance equations with fixed values

   b) manually solving mass balance equations with parameters

   c) using the `stoichcalc` package based on the SVD theorem

Open questions?

Open questions?

Questions

1. How do you find out, whether you need additional constraints to elemental mass balance and charge? What could be a drawback of the simplified approach to this question?

2. Where to get the required additional constraints from (if needed)?

3. Why do we add H^+, but not OH^- to the compounds considered for the calculation of stoichiometric coefficients?

Process	HPO$_4^{2-}$ gP	NH$_4^+$ gN	NO$_3^-$ gN	O$_2$ gO	ALG gDM	ZOO gDM	POMD gDM	POMI gDM	SPOMD gDM	SPOMI gDM	Rate
Growth of algae NO$_3^-$	$-$		$-$	$+$	1						$\rho_{\mathrm{gro,ALG,NO_3^-}}$
Growth of algae NH$_4^+$	$-$	$-$		$+$	1						$\rho_{\mathrm{gro,ALG,NH_4^+}}$
Respiration of algae	$+$	$+$		$-$	-1						$\rho_{\mathrm{resp,ALG}}$
Death of algae	0/+	0/+		0/+	-1		$(1-f_{\mathrm{I}})Y_{\mathrm{ALG,death}}$	$f_{\mathrm{I}}Y_{\mathrm{ALG,death}}$			$\rho_{\mathrm{death,ALG}}$
Growth of zooplankton	$+$	$+$		$-$	$\dfrac{-1}{Y_{\mathrm{ZOO}}}$	1	$\dfrac{(1-f_{\mathrm{I}})f_{\mathrm{e}}}{Y_{\mathrm{ZOO}}}$	$\dfrac{f_{\mathrm{I}}f_{\mathrm{e}}}{Y_{\mathrm{ZOO}}}$			$\rho_{\mathrm{gro,ZOO}}$
Respiration of zoopl.	$+$	$+$		$-$		-1					$\rho_{\mathrm{resp,ZOO}}$
Death of zooplankton	0/+	0/+		0/+		-1	$(1-f_{\mathrm{I}})Y_{\mathrm{ZOO,death}}$	$f_{\mathrm{I}}Y_{\mathrm{ZOO,death}}$			$\rho_{\mathrm{death,ZOO}}$
Nitrification		-1	$+$	$-$							ρ_{nitri}
Oxic mineral. of org. part.	$+$	$+$		$-$			-1				$\rho_{\mathrm{miner,ox,POMD}}$
Ox. min. of org. part. in sed.	$+$	$+$		$-$					-1		$\rho_{\mathrm{miner,ox,SPOMD}}$
Anox. min. of org. part. in sed.	$+$	$+$	$-$						-1		$\rho_{\mathrm{miner,anox,SPOMD}}$
Sed. of deg. org. part.							-1		1		$\rho_{\mathrm{sed,POMD}}$
Sed. of inert org. part.								-1		1	$\rho_{\mathrm{sed,POMI}}$

Table 11.9: Process table of the model for biogeochemical cycles in a lake.

process rates:
how fast are
the processes

Transformation Rates

How many cakes can we bake per day?

it depends!

On what does it depend?

on the temperature of the oven!

what else?

on our supply chain for the ingredients!

how fast is each process?

rate
parameter
for standard
conditions
[1/t]

temperature
dependence
[-]

dependence
on other
env. factors
[-]

$$\rho_{\text{gro,ALG,NH}_4^+} = k_{\text{gro,ALG},T_0} \cdot f_{\text{temp}}(T) \cdot f_{\text{rad}}(I)$$

process rate
[M/(L³t)]

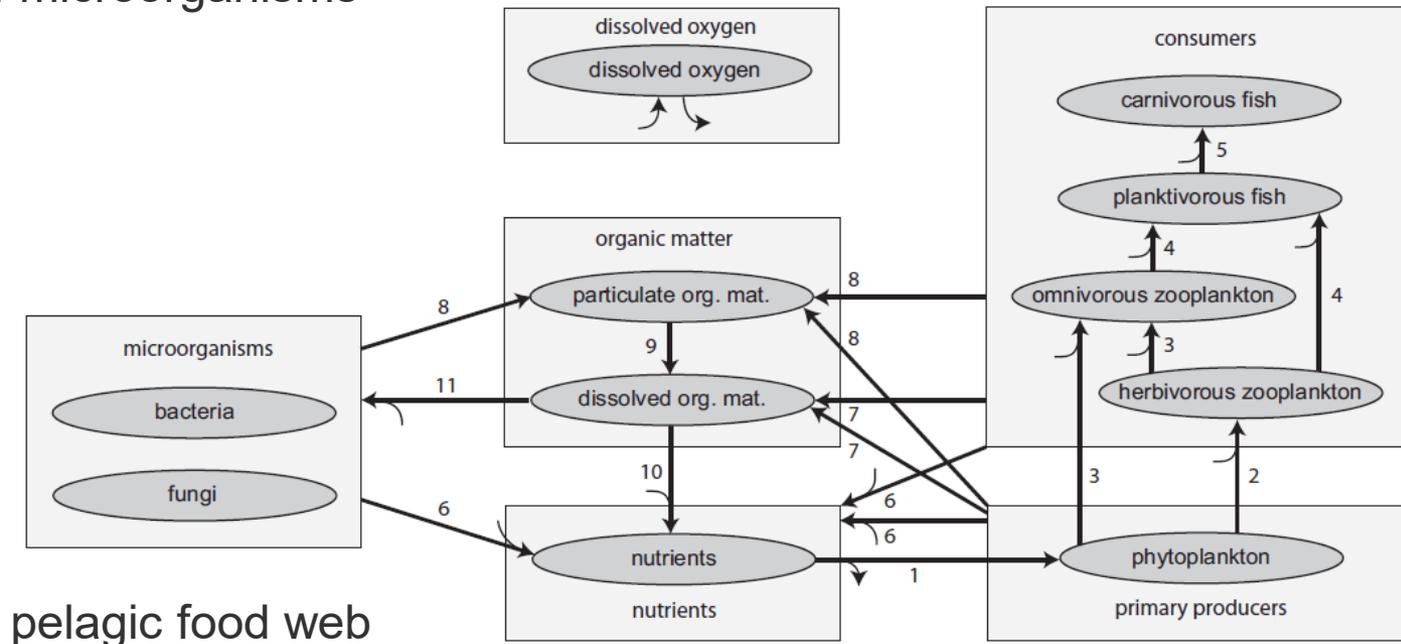$$\cdot f_{\lim}(C_{\text{HPO}_4^{2-}}, C_{\text{NH}_4^+}, C_{\text{NO}_3^-}) \cdot C_{\text{ALG}}$$

