Exercise 2

Modelling Aquatic Ecosystems FS24

Today’s agenda

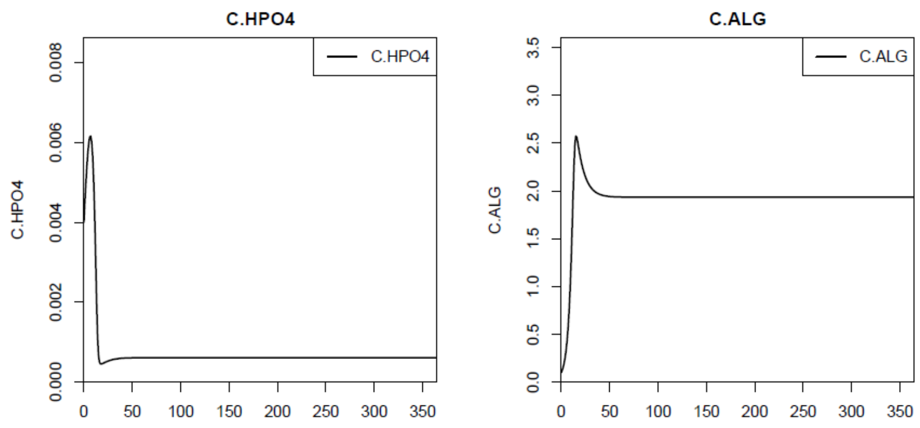
- Q&A of last week’s exercise
- Intro to phytoplankton – zooplankton model
- Recap on elements in process rates
- Break
- Work on the exercise on your own
- Discussion of theory questions

Q&A of last week’s exercise

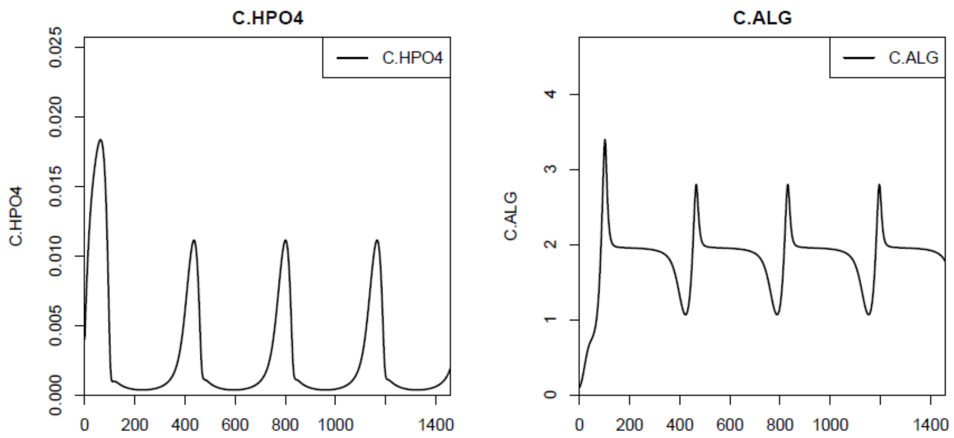
Are there any open questions on Exercise 1?

Homework solution visualization:

constant external conditions:



seasonally varying external conditions:



Reminder: The solutions are available on Mondays on the course website
https://www.eawag.ch/en/department/siam/teaching/modelling-aquatic-ecosystems/#c21285

Question 1

How can you derive the total (net) transformation rate of $C_{\mathrm{HPO}_4^{-2}}$ and C_{ALG} from the process table (Table 11.1) and the process rates (Table 11.2)?

Hint: see equation (4.1) in the manuscript. What are the units?

