

Exercise 4

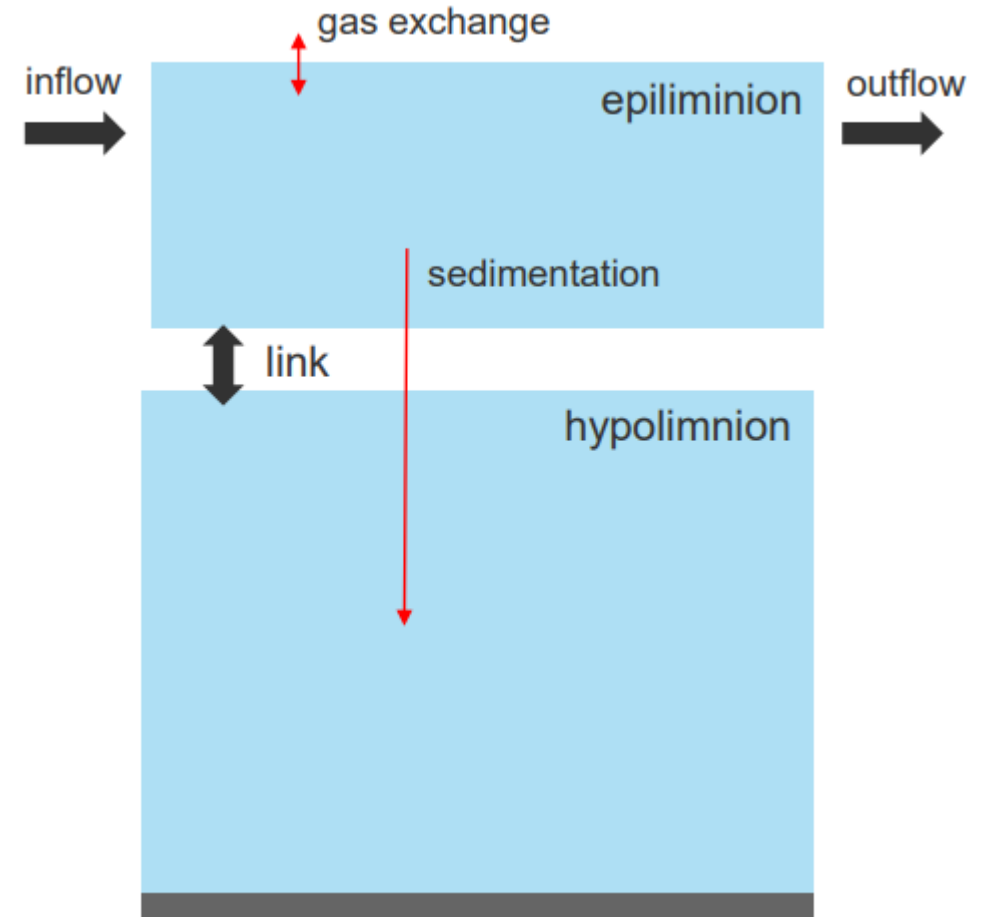
Modelling Aquatic Ecosystems FS26

Today's agenda

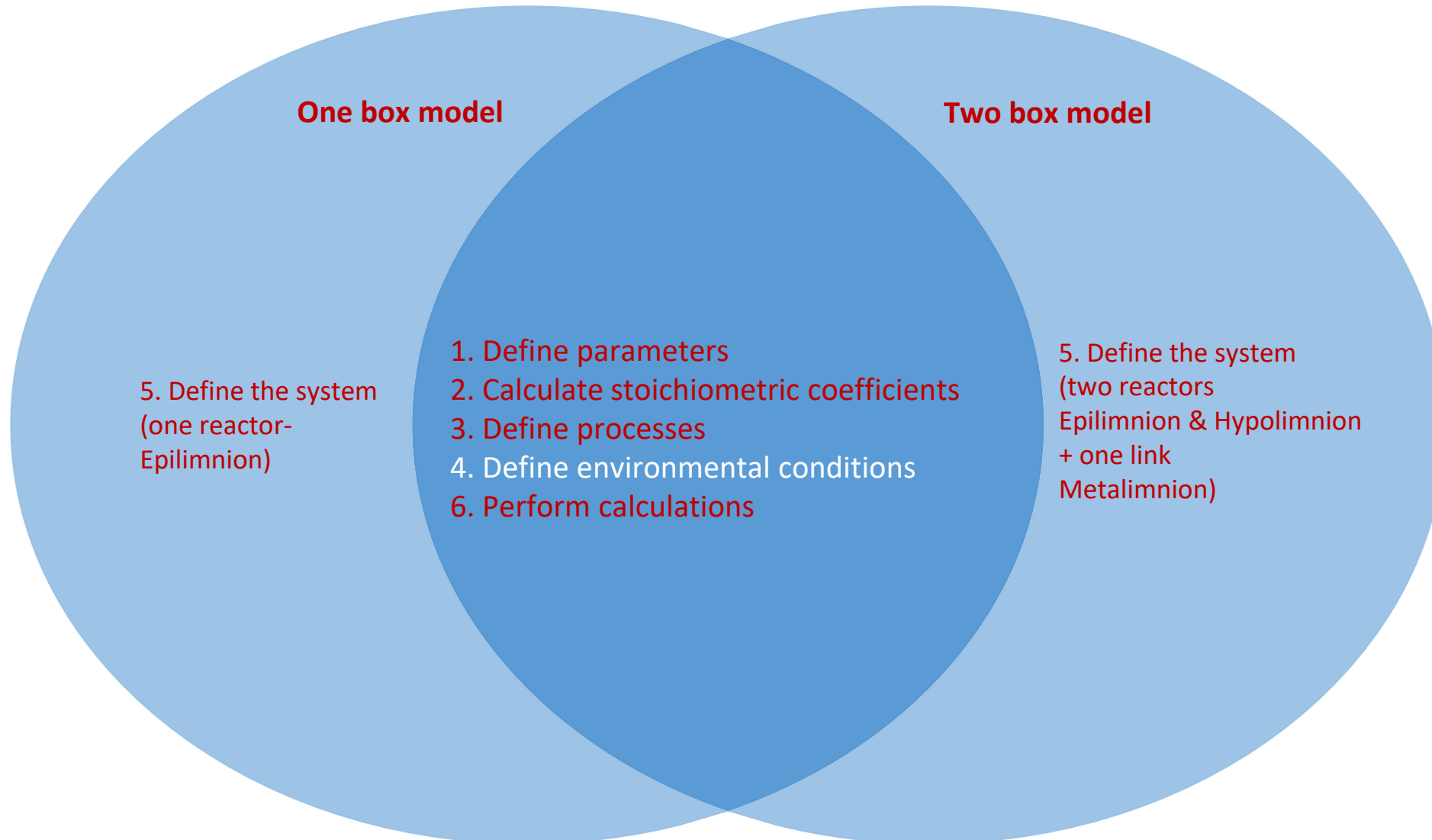
- Quick recap of last week's lecture
- Introduction to today's model 11.4
- Work on the exercise
- Break
- Discuss the results and the questions of the exercise
- Work on your project topics and take the opportunity to ask questions