limitation terms for all "substances"
that have a negative stoich. coefficient
[-]

dependence on the
concentration of the
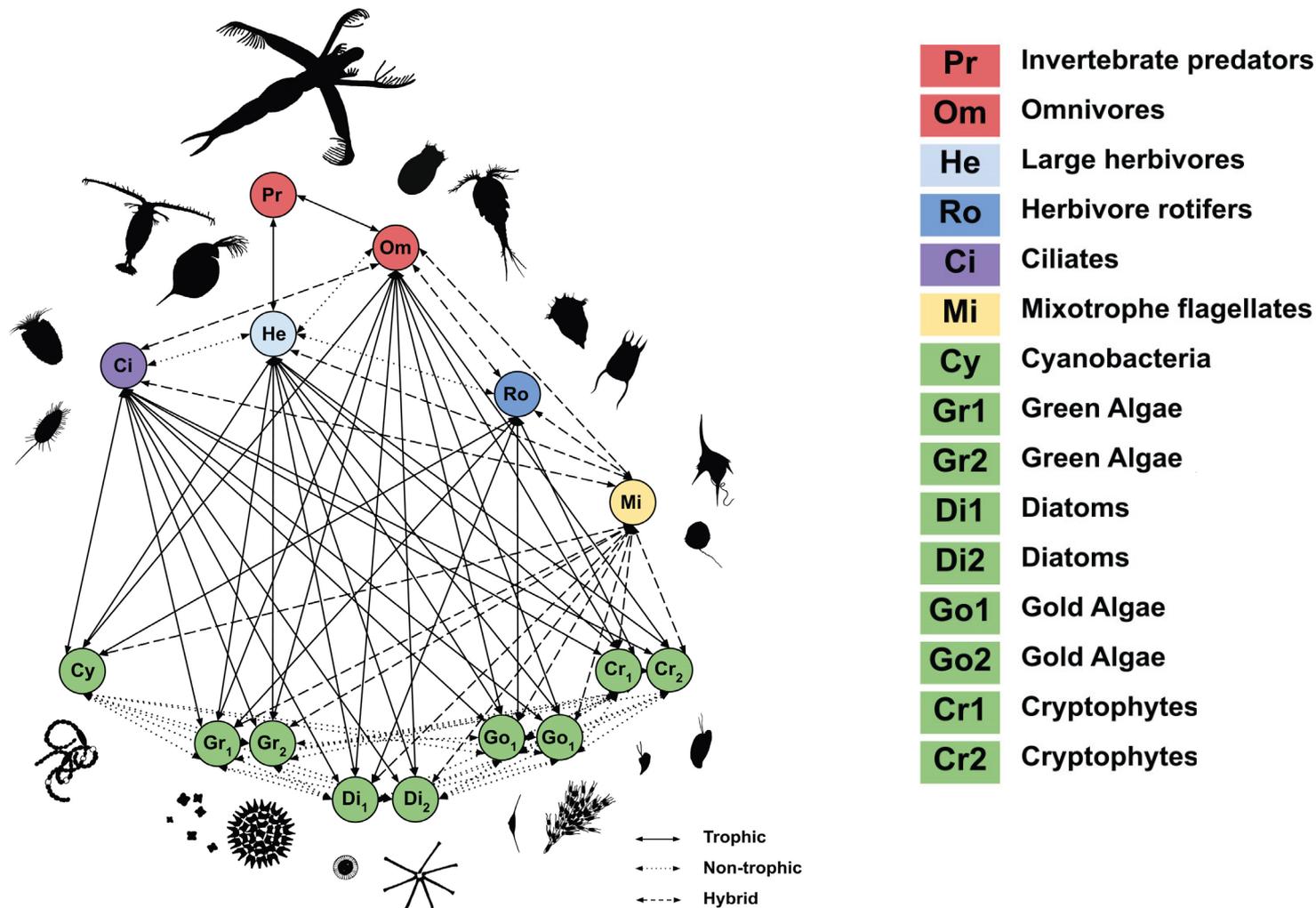substance to which
the stoichiometry
was normalized
[M/L³]

+ maybe inhibition terms

1 primary production (= growth of algae populations)
2,3,4,5 consumption (= growth of consumer populations
incl. somatic growth and reproduction)
6 respiration (= breathing)
7 release of dissolved organic matter by excretion and sloppy feeding
8 death (= conversion of living organism to dead organic particles)
9 hydrolysis (= conversion of particulate to dissolved organic matter)
10 mineralization (conversion of organic matter to nutrients)
11 growth of microorganisms

pelagic food web

eawag
aquatic research

More realistic lake food web

Pr	Invertebrate predators
Om	Omnivores
He	Large herbivores
Ro	Herbivore rotifers
Ci	Ciliates
Mi	Mixotrophe flagellates
Cy	Cyanobacteria
Gr1	Green Algae
Gr2	Green Algae
Di1	Diatoms
Di2	Diatoms
Go1	Gold Algae
Go2	Gold Algae
Cr1	Cryptophytes
Cr2	Cryptophytes

Trophic
Non-trophic
Hybrid

from: Ewa Merz et al., 2023 *Nature Climate Change*. doi.org/10.1038/s41558-023-01615-6

It's your turn:

Idea: safer space to practice for the oral exam

1. What happens in the process from a biological point of view?

   Which substances/organisms are involved?

2. How can we derive the stoichiometric coefficients for this process?

   Explain the qualitative stoichiometry

   (process table, which substances are involved?).

   Do we need additional constraints?

3. Explain how to formulate the process rate.

4. Anything special?

Primary production

What happens?   chapter 8.1

Primary production is the production of organic material from inorganic nutrients through photosynthesis.

This process provides the food for the subsequent trophic levels of the ecosystem food web.

Algae can use nitrate or ammonia as a nitrogen source.
We implement them as separated processes.

The process rates have most terms in common and include a preference factor that depends on the concentration of all food sources.

Preference Among Different Food Sources

Simplest conceptually satisfying expression:

$$f_{\mathrm{pref}}^{i}(C_1, ..., C_n) = \frac{p_i C_i}{\sum_{j=1}^{n} p_j C_j}$$

n: food sources with concentrations $C_1, ..., C_n$,

p_j: preference coefficient for food source j.

Note that the preference terms of all food sources sum up to 1,
so organisms don't grow faster if we resolve there food sources better.