Question 1 - Answer

Process Table

Process	Substances / Organisms HPO4 $[gP/m^3]$	ALG $[gDM/m^3]$	Rate
Growth of algae	$-\alpha_{P,ALG}$	1	$\rho_{gro,ALG} = k_{gro,ALG} \frac{C_{HPO_4^{2-}}}{K_{HPO_4^{2-},ALG} + C_{HPO_4^{2-}}} C_{ALG}$
Death of algae		-1	$\rho_{death,ALG} = k_{death,ALG} C_{ALG}$

$\alpha_{P,ALG}$ units of phosphate are consumed to produce one unit of algae

linear growth rate modified by limitation term in phosphate (phosphate is consumed, rate has to go to zero if phosphate declines)

linear death rate

one unit of algae disappears from the modelled part of the system (no mass conservation!)

$$r_j = \sum_{i=1}^{n_p} \nu_{ij} \rho_i$$

r = Net transformation rate

ν = Substance-specific stoichiometric coefficients

ρ = Process rate

j = Substance

i = Process

Question 1 - Answer

$$r_{Alg} = k_{gro,\,Alg} \times \frac{C_P}{K + C_P} \times C_{Alg} - k_{death,\,Alg} \times C_{Alg}$$

$$[r_{Alg}] = \frac{1}{d} \times unitless \times \frac{gDM}{m^3} - \frac{1}{d} \times \frac{gDM}{m^3} = \frac{gDM}{d \times m^3}$$

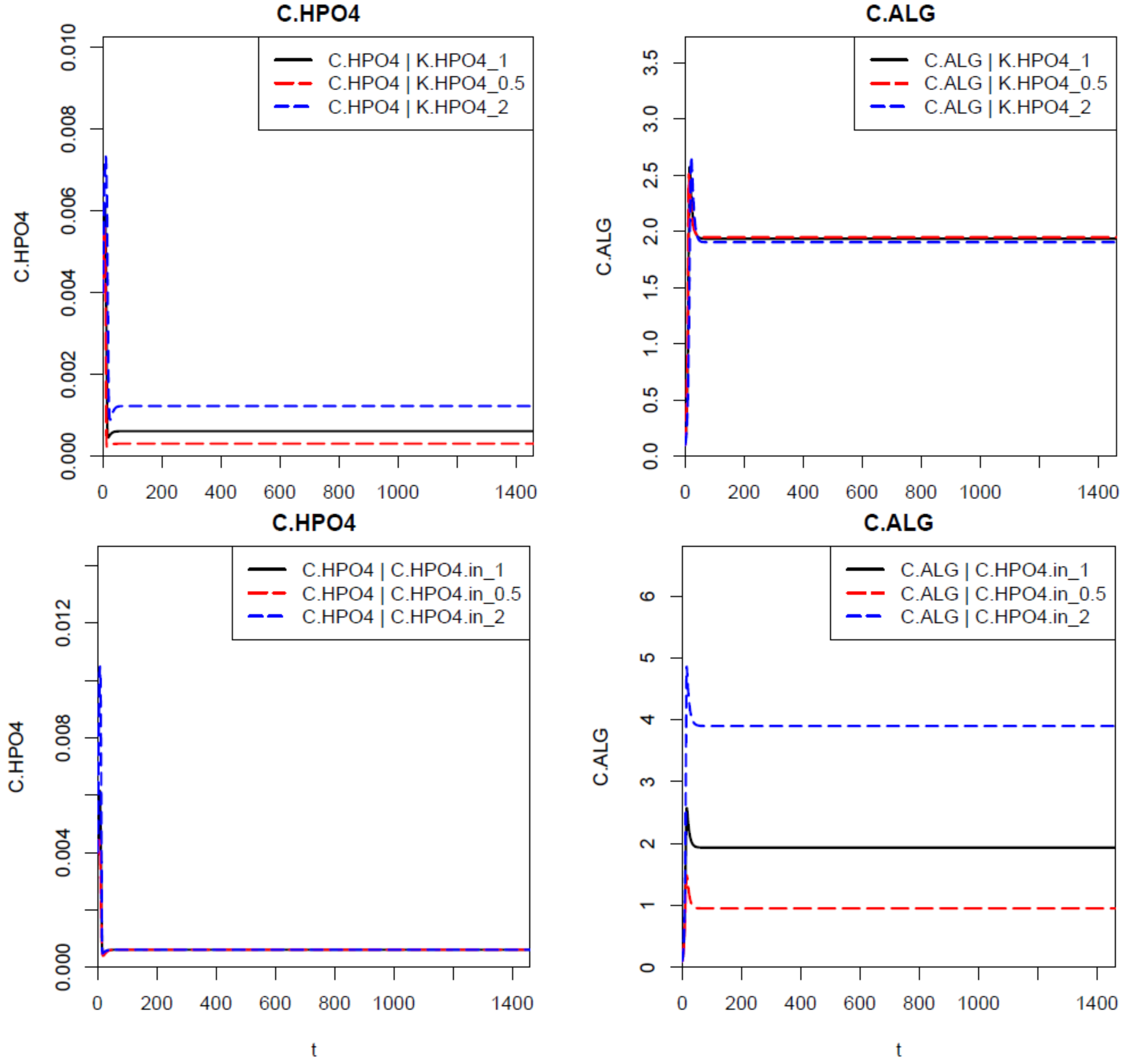
$$r_P = -\alpha_{P,Alg} \times k_{gro,\,Alg} \times \frac{C_P}{K + C_P} \times C_{Alg}$$