Recap of last week's theory

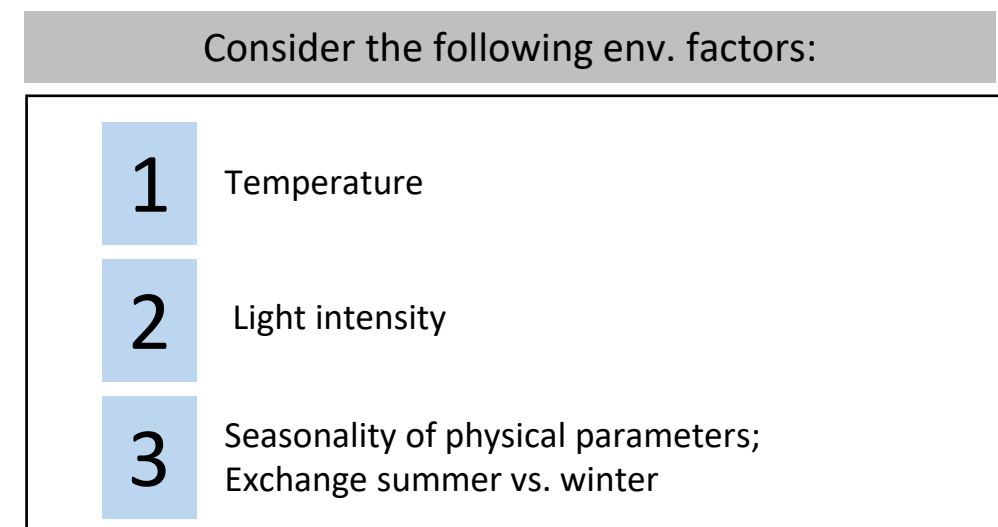
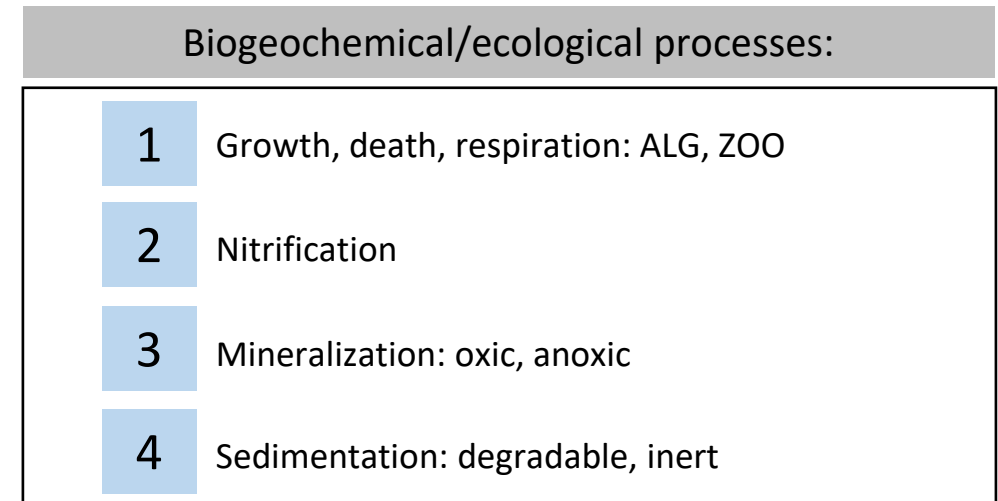
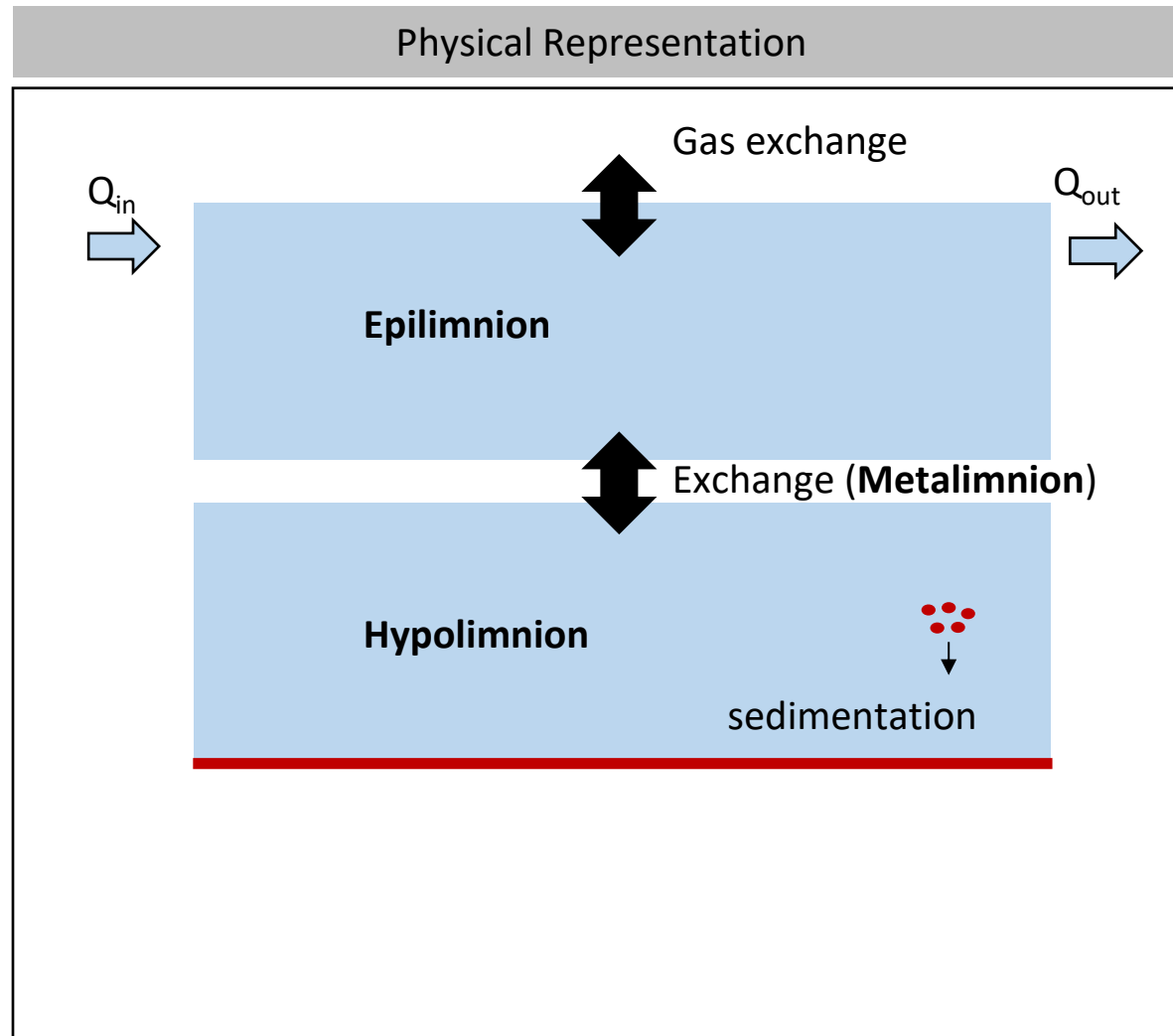
- Mass balance in a continuous multi-reactor system (sections 3.3 and 3.4)
- Transport and mixing in lakes- Physical processes (sections 6.1 to 6.3)
 - Plunging of inflows
 - Horizontal mixing
 - Stratification / Vertical mixing
- Sedimentation
- Gas exchange
- Two box lake model (today's exercise sections 11.3 and 11.4)