Primary production

Stoichiometry:

Process	Substances / Organisms								Rate
	NH_4^+ gN	NO_3^- gN	HPO_4^{2-} gP	HCO_3^- gC	O_2 gO	H^+ mol	H_2O mol	ALG gDM	
Pri. prod. NH_4^+	−		−	−	+	?	?	1	$\rho_{gro,ALG,NH4}$
Pri. prod. NO_3^-		−	−	−	+	?	?	1	$\rho_{gro,ALG,NO3}$

Six unknown stoichiometric coefficients.

Conservation of C, H, O, N, P and charge: six mass balance equations.

No additional constraints needed.

Process rate:

limitation term
for the sum of both
nitrogen sources

$$\rho_{\mathrm{gro,ALG,NH_4^+}} = k_{\mathrm{gro,ALG},T_0} \cdot \exp\Big(\beta_{\mathrm{ALG}}(T - T_0)\Big) \cdot \frac{I}{K_I + I}$$

$$\cdot \min\left(\frac{C_{\mathrm{HPO_4^{2-}}}}{K_{\mathrm{HPO_4^{2-},ALG}} + C_{\mathrm{HPO_4^{2-}}}}, \frac{C_{\mathrm{NH_4^+}} + C_{\mathrm{NO_3^-}}}{K_{\mathrm{N,ALG}} + C_{\mathrm{NH_4^+}} + C_{\mathrm{NO_3^-}}}\right)$$

$$\cdot \frac{p_{\mathrm{NH_4^+}} C_{\mathrm{NH_4^+}}}{p_{\mathrm{NH_4^+}} C_{\mathrm{NH_4^+}} + C_{\mathrm{NO_3^-}}} \cdot C_{\mathrm{ALG}}$$

with $p_{\mathrm{NO_3^-}} = 1$

$$\rho_{\mathrm{gro,ALG,NO_3^-}} = k_{\mathrm{gro,ALG},T_0} \cdot \exp\Big(\beta_{\mathrm{ALG}}(T - T_0)\Big) \cdot \frac{I}{K_I + I}$$

$$\cdot \min\left(\frac{C_{\mathrm{HPO_4^{2-}}}}{K_{\mathrm{HPO_4^{2-},ALG}} + C_{\mathrm{HPO_4^{2-}}}}, \frac{C_{\mathrm{NH_4^+}} + C_{\mathrm{NO_3^-}}}{K_{\mathrm{N,ALG}} + C_{\mathrm{NH_4^+}} + C_{\mathrm{NO_3^-}}}\right)$$

$$\cdot \frac{C_{\mathrm{NO_3^-}}}{p_{\mathrm{NH_4^+}} C_{\mathrm{NH_4^+}} + C_{\mathrm{NO_3^-}}} \cdot C_{\mathrm{ALG}}$$

Process rate:

$$\rho_{\text{gro,ALG,NH}_4^+} = k_{\text{gro,ALG},T_0} \cdot \exp\Big(\beta_{\text{ALG}}(T - T_0)\Big) \cdot \frac{I}{K_I + I}$$

$$\cdot \min\left(\frac{C_{\text{HPO}_4^{2-}}}{K_{\text{HPO}_4^{2-},\text{ALG}} + C_{\text{HPO}_4^{2-}}}, \frac{C_{\text{NH}_4^+} + C_{\text{NO}_3^-}}{K_{\text{N,ALG}} + C_{\text{NH}_4^+} + C_{\text{NO}_3^-}}\right)$$

$$\cdot \frac{p_{\text{NH}_4^+} C_{\text{NH}_4^+}}{p_{\text{NH}_4^+} C_{\text{NH}_4^+} + C_{\text{NO}_3^-}} \cdot C_{\text{ALG}}$$

$$\rho_{\text{gro,ALG,NO}_3^-} = k_{\text{gro,ALG},T_0} \cdot \exp\Big(\beta_{\text{ALG}}(T - T_0)\Big) \cdot \frac{I}{K_I + I}$$

$$\cdot \min\left(\frac{C_{\text{HPO}_4^{2-}}}{K_{\text{HPO}_4^{2-},\text{ALG}} + C_{\text{HPO}_4^{2-}}}, \frac{C_{\text{NH}_4^+} + C_{\text{NO}_3^-}}{K_{\text{N,ALG}} + C_{\text{NH}_4^+} + C_{\text{NO}_3^-}}\right)$$

$$\cdot \frac{C_{\text{NO}_3^-}}{p_{\text{NH}_4^+} C_{\text{NH}_4^+} + C_{\text{NO}_3^-}} \cdot C_{\text{ALG}}$$

preference term with $p_{\text{NO}_3^-} = 1$

Respiration

What happens?   chapter 8.2

Respiration is the inverse process of photosynthesis,

it consumes O_2 and produces CO_2 and energy.

Respiration is an important process for the survival of organisms

as it provides energy for live maintenance processes.

Respiration leads to cycling of nutrients between the organically bound and

inorganic phases.

Stoichiometry:

Process	Substances / Organisms							Rate
	NH_4^+ gN	HPO_4^{2-} gP	HCO_3^- gC	O_2 gO	H^+ mol	H_2O mol	ALG gDM	
Respiration	+	+	+	−	?	?	−1	$\rho_{\mathrm{resp,ALG}}$

Six unknown stoichiometric coefficients.
Conservation of C, H, O, N, P and charge: 6 equations.
No additional constraints needed.

Process rate:

$$\rho_{\mathrm{resp,ALG}} = k_{\mathrm{resp,ALG}} \cdot \exp\Big(\beta_{\mathrm{ALG}}(T - T_0)\Big) \cdot \frac{C_{\mathrm{O2}}}{K_{\mathrm{O2}} + C_{\mathrm{O2}}} \cdot C_{\mathrm{ALG}}$$

What happens?   chapter 8.3

Death transfers living organisms into dead organic particles.

Different organisms can have **different compositions**.
To avoid introducing many types of POM, we have to account for a different composition of the living organisms and the dead organic particles (the dead bodies).
To respect the **mass balance principle**, we introduce a **yield** that leads to a **partial mineralization** during the death process. The yield is chosen so that as much as possible of the living organism is transferred to POM and the rest is mineralized.

Natural organic particles have a wide spectrum of biodegradability.
In models of ecological systems, this is often represented by a (quickly) **degradable** and an **inert** (slowly degradable) fraction of organic matter.