$$[r_P] = \frac{gP}{gDM} \times \frac{1}{d} \times unitless \times \frac{gDM}{m^3} = \frac{gP}{d \times m^3}$$

Question 2

Look at the state variables $C_{\mathrm{HPO_4^{2-}}}$ and C_{ALG}. Which of them is more sensitive to the parameter $K_{\mathrm{HPO_4^{2-},\ ALG}}$ and which of them is more sensitive to $C_{\mathrm{in,\ HPO_4^{2-}}}$? Do you understand why?

Question 2 - Visualization



Look at the solution of the ODE in the chapter 11.1
→ equations 11.12 and 11.13

Solution of the ODE in the chapter 11.1, equations 11.12 and 11.13

$$C^{\mathrm{fix},2}_{\mathrm{HPO}_4^{2-}} = \frac{K_{\mathrm{HPO}_4^{2-},\mathrm{ALG}}}{\frac{k_{\mathrm{gro,ALG}}}{k_{\mathrm{death,ALG}} + \frac{Q_{\mathrm{in}}}{V}} - 1} \quad , \tag{11.12}$$

$$C^{\mathrm{fix},2}_{\mathrm{ALG}} = \frac{1}{\alpha_{\mathrm{P,ALG}}} \frac{\frac{Q_{\mathrm{in}}}{V}}{k_{\mathrm{death,ALG}} + \frac{Q_{\mathrm{in}}}{V}} \left(C_{\mathrm{in,HPO}_4^{2-}} - \frac{K_{\mathrm{HPO}_4^{2-},\mathrm{ALG}}}{\frac{k_{\mathrm{gro,ALG}}}{k_{\mathrm{death,ALG}} + \frac{Q_{\mathrm{in}}}{V}} - 1} \right) \quad . \tag{11.13}$$

Intro to phytoplankton – zooplankton model
Chapter 11.2

$\alpha_{P,ALG}$ units of phosphate are consumed to produce one unit of algae (units indicated above)

one unit of algae disappears from the modelled part of the system (no mass conservation!)

Process	Substances / Organisms			Rate
	HPO_4^{2-}	ALG	ZOO	
	gP	gDM	gDM	
Growth of algae	$-\alpha_{P,ALG}$	1		$\rho_{gro,ALG}$
Death of algae		-1		$\rho_{death,ALG}$
Growth of zooplankton		$-\frac{1}{Y_{ZOO}}$	1	$\rho_{gro,ZOO}$
Death of zooplankton			-1	$\rho_{death,ZOO}$

process rates **???**

$1/Y_{ZOO}$ (> 1) units of algae are consumed to produce one unit of zooplankton (no mass conservation!)

one unit of zooplanktion disappears from the modelled part of the system (no mass conservation!)

What constitute process rates ?