One box model vs. Two box model



Two box biogeochemical-ecological lake model



Process table

Process	Substances / Organisms										Rate
	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	
Growth of algae NO ₃ ⁻	-		-	+	1						$\rho_{\text{gro,ALG,NO}_3^-}$
Growth of algae NH ₄ ⁺	-	-		+	1						$\rho_{\text{gro,ALG,NH}_4^+}$
Respiration of algae	+	+		-	-1						$\rho_{\text{resp,ALG}}$
Death of algae	0/+	0/+		0/+	-1		$(1 - f_I)Y_{\text{ALG,death}}$	$f_I Y_{\text{ALG,death}}$			$\rho_{\text{death,ALG}}$
Growth of zooplankton	+	+		-	$\frac{-1}{Y_{\text{ZOO}}}$	1	$\frac{(1 - f_I)f_e}{Y_{\text{ZOO}}}$	$\frac{f_I f_e}{Y_{\text{ZOO}}}$			$\rho_{\text{gro,ZOO}}$
Respiration of zoopl.	+	+		-		-1					$\rho_{\text{resp,ZOO}}$
Death of zooplankton	0/+	0/+		0/+		-1	$(1 - f_I)Y_{\text{ZOO,death}}$	$f_I Y_{\text{ZOO,death}}$			$\rho_{\text{death,ZOO}}$
Nitrification							$\text{NH}_4^+ + 2\text{O}_2 \rightarrow \text{NO}_3^- + 2\text{H}^+ + \text{H}_2\text{O}$				ρ_{nitri}
Oxic mineral. of org. part.							$\text{POMD} + \text{O}_2 \rightarrow \text{NH}_4^+ + \text{HPO}_4^{2-} + \text{CO}_2 + \text{H}_2\text{O}$				$\rho_{\text{miner,ox,POMD}}$
Ox. min. of org. part. in sed.							$\text{SPOMD} + \text{O}_2 \rightarrow \text{NH}_4^+ + \text{HPO}_4^{2-} + \text{CO}_2 + \text{H}_2\text{O}$				$\rho_{\text{miner,ox,SPOMD}}$
Anox. min. of org. part. in sed.							$\text{SPOMD} + \text{NO}_3^- \rightarrow \text{NH}_4^+ + \text{HPO}_4^{2-} + \text{CO}_2 + \text{H}_2\text{O}$				$\rho_{\text{miner,anox,SPOMD}}$
Sed. of deg. org. part.							$\text{POMD} \rightarrow \text{SPOMD}$				$\rho_{\text{sed,POMD}}$
Sed. of inert org. part.							$\text{POMI} \rightarrow \text{SPOMI}$				$\rho_{\text{sed,POMI}}$

Rate	Rate expression
$\rho_{\text{gro,ALG,NH}_4^+}$	$k_{\text{gro,ALG},T_0} \cdot \exp(\beta_{\text{ALG}}(T - T_0)) \cdot \frac{1}{\lambda h} \log\left(\frac{K_I + I_0}{K_I + I_0 \exp(-\lambda h)}\right) \cdot \min\left(\frac{C_{\text{HPO}_4^{2-}}}{K_{\text{HPO}_4^{2-},\text{ALG}} + C_{\text{HPO}_4^{2-}}}, \frac{C_{\text{NH}_4^+} + C_{\text{NO}_3^-}}{K_{\text{N,ALG}} + C_{\text{NH}_4^+} + C_{\text{NO}_3^-}}\right) \cdot \frac{p_{\text{NH}_4^+} C_{\text{NH}_4^+}}{p_{\text{NH}_4^+} C_{\text{NH}_4^+} + C_{\text{NO}_3^-}} \cdot C_{\text{ALG}}$
$\rho_{\text{gro,ALG,NO}_3^-}$	$k_{\text{gro,ALG},T_0} \cdot \exp(\beta_{\text{ALG}}(T - T_0)) \cdot \frac{1}{\lambda h} \log\left(\frac{K_I + I_0}{K_I + I_0 \exp(-\lambda h)}\right) \cdot \min\left(\frac{C_{\text{HPO}_4^{2-}}}{K_{\text{HPO}_4^{2-},\text{ALG}} + C_{\text{HPO}_4^{2-}}}, \frac{C_{\text{NH}_4^+} + C_{\text{NO}_3^-}}{K_{\text{N,ALG}} + C_{\text{NH}_4^+} + C_{\text{NO}_3^-}}\right) \cdot \frac{C_{\text{NO}_3^-}}{p_{\text{NH}_4^+} C_{\text{NH}_4^+} + C_{\text{NO}_3^-}} \cdot C_{\text{ALG}}$
$\rho_{\text{resp,ALG}}$	$k_{\text{resp,ALG},T_0} \cdot \exp(\beta_{\text{ALG}}(T - T_0)) \cdot \frac{C_{\text{O}_2}}{K_{\text{O}_2,\text{ALG}} + C_{\text{O}_2}} \cdot C_{\text{ALG}}$
$\rho_{\text{death,ALG}}$	$k_{\text{death,ALG}} \cdot C_{\text{ALG}}$
$\rho_{\text{gro,ZOO}}$	$k_{\text{gro,ZOO},T_0} \cdot \exp(\beta_{\text{ZOO}}(T - T_0)) \cdot \frac{C_{\text{O}_2}}{K_{\text{O}_2,\text{ZOO}} + C_{\text{O}_2}} \cdot C_{\text{ALG}} \cdot C_{\text{ZOO}}$
$\rho_{\text{resp,ZOO}}$	$k_{\text{resp,ZOO},T_0} \cdot \exp(\beta_{\text{ZOO}}(T - T_0)) \cdot \frac{C_{\text{O}_2}}{K_{\text{O}_2,\text{ZOO}} + C_{\text{O}_2}} \cdot C_{\text{ZOO}}$
$\rho_{\text{death,ZOO}}$	$k_{\text{death,ZOO}} \cdot C_{\text{ZOO}}$
ρ_{nitri}	
$\rho_{\text{miner,ox,POMD}}$	
$\rho_{\text{miner,ox,SPOMD}}$	
$\rho_{\text{miner,anox,SPOMD}}$	
$\rho_{\text{sed,POMD}}$	
$\rho_{\text{sed,POMI}}$	