Stoichiometry:

Process	NH$_4^+$ gN	HPO$_4^{2-}$ gP	HCO$_3^-$ gC	O$_2$ gO	H$^+$ mol	H$_2$O mol	ALG gDM	POMD gDM	POMI gDM
Death	0/+	0/+	0/+	0/+	?	?	-1	$(1-f_I)$ $\cdot Y_{\mathrm{ALG,death}}$	f_I $\cdot Y_{\mathrm{ALG,death}}$

Eight unknown stoichiometric coefficients.
Conservation of C, H, O, N, P and charge: 6 equations.
Two additional constraints needed:

$$Y_{\mathrm{death}} = \frac{-(\nu_{\mathrm{death\ POMD}} + \nu_{\mathrm{death\ POMI}})}{\nu_{\mathrm{death\ ALG}}}$$

Y_{death} = how much particles are produced per unit of dying algae

$$\nu_{\mathrm{death\ ALG}} \cdot Y_{\mathrm{death}} + \nu_{\mathrm{death\ POMD}} + \nu_{\mathrm{death\ POMI}} = 0$$

$$f_I = \frac{\nu_{\mathrm{death\ POMI}}}{\nu_{\mathrm{death\ POMI}} + \nu_{\mathrm{death\ POMD}}}$$

f_I = fraction of produced particles that are inert

$$\nu_{\mathrm{death\ POMD}}\ f_I - \nu_{\mathrm{death\ POMI}}(1 - f_I) = 0$$

Death

Process rate:

$$\rho_{\text{death,ALG}} = k_{\text{death,ALG}} \cdot C_{\text{ALG}}$$

Consumption

What happens?

chapter 8.4

Secondary producers consume organic food sources

(living organisms or dead organic matter).

This process produces dead organic matter

due to sloppy feeding and excretion.

Our example here is zooplankton growth on algae.

Stoichiometry:

Process	Substances / Organisms									
	NH_4^+ gN	HPO_4^{2-} gP	HCO_3^- gC	O_2 gO	H^+ mol	H_2O mol	ALG gDM	ZOO gDM	POMD gDM	POMI gDM
Growth ZOO	+	+	+	−	?	?	−	1	+	+

Process formulation with fast **d**egradable and "**i**nert" (=slowly degradable) particle production due to sloppy feeding and excretion and partial mineralization.

Nine unknown stoichiometric coefficients.
Conservation of C, H, O, N, P and charge: 6 equations.
Three additional constraints needed:

$$1ALG \rightarrow Y_{ZOO}ZOO + f_e POM + (1 - Y_{ZOO} - f_e)\ \text{nutrients}$$

$$POM = f_I POMI + (1 - f_I)POMD$$

Consumption

3 constraints:

$$Y_{\text{Zoo}} = \frac{-\nu_{\text{gro,ZOO ZOO}}}{\nu_{\text{gro,ZOO ALG}}}$$

fraction of consumed algae that are converted to consumer biomass

$$\nu_{\text{gro,ZOO ZOO}} + \nu_{\text{gro,ZOO ALG}} Y_{\text{ZOO}} = 0$$

$$f_{\text{e}} = \frac{-(\nu_{\text{gro,ZOO POMD}} + \nu_{\text{gro,ZOO POMI}})}{\nu_{\text{gro,ZOO ALG}}}$$

fraction of consumed algae that are excreted

$$\nu_{\text{gro,ZOO POMD}} + \nu_{\text{gro,ZOO POMI}} + \nu_{\text{gro,ZOO ALG}} f_{\text{e}} = 0$$

$$f_{\text{I}} = \frac{\nu_{\text{gro,ZOO POMI}}}{\nu_{\text{gro,ZOO POMI}} + \nu_{\text{gro,ZOO POMD}}}$$

fraction of produced particles that are inert

$$\nu_{\text{gro,ZOO POMD}} f_{\text{I}} - \nu_{\text{gro,ZOO POMI}} (1 - f_{\text{I}}) = 0$$

Process	Substances / Organisms									
	NH_4^+	HPO_4^{2-}	HCO_3^-	O_2	H^+	H_2O	ALG	ZOO	POMD	POMI
	gN	gP	gC	gO	mol	mol	gDM	gDM	gDM	gDM
Growth ZOO	+	+	+	−	?	?	$\dfrac{-1}{Y_{\text{ZOO}}}$	1	$\dfrac{(1-f_{\text{I}})f_{\text{e}}}{Y_{\text{ZOO}}}$	$\dfrac{f_{\text{I}}f_{\text{e}}}{Y_{\text{ZOO}}}$

Consumption

Process rate:

with Monod-limitation for food:

$$\rho_{\mathrm{gro,ZOO}} = k_{\mathrm{gro,ZOO},T_0} \cdot \exp\Big(\beta_{\mathrm{ZOO}}(T-T_0)\Big) \cdot \frac{C_{\mathrm{O_2}}}{K_{\mathrm{O_2,ZOO}} + C_{\mathrm{O_2}}} \cdot \frac{C_{\mathrm{ALG}}}{K_{\mathrm{ALG,ZOO}} + C_{\mathrm{ALG}}} \cdot C_{\mathrm{ZOO}}$$

[1/d]   [-]

with linear dependence on food:

$$\rho_{\mathrm{gro,ZOO}} = k'_{\mathrm{gro,ZOO},T_0} \cdot \exp\Big(\beta_{\mathrm{ZOO}}(T-T_0)\Big) \cdot \frac{C_{\mathrm{O_2}}}{K_{\mathrm{O_2,ZOO}} + C_{\mathrm{O_2}}} \cdot C_{\mathrm{ALG}} \cdot C_{\mathrm{ZOO}}$$

[m³/gDM/d]   [gDM/ m³]

! affects the unit of the specific growth rate $k_{gro,ZOO,T0}$ / $k'_{gro,ZOO,T0}$

Consumption

Reminder: implementation of constraints in `stoichcalc`

```
# Growth of zooplankton:

nu.gro.ZOO <-
    calc.stoich.coef(alpha         = alpha,
                     name          = "gro.ZOO",
                     subst         = c("C.NH4","C.HPO4","C.HCO3","C.O2","C.H",
                                       "C.H2O","C.ALG","C.ZOO","C.POMD","C.POMI"),
                     subst.norm    = "C.ZOO",
                     nu.norm       = 1,
                     constraints = list(c("C.ZOO"  = 1,
                                          "C.ALG"  = param$Y.ZOO),
                                        c("C.POMD" = 1,
                                          "C.POMI" = 1,
                                          "C.ALG"  = param$f.e),
                                        c("C.POMD" = -param$f.I,
                                          "C.POMI" = 1-param$f.I)))
```

$$v_i \cdot \left(\gamma_{(i)}\right)^{\mathrm{T}} = 0 \qquad v_{\mathrm{gro,ZOO\ ZOO}}\ 1 + v_{\mathrm{gro,ZOO\ ALG}}\ Y_{\mathrm{ZOO}} = 0$$

$$\text{with } v_{\mathrm{gro,ZOO\ ZOO}} = 1: \qquad v_{\mathrm{gro,ZOO\ ALG}} = -\frac{1}{Y_{\mathrm{ZOO}}}$$

Mineralization

What happens?

chapter 8.5

Oxic mineralization transforms organic matter to dissolved nutrients and carbon dioxide under **consumption of oxygen**.