Process Rates (4.2)

Process rates typically depend

a) linearly on the concentration [g/m3] (or density) of the state variable (e.g. substance or organism), for which the stoichiometric coefficient was set to a fixed value (usually +1 or -1)

b) on a rate parameter that describes the speed of the process under standard conditions (*k*) [1/t]

c) on external drivers, e.g. environmental conditions (e.g. temperature, light, ...)

e) on additional limiting or inhibiting factors (e.g. limitation terms for all substances/organisms that are consumed during the process)

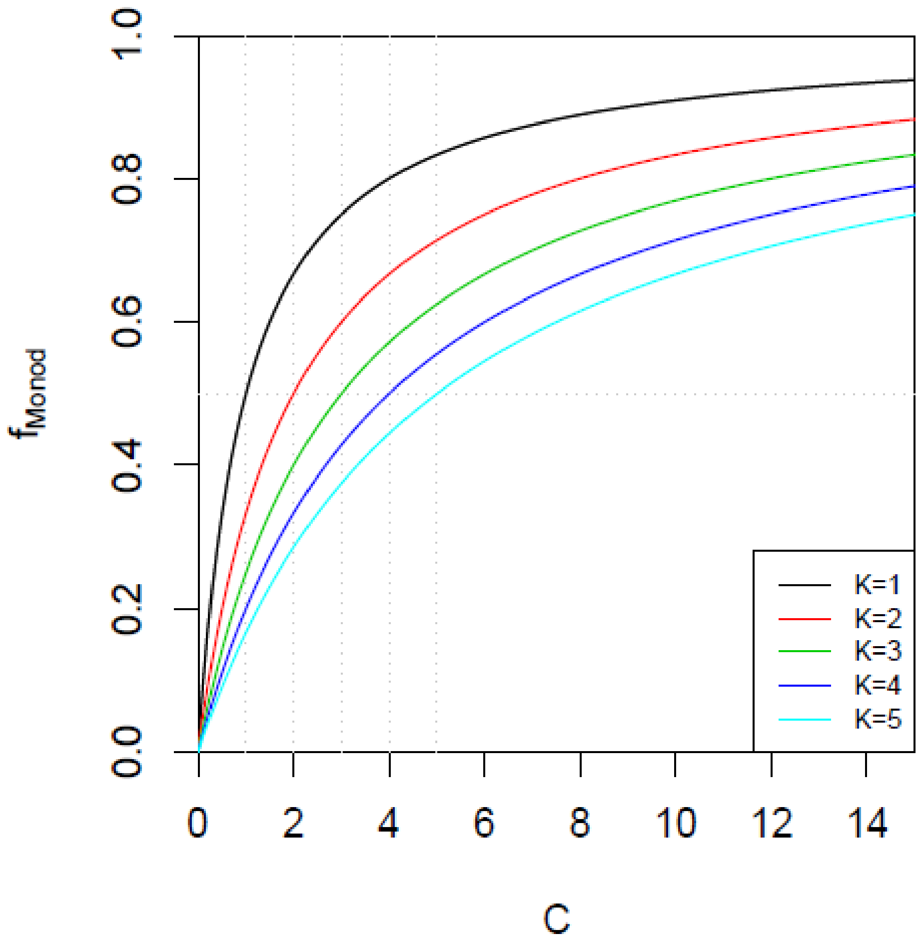
$$\rho_{\mathrm{gro,ALG,NH_4^+}} = \overbrace{k_{\mathrm{gro,ALG},T_0}}^{\text{rate parameter}} \cdot \overbrace{f_{\mathrm{temp}}(T)}^{\text{temperature dependence}} \cdot \overbrace{f_{\mathrm{rad}}(I)}^{\text{light dependence}}$$

$$\cdot \underbrace{f_{\mathrm{lim}}(C_{\mathrm{HPO_4^{2-}}}, C_{\mathrm{NH_4^+}}, C_{\mathrm{NO_3^-}})}_{\text{nutrient limitation}} \cdot \underbrace{C_{\mathrm{ALG}}}_{\text{rate linear in algae concentration}}$$

Process Rates (4.2.2)