Specific maximum process rate term k
+ Temperature dependence term
+ Substance limitation term(s)

Implementation of Stratification/Vertical mixing

parameters for the coefficient
of vertical turbulent diffusion Kz

```
Kz.summer = 0.02, # m2/d  
Kz.winter = 20, # m2/d
```

chapter 6.1.1

```
# Definition of environmental conditions:  
  
cond.epi <- list(I0 = expression( 0.5*(I0.min+I0.max)  
                                +0.5*(I0.max-I0.min)  
                                *cos(2*pi/365.25*(t-t.max))),  
                T = expression( 0.5*(T.min+T.max)  
                                +0.5*(T.max-T.min)  
                                *cos(2*pi/365.25*(t-t.max))),  
                C.O2.sat = expression(exp(7.7117-1.31403*log(T+45.93))  
                                       *p/101325))
```

```
cond.hypo <- list(I0 = 0,  
                 T = 5)
```

seasonal pattern of Kz

```
cond.gen <- list(Kz=expression( 0.5*(Kz.summer+Kz.winter)  
                               -0.5*(Kz.winter-Kz.summer)  
                               *sign(cos(2*pi/365.25*(t-t.max))+0.4)))
```

Implementation of Stratification/Vertical mixing

chapter 6.1.1

#Definition of the Lake system:

```
system.11.4 <- new(Class = "system",
                  name   = "Lake",
                  reactors = list(epilimnion, hypolimnion),
                  links   = list(metalimnion),
                  cond     = cond.gen,
                  param    = param,
                  t.out    = seq(0, 730, by=1)) #number of days 365, 730, 1095, 1460
```

make the definition of K_z available for the whole system

Definition of links:

Exchange between epilimnion and hypolimnion:

```
metalimnion <-
  new(Class = "link",
       name  = "Metalimnion",
       from  = "Epi",
       to    = "Hypo",
       qadv.spec = list(C.POMD = expression(v.sed.POM*A),
                       C.POMI = expression(v.sed.POM*A)),
       qdiff.gen = expression(A/h.meta*Kz))
```

(eq. 6.1.3)
general diffusive exchange coefficient
between epi- and hypolimnion,
(general = applies to all dissolved and suspended substances)

Implementation of Gas exchange

chapter 6.3

```
# Definition of environmental conditions:

cond.epi <- list(I0      = expression( 0.5*(I0.min+I0.max)
                                         +0.5*(I0.max-I0.min)
                                         *cos(2*pi/365.25*(t-t.max))),
               T        = expression( 0.5*(T.min+T.max)
                                         +0.5*(T.max-T.min)
                                         *cos(2*pi/365.25*(t-t.max))),
               C.O2.sat = expression(exp(7.7117-1.31403*log(T+45.93))
                                         *p/101325))

cond.hypo <- list(I0 = 0,
                 T  = 5)

cond.gen <- list(Kz=expression( 0.5*(Kz.summer+Kz.winter)
                               -0.5*(Kz.winter-Kz.summer)
                               *sign(cos(2*pi/365.25*(t-t.max))+0.4)))
```

(eq 6.76)

Implementation of Gas exchange

chapter 6.3

```
# Epilimnion:

epilimnion <-
  new(Class      = "reactor",
       name      = "Epi",
       volume.ini = expression(A*h.epi),
       conc.pervol.ini = list(C.HPO4 = expression(C.HPO4.ini), # gP/m3
                              C.NH4  = expression(C.NH4.ini),  # gN/m3
                              C.NO3  = expression(C.NO3.ini),  # gN/m3
                              C.O2   = expression(C.O2.ini),   # gO/m3
                              C.ALG   = expression(C.ALG.ini),  # gDM/m3
                              C.ZOO   = expression(C.ZOO.ini),  # gDM/m3
                              C.POMD  = expression(C.POMD.ini), # gDM/m3
                              C.POMI  = expression(C.POMI.ini)), # gDM/m3
       input     = list(C.O2 = expression(v.ex.O2*A
                                           *(C.O2.sat-C.O2))), # gas ex.
       inflow    = expression(Q.in*86400), # m3/d
       inflow.conc = list(C.HPO4 = expression(C.HPO4.in),
```

(eq 6.73)

Implementation of Sedimentation

chapter 6.2

Because we have no separate sediment reactor, **sedimentation within each reactor** is implemented as a transformation process from C.POM to D.POM:

Stoichiometry

```
# Sedimentation of degradable organic particles:

nu.sed.POMD <-
  calc.stoich.coef(alpha      = alpha,
                  name       = "sed.POMD",
                  subst      = c("C.POMD", "D.POMD"),
                  subst.norm  = "C.POMD",
                  nu.norm    = -1)

# Sedimentation of inert organic particles:

nu.sed.POMI <-
  calc.stoich.coef(alpha      = alpha,
                  name       = "sed.POMI",
                  subst      = c("C.POMI", "D.POMI"),
                  subst.norm  = "C.POMI",
                  nu.norm    = -1)
```