In the absence of dissolved oxygen (primarily in the sediment), mineralization can use **nitrate (=anoxic)**, **manganese** oxide, **iron** hydroxide or **sulfate** for oxidizing organic matter (=**anaerobic**). Finally, **methanogenesis** can convert organic matter to nutrients, carbon dioxide and methane.

As **mineralization is caused by bacteria** and bacterial concentrations vary considerably from one (part of the) system to another, mineralization rate coefficients vary over many orders of magnitude.

35

Oxic Mineralization

Stoichiometry:

Process	\multicolumn{7}{c	}{Substances / Organisms}	Rate
	NH_4^+ gN	HPO_4^{2-} gP	HCO_3^- gC	O_2 gO	H^+ mol	H_2O mol	POM gDM	
Oxic miner.	$+$	$+$	$+$	$-$	?	?	-1	$\rho_{\mathrm{miner,ox,POM}}$

Six unknown stoichiometric coefficients.
Conservation of C, H, O, N, P and charge: 6 equations.
No additional constraints needed.

Process rate:

$$\rho_{\mathrm{miner,ox,POM}} = k_{\mathrm{miner,ox,POM}} \cdot \exp\left(\beta_{\mathrm{BAC}}(T-T_0)\right) \cdot \frac{C_{\mathrm{O2}}}{K_{\mathrm{O2,miner}} + C_{\mathrm{O2}}} \cdot C_{\mathrm{POM}}$$

Stoichiometry:

Process		Substances / Organisms							Rate
	NH_4^+ gN	NO_3^- gN	N_2 gN	HPO_4^{2-} gP	HCO_3^- gC	H^+ mol	H_2O mol	POM gDM	
Anox. min.	$+$	$-$	$+$	$+$	$+$	?	?	-1	$\rho_{\mathrm{miner,anox,POM}}$

Seven unknown stoichiometric coefficients. Conservation of C, H, O, N, P and charge: 6 equations. One additional constraint needed:

$$\nu_{\mathrm{miner,anox\ NO3}} + \nu_{\mathrm{miner,anox\ N2}} = 0$$

Process rate:

$$\rho_{\mathrm{miner,anox,POM}} = k_{\mathrm{miner,anox,POM}} \cdot \exp\left(\beta_{\mathrm{BAC}}(T-T_0)\right) \cdot \frac{K_{\mathrm{O2,miner}}}{K_{\mathrm{O2,miner}} + C_{\mathrm{O2}}}$$

$$\cdot \frac{C_{\mathrm{NO3}}}{K_{\mathrm{NO3,miner}} + C_{\mathrm{NO3}}} \cdot C_{\mathrm{POM}}$$

Anaerobic Mineralization

Stoichiometry:

Process	Substances / Organisms							
	NH_4^+ gN	HPO_4^{2-} gP	HCO_3^- gC	Mn^{2+} mol	H^+ mol	H_2O mol	MnO_2 mol	POM gDM
Mn oxide red.	+	+	+	+	?	?	−	−1

Process	Substances / Organisms							
	NH_4^+ gN	HPO_4^{2-} gP	HCO_3^- gC	Fe^{2+} mol	H^+ mol	H_2O mol	FeOOH mol	POM gDM
Fe hydrox. red.	+	+	+	+	?	?	−	−1

Process	Substances / Organisms							
	NH_4^+ gN	HPO_4^{2-} gP	HCO_3^- gC	SO_4^{2-} mol	HS^- mol	H^+ mol	H_2O mol	POM gDM
Sulfate reduction	+	+	+	−	+	?	?	−1

7 unknowns and 6+1 (Mn/Fe/S) mass balance equations
= no additional constraint needed

38

Anaerobic Mineralization

Stoichiometry:

Process	Substances / Organisms						
	NH_4^+	HPO_4^{2-}	HCO_3^-	CH_4	H^+	H_2O	POM
	gN	gP	gC	gC	mol	mol	gDM
Methanogenesis	+	+	+	+	?	?	−1

6 unknowns and 6 mass balance equations = no additional constraint needed

The process rates need additional limitation and inhibition terms!

Nitrification

What happens?   chapter 8.6

Nitrification leads to a **transformation** of **ammonia** to **nitrite** and **nitrate**.

This is done be chemoautotrophic bacteria that gain energy by this transformation process.

It can be modelled as a 1 or 2 step process.

As an alternative, we can model the growth, respiration, and death of the nitrifying bacteria (see chapter 8.8.2).

One step model:

Process	Substances / Organisms				
	NH_4^+	NO_3^-	O_2	H^+	H_2O
	gN	gN	gO	mol	mol
Nitrification	-1	$+$	$-$	?	?

4 unknowns,
4 equations for N,H,O,e[-]
no constraints needed

$$NH_4^+ + 2\,O_2 \rightarrow NO_3^- + 2\,H^+ + H_2O$$

Rate:

$$\rho_{\mathrm{nitri}} = k_{\mathrm{nitri}} \cdot \exp\left(\beta_{\mathrm{BAC}}(T - T_0)\right) \cdot \min\left(\frac{C_{\mathrm{NH4}}}{K_{\mathrm{NH4,nitri}} + C_{\mathrm{NH4}}}, \frac{C_{\mathrm{O2}}}{K_{\mathrm{O2,nitri}} + C_{\mathrm{O2}}}\right)$$

Two steps model:

Process	Substances / Organisms					
	NH_4^+ gN	NO_2^- gN	NO_3^- gN	O_2 gO	H^+ mol	H_2O mol
Ammonium oxidation	-1	$+$		$-$	?	?
Nitrite oxidation		-1	$+$	$-$	?	?

$$NH_4^+ + \frac{3}{2}\,O_2 \rightarrow NO_2^- + 2\,H^+ + H_2O$$

$$NO_2^- + \frac{1}{2}\,O_2 \rightarrow NO_3^-$$
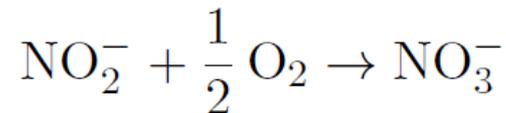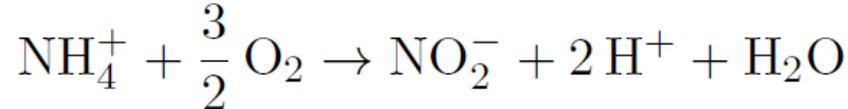
4 unknowns,
4 equations for N,H,O,e⁻
no constraints needed