Nutrient limitation

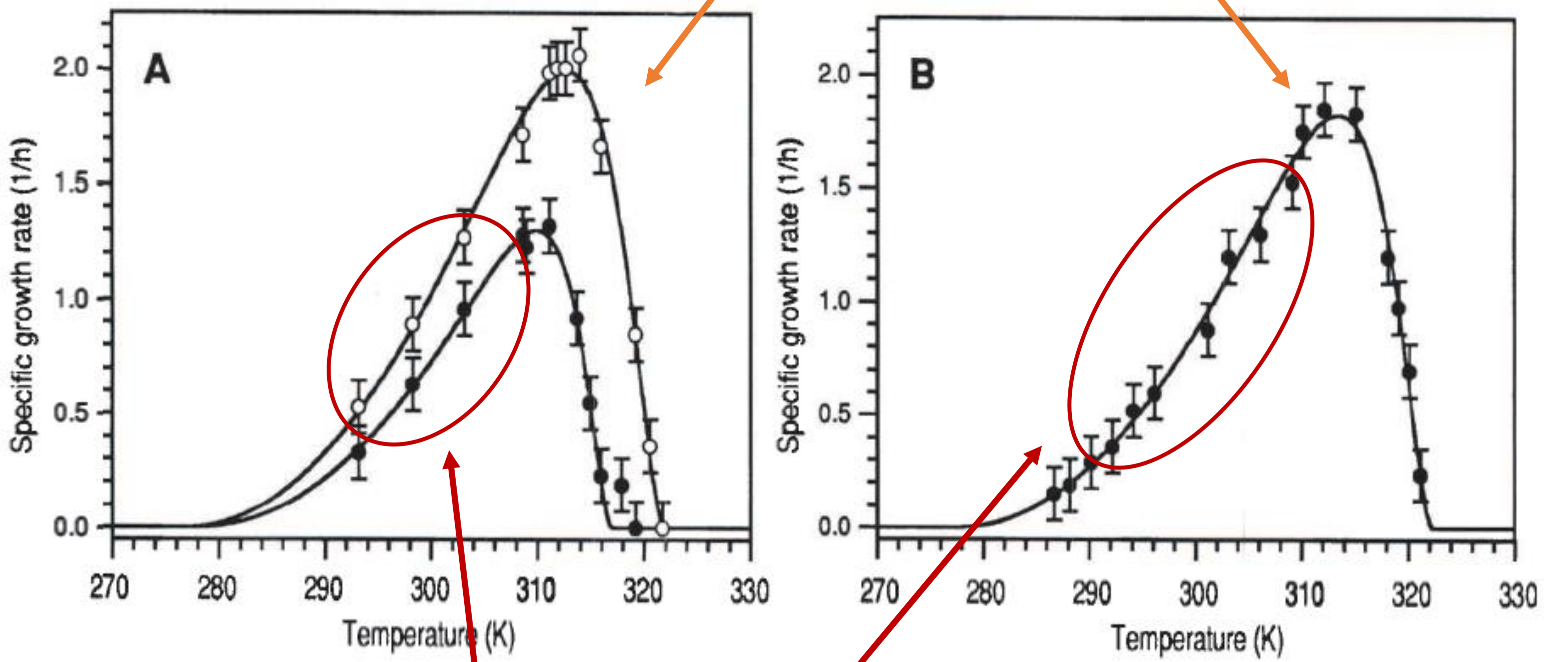
$$f_{\lim}^{\text{Monod}}(C) = \frac{C}{K + C}$$



Process Rates (4.2.1)

Temperature dependence

typical behavior of biological reactions to temperature → an increase from a minimum to an optimum, followed by a decrease, described in equation 4.9



natural systems are usually limited in their temperature range, so we only describe the inclining branch:

reference temperature at which the factor is unity

$$f^{\mathrm{exp}}_{\mathrm{temp}}(T) = \exp\left(\beta(T - T_0)\right)$$

coefficient of temperature dependence

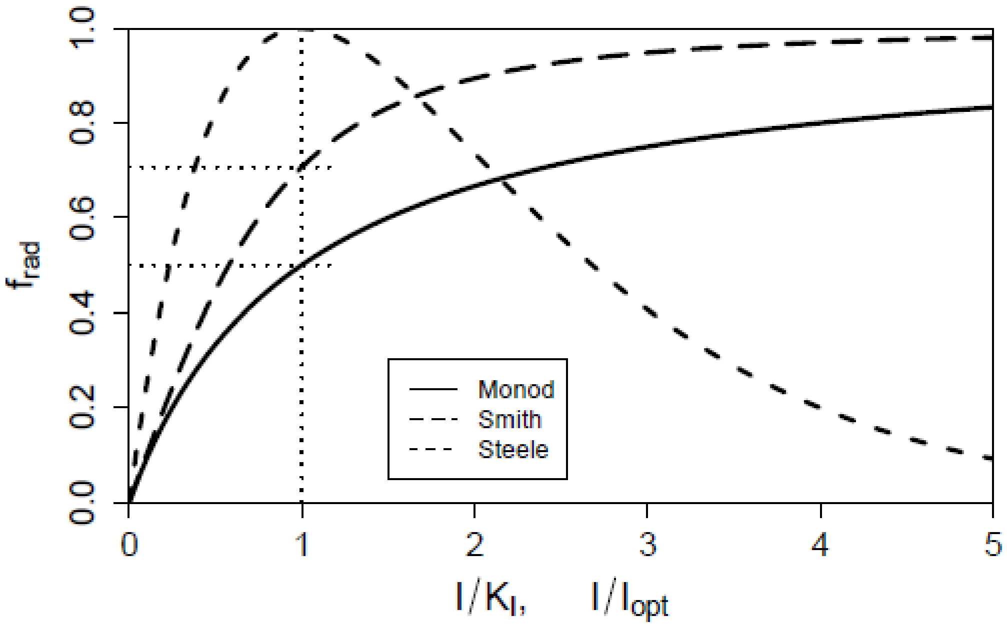
Process Rates (4.2.4)

Light dependence **at a specific depth** (e.g., at bottom of the river)

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

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

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

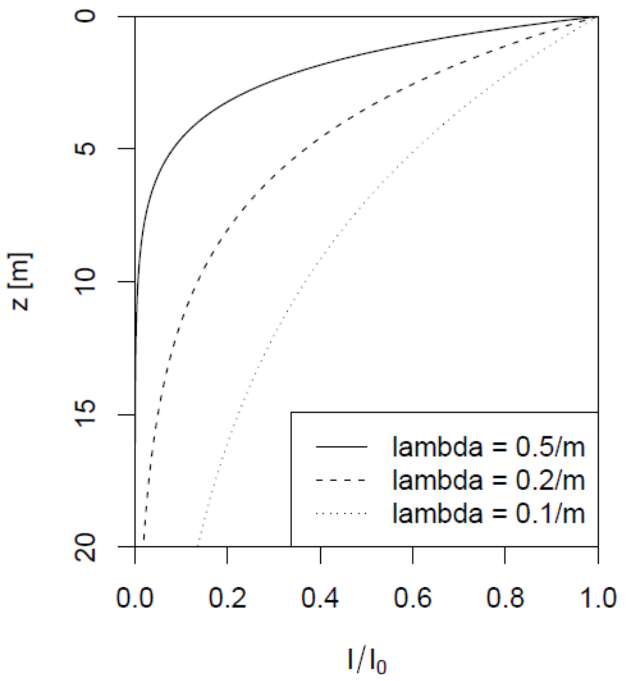


Light is needed for algae growth, but high intensities may still be inhibiting.

Process Rates (4.2.4)

Light dependence **over depth**

Averaging rate (factor) over depth of the mixed box:



$$I = I_0 \exp(-\lambda z) \qquad \lambda = \lambda_1 + \lambda_2 \cdot C_{\mathrm{ALG}}$$

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

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

→ Rate (factor) averaging is needed if the model does not resolve the depth continuously.

Process Rates (11.2)

Model with constant driving forces (Table 11.5):

Rate	Rate expression
$\rho_{\text{gro,ALG}}$	$k_{\text{gro,ALG}} \dfrac{C_{\text{HPO}_4^{2-}}}{K_{\text{HPO}_4^{2-},\text{ALG}} + C_{\text{HPO}_4^{2-}}} C_{\text{ALG}}$
$\rho_{\text{death,ALG}}$	$k_{\text{death,ALG}} C_{\text{ALG}}$
$\rho_{\text{gro,ZOO}}$	$k_{\text{gro,ZOO}} C_{\text{ALG}} C_{\text{ZOO}}$
$\rho_{\text{death,ZOO}}$	$k_{\text{death,ZOO}} C_{\text{ZOO}}$