Process rate

```
# Sedimentation of degradable organic particles:

sed.POMD <-
  new(Class = "process",
      name  = "sed.POMD",
      rate  = expression(v.sed.POM/h.hypo*C.POMD),
      stoich = as.list(nu["sed.POMD",]))

# Sedimentation of inert organic particles:

sed.POMI <-
  new(Class = "process",
      name  = "sed.POMI",
      rate  = expression(v.sed.POM/h.hypo*C.POMI),
      stoich = as.list(nu["sed.POMI",]))
```

Implementation of Sedimentation

chapter 6.2

sedimentation from epilimnion to hypolimnion:

```
# Definition of links:

# Exchange between epilimnion and hypolimnion:

metalimnion <-
  new(Class      = "link",
       name      = "Metalimnion",
       from      = "Epi",
       to        = "Hypo",
       qadv.spec = list(C.POMD = expression(v.sed.POM*A),
                       C.POMI = expression(v.sed.POM*A)),
       qdiff.gen = expression(A/h.meta*Kz))
```

Note on numerical solution of ODE (section 5.4)

- In `ecosim`, we use the R package `deSolve` that builds an interface to a large number of very sophisticated numerical ordinary differential equations solvers.
- You can always get the description of R packages by entering the address
 - <https://cran.r-project.org/package=deSolve>
 - <https://cran.r-project.org/package=ecosim>
- The function `ode` in `deSolve` has a long list of numerical integrators available:

```
ode(y, times, func, parms,  
method = c("lsoda", "lsode", "lsodes", "lsodar", "vode", "daspk",  
           "euler", "rk4", "ode23", "ode45", "radau",  
           "bdf", "bdf_d", "adams", "impAdams", "impAdams_d", "iteration"), ...)
```

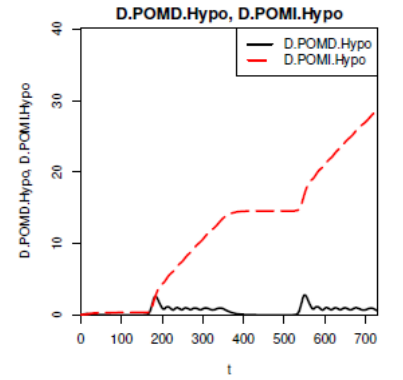
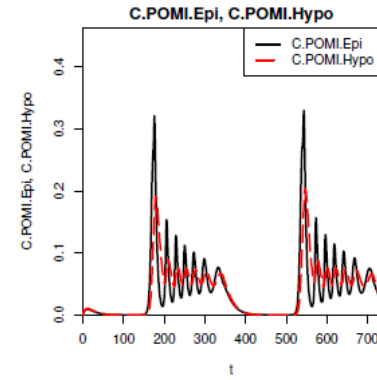
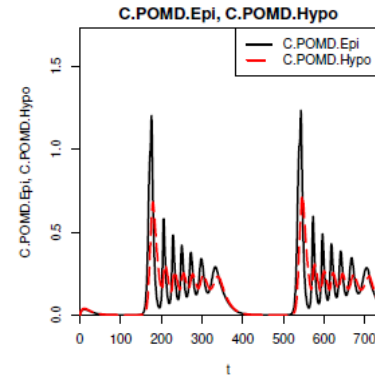
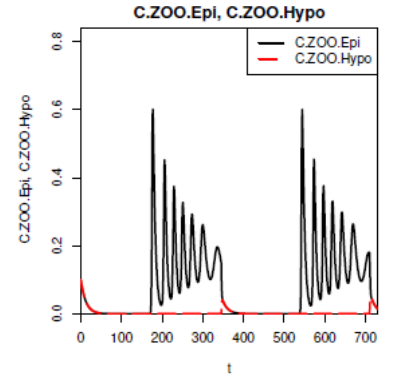
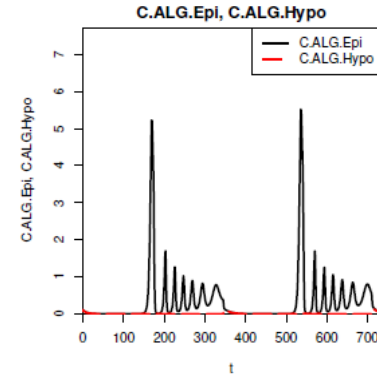
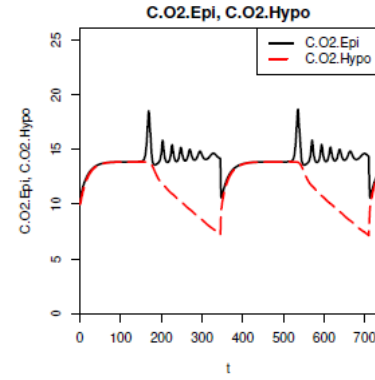
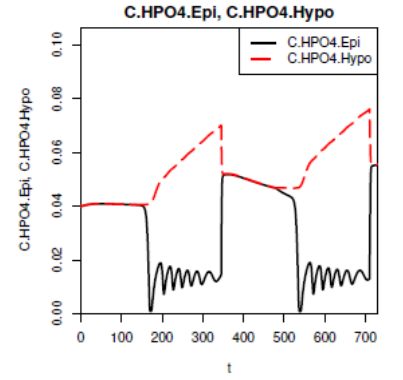
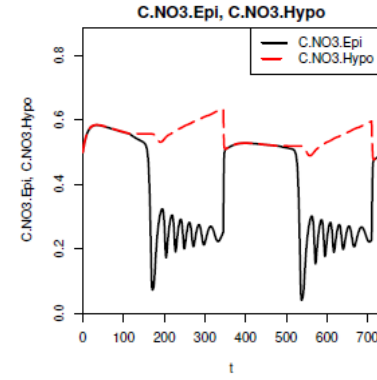
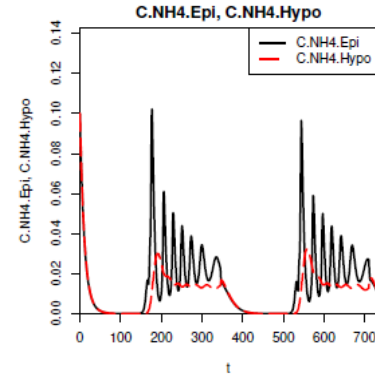
- The function `calcrec` in `ecosim` allows you to choose the method and passes further arguments to `ode (...)`:

```
calcrec(system, method="lsoda", ...)
```