Rate:

$$\rho_{nitri1} = k_{nitri1,T_0} \cdot \exp\left(\beta_{N1}(T - T_0)\right) \cdot \min\left(\frac{C_{NH_4^+}}{K_{NH_4^+,nitri} + C_{NH_4^+}}, \frac{C_{O_2}}{K_{O_2,nitri} + C_{O_2}}\right)$$

$$\rho_{nitri2} = k_{nitri2,T_0} \cdot \exp\left(\beta_{N2}(T - T_0)\right) \cdot \min\left(\frac{C_{NO_2^-}}{K_{NO_2^-,nitri} + C_{NO_2^-}}, \frac{C_{O_2}}{K_{O_2,nitri} + C_{O_2}}\right)$$

Hydrolysis

What happens?   chapter 8.7

In this process, particulate organic matter is transformed into dissolved organic matter, which can be consumed by heterotrophic bacteria.

It is a chemical process, where a water molecule or hydroxide ion substitutes for another atom or group of atoms in an organic molecule.

Hydrolysis

Stoichiometry:

Process	Substances / Organisms							
	NH_4^+	HPO_4^{2-}	HCO_3^-	O_2	H^+	H_2O	POM	DOM
	gN	gP	gC	gO	mol	mol	gDM	g
Hydrolysis	0/+	0/+	0/+	0/+	?	?	−1	Y_{hyd}

The 0/+ indicates that the stoichiometric coefficient should not be negative.
7 unknowns and 6 equations: 1 additional constraint is needed.

$$\nu_{hyd\,DOM} + \nu_{hyd\,POM} Y_{hyd} = 0$$

Y_{hyd} specifies which fraction of POM is transferred to DOM

→ can be max. 1 if the elemental composition is the same,
   then all other unknowns are 0.

Hydrolysis

Process rate:

$$\rho_{\mathrm{hyd,POM}} = k_{\mathrm{hyd,POM},T_0} \cdot \exp\left(\beta_{\mathrm{hyd}}(T - T_0)\right) \cdot C_{\mathrm{POM}}$$

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. Stochasticity, uncertainty, Parameter estimation
Exercise: uncertainty, stochasticity

7. Existing models and applications in research and practice, examples and case studies, preparation of the oral exam, feedback

- read chapter 3.3 (mass balance in multi-reactor system)

- read chapter 6.1.1 (transport and mixing in lakes)

- read chapters 11.3 and 11.4 (two-box model lake models)

- voluntary bonus: if you are interested in chemical processes read chapter 6

... about components of process rates (repetition chapter 4)

Light dependence factor

Monod:

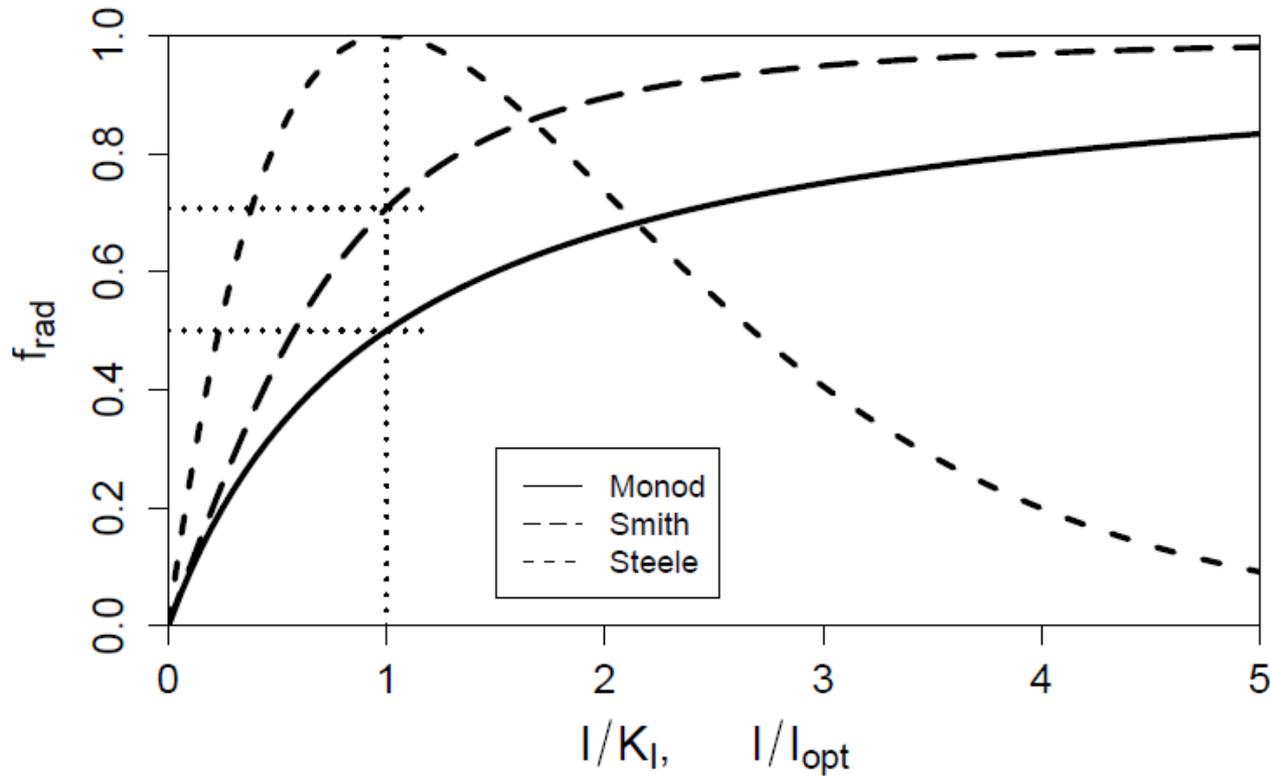$$f_{\text{rad}}^{\text{Monod}}(I) = \frac{I}{K_I + I}$$
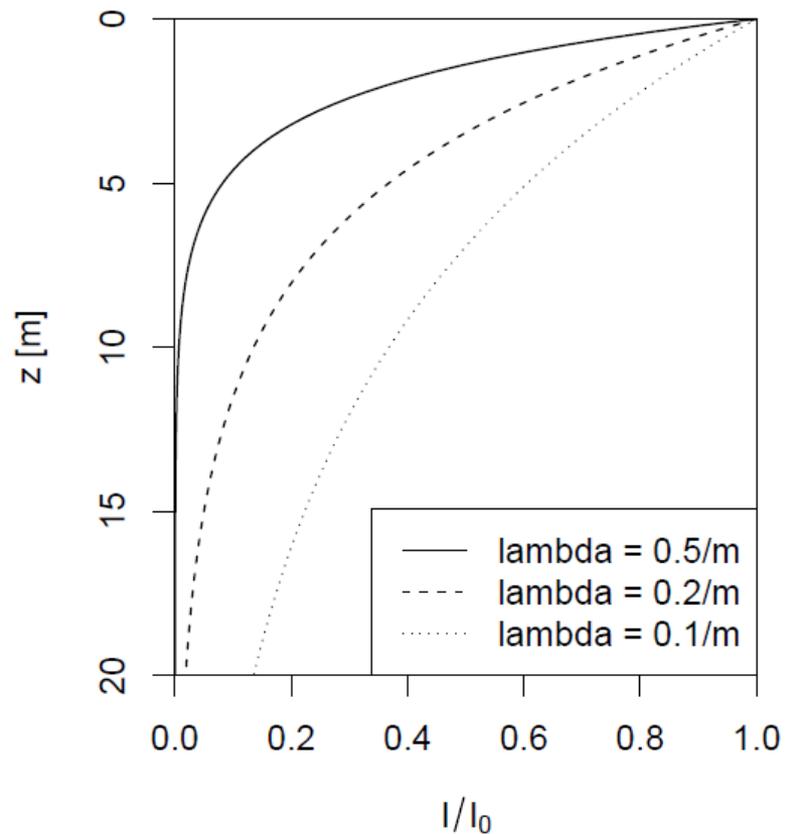
Smith:

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

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:

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

Smith:

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

Steele:

$$\bar{f}_{\text{rad}}^{\text{Steele}}(I_0, \lambda, h) = \frac{e}{\lambda h} \left[\exp \left(-\frac{I_0 \exp(-\lambda h)}{I_{\text{opt}}} \right) - \exp \left(-\frac{I_0}{I_{\text{opt}}} \right) \right]$$
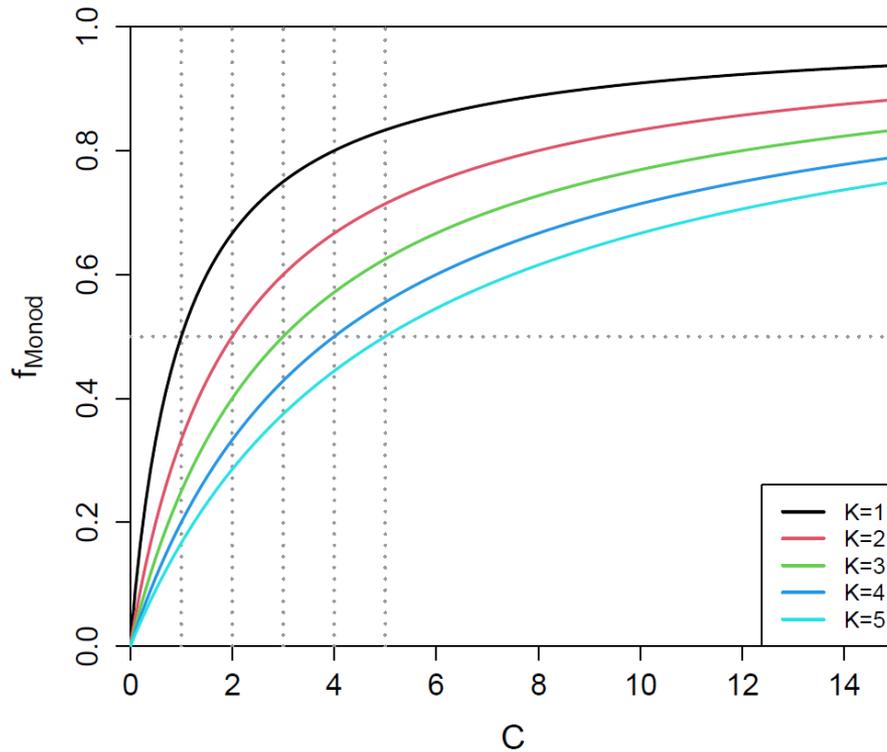
Typical Elements of Process Rates

Temperature dependence factor
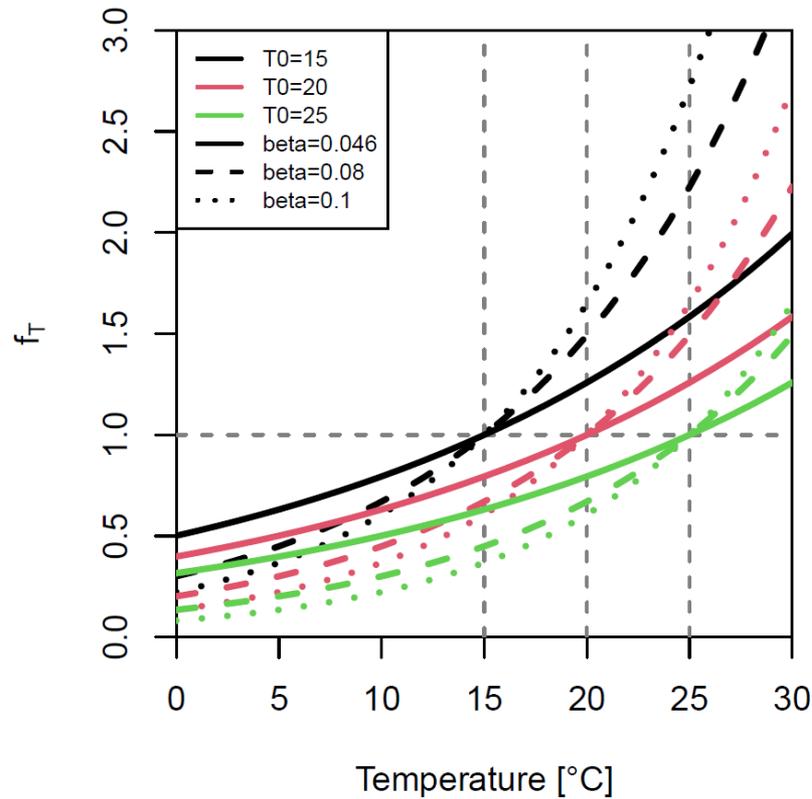
Exponential:

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

54

Limitation by substance concentrations

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

Limitation by multiple substances

Product:

$$f_N(C_{\text{HPO4}}, C_{\text{NH4}}, C_{\text{NO3}})$$

$$= \frac{C_{\text{HPO4}}}{K_{\text{HPO4}} + C_{\text{HPO4}}} \cdot \frac{C_{\text{NH4}} + C_{\text{NO3}}}{K_{\text{N}} + C_{\text{NH4}} + C_{\text{NO3}}}$$

Minimum (Liebig's Law):

$$f_N(C_{\text{HPO4}}, C_{\text{NH4}}, C_{\text{NO3}})$$

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

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:

$$f_{\mathrm{pref}}^{i}(C_1, ..., C_n) = \frac{p_i C_i}{\displaystyle\sum_{j=1}^{n} p_j C_j}$$

n: food sources with concentrations $C_1, ..., C_n$,

p_j: preference coefficient for food source j.

Inhibition by substance concentrations

Monod:

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

Exponential:

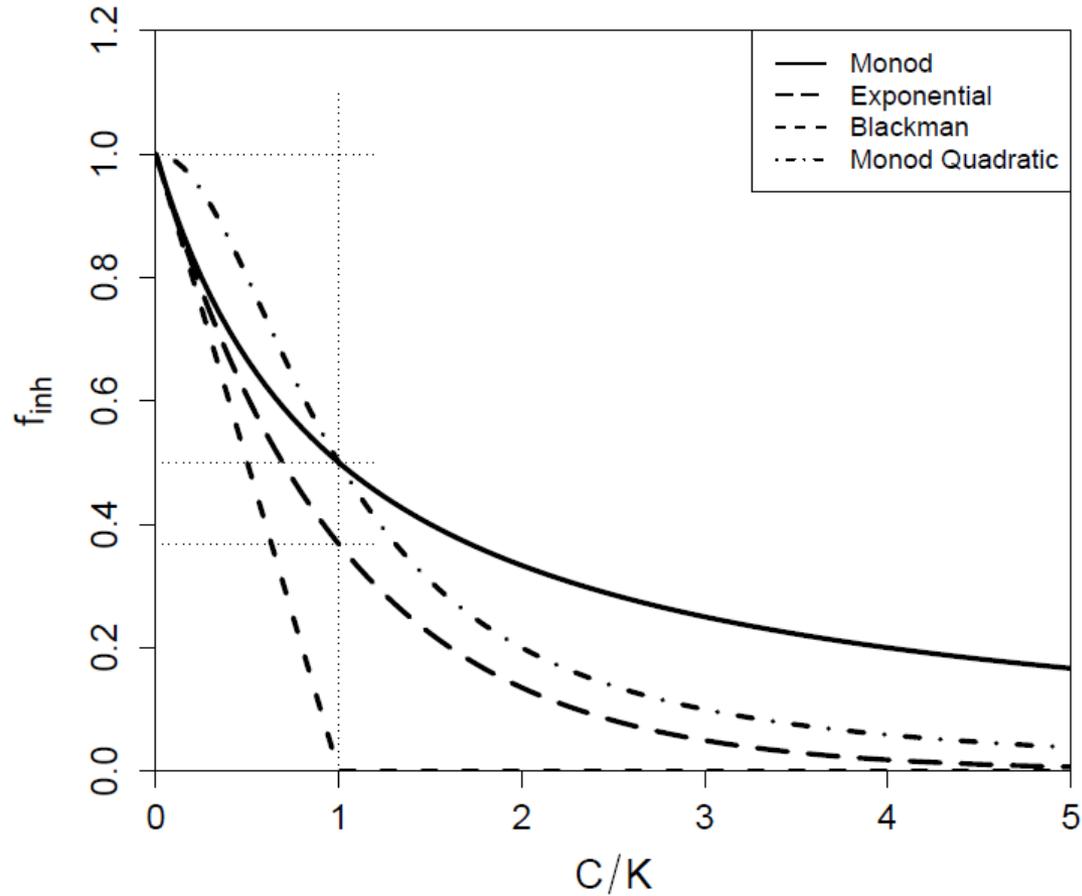$$f_{\text{inh}}^{\text{exp}}(C) = \exp\left(-\frac{C}{K}\right)$$

Blackman:

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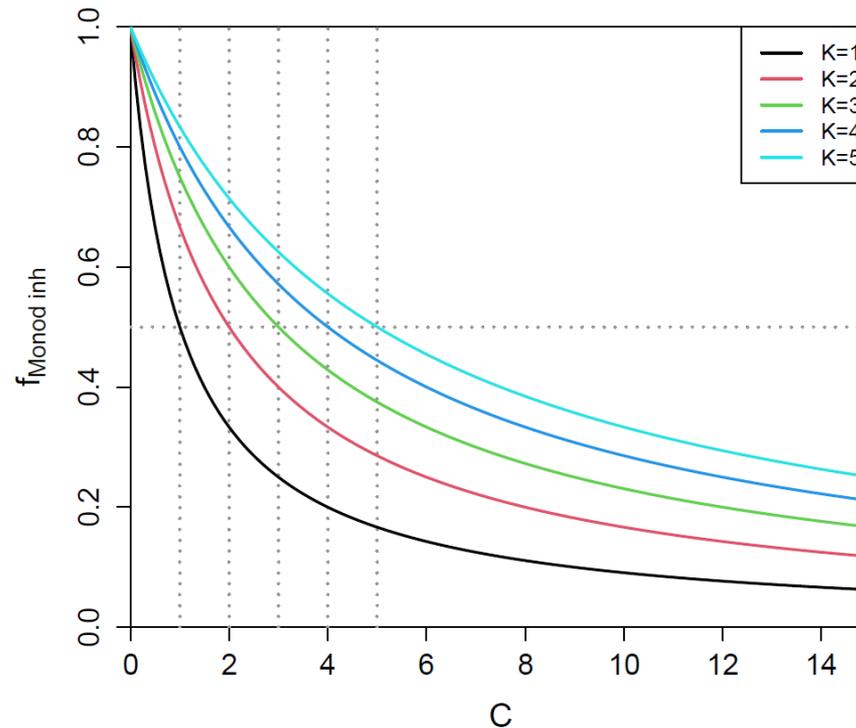
Monod Quadratic:

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

Inhibition by substance concentrations

Inhibition by substance concentrations

$$f_{\text{inh}}^{\text{Monod}}(C) = \frac{K}{K+C} = 1 - \frac{C}{K+C}$$