phosphate limitation of algae growth

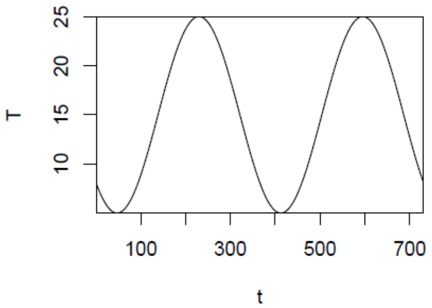
zooplankton growth rate linear in zooplankton with a linear limitation in algae

linear death rate

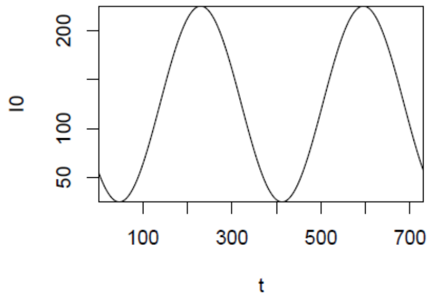
Process Rates (11.2)

Model with seasonally varying driving forces (Table 11.6):

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



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



Rate	Rate expression
$\rho_{\mathrm{gro,ALG}}$	$k_{\mathrm{gro,ALG},T_0} \cdot \exp\left(\beta_{\mathrm{ALG}}(T - T_0)\right) \cdot \frac{1}{\lambda h} \log\left(\frac{K_I + I_0}{K_I + I_0 \exp(-\lambda h)}\right) \cdot \frac{C_{\mathrm{HPO_4^{2-}}}}{K_{\mathrm{HPO_4^{2-},ALG}} + C_{\mathrm{HPO_4^{2-}}}} \cdot C_{\mathrm{ALG}}$
$\rho_{\mathrm{death,ALG}}$	$k_{\mathrm{death,ALG}}\, C_{\mathrm{ALG}}$
$\rho_{\mathrm{gro,ZOO}}$	$k_{\mathrm{gro,ZOO},T_0} \cdot \exp\left(\beta_{\mathrm{ZOO}}(T - T_0)\right) \cdot C_{\mathrm{ALG}}\, C_{\mathrm{ZOO}}$
$\rho_{\mathrm{death,ZOO}}$	$k_{\mathrm{death,ZOO}}\, C_{\mathrm{ZOO}}$

temperature dependence

light dependence

Note on class definition in Ecosim

The classes (processes, reactors, links, systems) have pre-defined elements (e.g., name, rate, stoich, …) to be declared when we define them. These elements have specific types, for instance;

- “rate” must be an “expression” to explicit that it’s a mathematical formula that will be calculated later when this process will be called with a vector of parameters and numerical values,
- “stoich” must be a list of numbers or “expression”, etc.

More information on Ecosim and its classes in Chapter 16 of the manuscript.

Process	Substances / Organisms HPO_4^{2-} gP	ALG gDM	ZOO gDM	Rate
Growth of algae	$-\alpha_{P,ALG}$	1		$\rho_{gro,ALG}$

Process table, Table 11.4

```
# growth of algae:

gro.ALG    <- new(Class   = "process",
                  name    = "Growth of algae",
                  rate    = expression(k.gro.ALG
                                       *C.HPO4/(K.HPO4+C.HPO4)
                                       *C.ALG),
                  stoich  = list(C.ALG  = expression(1),              # gDM/gDM
                                 C.HPO4 = expression(-alpha.P.ALG)))  # gP/gDM
```

Definition of ALG growth rate, script Rmd

Elements of class “process”

Name	Type	Meaning
name	string	Name of process.
rate	expression	Expression for the dependence of the process rate on substance concentrations, model parameters, and external influence factors.
stoich	list	List of numbers or expressions for stoichiometric coefficients. Substances are identified by their names.
pervol	logical	Type of process rate: mass per volume and time (TRUE) or per area and time (FALSE).