Time to work on Exercise 4

Discuss the results

Process	Substances / Organisms											Rate
	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		
Growth of algae NO ₃ ⁻	-		-	+	1							ρ_{gro,ALG,NO_3^-}
Growth of algae NH ₄ ⁺	-	-		+	1							ρ_{gro,ALG,NH_4^+}
Respiration of algae	+	+		-	-1							$\rho_{resp,ALG}$
Death of algae	0/+	0/+		0/+	-1	$(1-f_i)Y_{ALG,death}$	$f_iY_{ALG,death}$					$\rho_{death,ALG}$
Growth of zooplankton	+	+		-	$\frac{-1}{Y_{ZOO}}$	1	$\frac{(1-f_i)f_e}{Y_{ZOO}}$	$\frac{f_i f_e}{Y_{ZOO}}$				$\rho_{gro,ZOO}$
Respiration of zoopl.	+	+		-	-1							$\rho_{resp,ZOO}$
Death of zooplankton	0/+	0/+		0/+	-1	$(1-f_i)Y_{ZOO,death}$	$f_iY_{ZOO,death}$					$\rho_{death,ZOO}$
Nitrification			-1	+								ρ_{nitri}
Oxic mineral. of org. part.	+	+		-			-1					$\rho_{miner,ox,POMD}$
Ox. min. of org. part. in sed.	+	+		-					-1			$\rho_{miner,ox,SPOMD}$
Anox. min. of org. part. in sed.	+	+		-						-1		$\rho_{miner,anox,SPOMD}$
Sed. of deg. org. part.							-1			1		$\rho_{sed,POMD}$
Sed. of inert org. part.								-1			1	$\rho_{sed,POMI}$



1. Why is it important that some stoichiometric coefficients are indicated as 0/+?

- 1) Allows for conditional release of substances
 - a. For example, during the death of algae, nutrients (like NH_4^+ and HPO_4^{2-}) and oxygen might be released — but not necessarily.
 - b. If they're 0, it means **all organic matter goes to detritus.**
 - c. If they're greater than 0, it means **a portion of organic matter is mineralized.**
 - d. **If they're negative, it means the death process leads to a consumption of nutrients. It's biologically non-sense.**

Substances	Condition of stoichiometric coefficients	Biological meaning
Nutrients (NH_4^+ , HPO_4^{2-}) and Oxygen(O_2)	$v = 0$	All organic matter goes to detritus.
	$v > 0$	A portion of organic matter is mineralized.
	$v < 0$	The death process leads to a consumption of nutrients.

- 2) Helps the model remain mass-balanced under different assumptions

2. How is the metalimnion represented in the model?

- A 'Link' between reactors

```
# Definition of links:

# Exchange between epilimnion and hypolimnion:

metalimnion <-
  new(Class      = "link",
       name      = "Metalimnion",
       from      = "Epi",
       to        = "Hypo",
       qadv.spec = list(C.POMD = expression(v.sed.POM*A),
                        C.POMI = expression(v.sed.POM*A)),
       qdiff.gen = expression(A/h.meta*Kz))
```

Vertical diffusive exchange expression
(depends on the concentration difference
between "Epi" and "Hypo")

Vertical "advective" flow with
sedimentation from epi. to hypo.

Usually advection means with the water
flow, here it just means directed flow
from "Epi" to "Hypo", which just
depends on the concentration in "Epi"

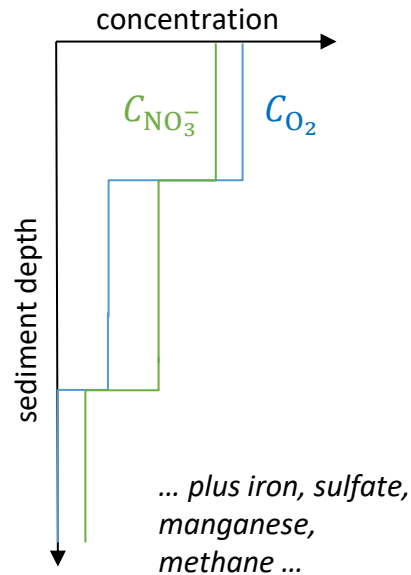
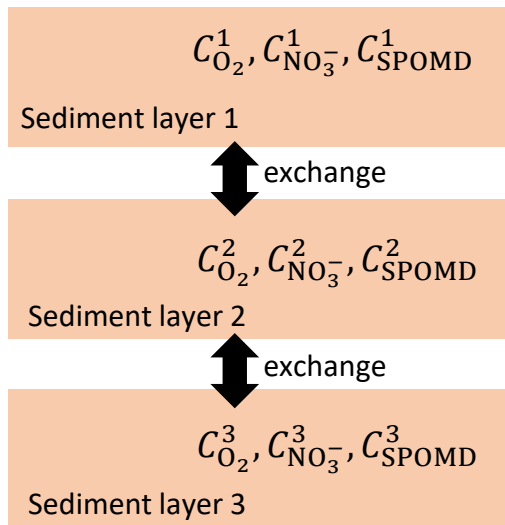
3. How and why do we differentiate oxic and anoxic mineralization ?