Definition of class “process”, Table 16.1

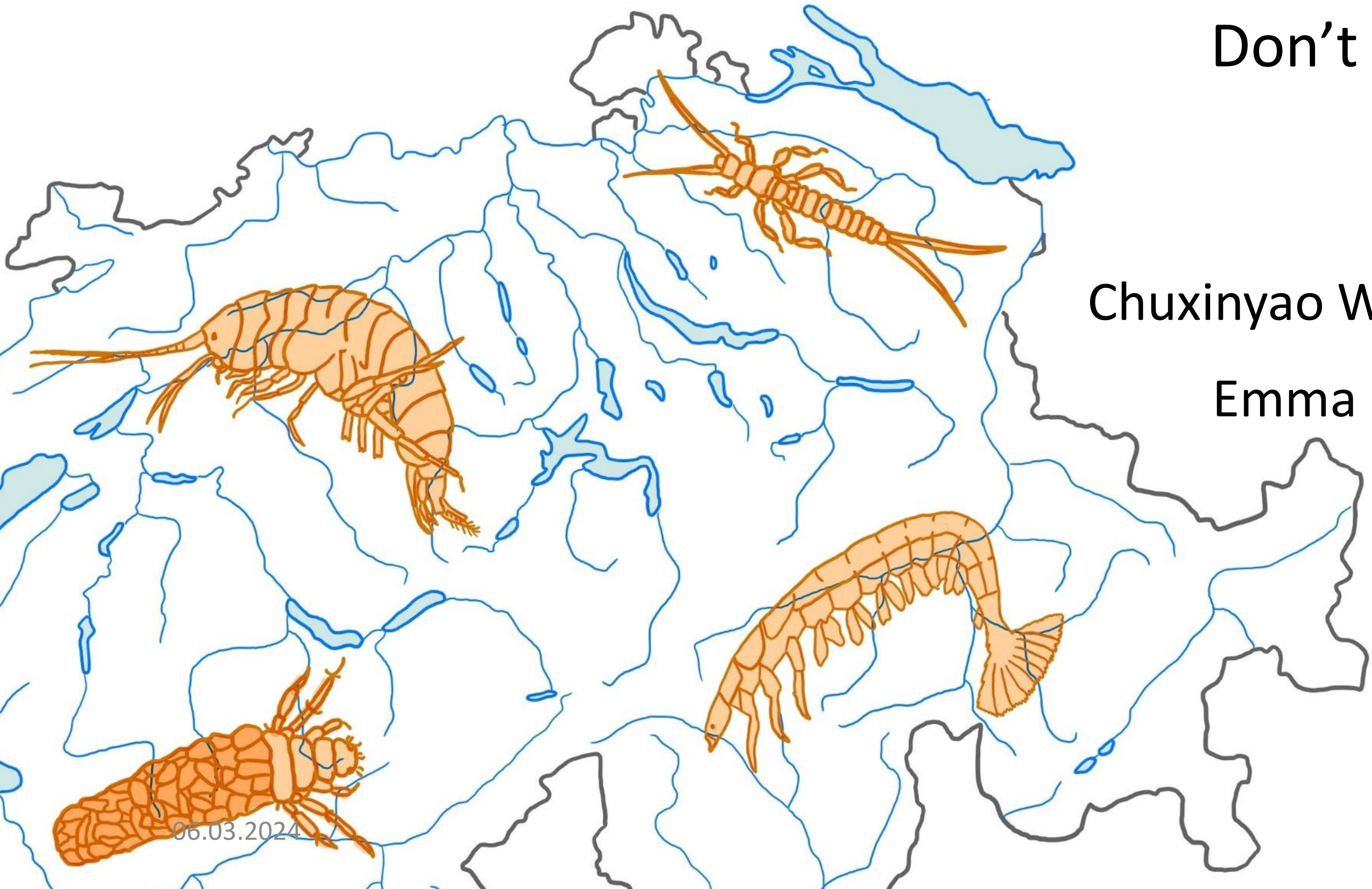
Time to work on Exercise 2

Theory questions

- Are the algae concentrations controlled bottom-up (by phosphate limitation) or top-down (by grazing of zooplankton)?
- What is the reason for oscillating concentrations under constant driving forces? What happens when you introduce periodic driving forces?
- What are the main deficits of the model compared to a real lake?
- What is your expectation regarding the response of the model to the change in each parameter, does the result match your expectation and can you explain the observed changes?

Homeworks:

- Task 4 – Sensitivity analysis
- Theory questions



Don't hesitate to send us an e-mail
if you have any questions.

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Have a nice sunny day !