In a more realistic model

Sediment is modelled as different discrete/continuous layers/depth, each with its in-situ substance concentrations:

$$\rho_{\text{miner,ox,SPOMD}} = k_{\text{miner,ox}} \cdot f_{\text{temp}}(T) \cdot f_{\text{lim}}(C_{\text{O}_2}) \cdot C_{\text{SPOMD}}$$

$$\rho_{\text{miner,anox,SPOMD}} = k_{\text{miner,anox}} \cdot f_{\text{temp}}(T) \cdot f_{\text{inh}}(C_{\text{O}_2}) \cdot f_{\text{lim}}(C_{\text{NO}_3^-}) \cdot C_{\text{SPOMD}}$$

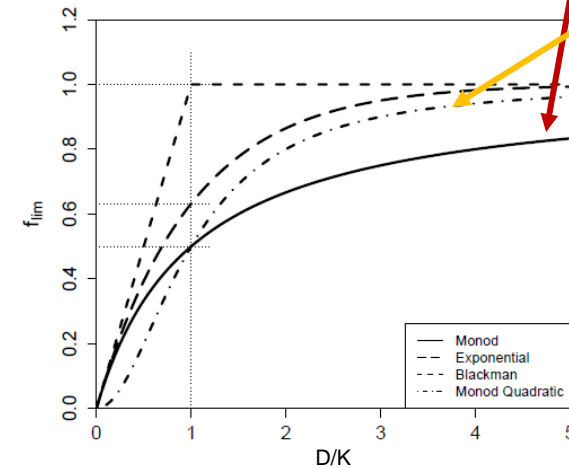


In our two-box model

Sediment is modelled as density of SPOMD at the bottom of the hypolimnion, with substance concentrations of this box:

$$\rho_{\text{miner,ox,SPOMD}} = k_{\text{miner,ox}} \cdot f_{\text{temp}}(T) \cdot f_{\text{lim}}(C_{\text{O}_2}) \cdot \frac{D_{\text{SPOMD}}}{K_{\text{SPOMD,miner}} + D_{\text{SPOMD}}}$$

$$\rho_{\text{miner,anox,SPOMD}} = k_{\text{miner,anox}} \cdot f_{\text{temp}}(T) \cdot f_{\text{lim}}(C_{\text{NO}_3^-}) \cdot \frac{D_{\text{SPOMD}}^2}{K_{\text{SPOMD,miner}}^2 + D_{\text{SPOMD}}^2}$$



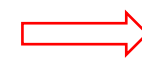
4. Look at the mass balance for P and N. If there is a difference between input and output + accumulation, where does it come from?

```
# Phosphorus mass balance:

nr.days <- (as.numeric(rownames(res.11.4)[nrow(res.11.4)])-as.numeric(rownames(res.11.4)[1]))
nr.steps <- (nrow(res.11.4)-1)

F.in.P <- c(HPO4 = param$Q.in*param$C.HPO4.in*nr.days*86400/1e6)
F.out.P <- c(HPO4 = sum(param$Q.in*res.11.4[, "C.HPO4.Epi"])*nr.days/nr.steps*86400/1e6,
            ALG = sum(param$Q.in*res.11.4[, "C.ALG.Epi"])*param$alpha.P.ALG*
                nr.days/nr.steps*86400/1e6,
            ZOO = sum(param$Q.in*res.11.4[, "C.ZOO.Epi"])*param$alpha.P.ZOO*
                nr.days/nr.steps*86400/1e6,
            POMD = sum(param$Q.in*res.11.4[, "C.POMD.Epi"])*param$alpha.P.POM*
                nr.days/nr.steps*86400/1e6,
            POMI = sum(param$Q.in*res.11.4[, "C.POMI.Epi"])*param$alpha.P.POM*
                nr.days/nr.steps*86400/1e6)

Acc.P <- c(HPO4 = param$A/1e6*
            ((param$h.epi*res.11.4[nrow(res.11.4), "C.HPO4.Epi"]+
              param$h.hypo*res.11.4[nrow(res.11.4), "C.HPO4.Hypo"])-
              (param$h.epi*res.11.4[1, "C.HPO4.Epi"]+
               param$h.hypo*res.11.4[1, "C.HPO4.Hypo"])),
            ALG = param$A/1e6*param$alpha.P.ALG*
            ((param$h.epi*res.11.4[nrow(res.11.4), "C.ALG.Epi"]+
              param$h.hypo*res.11.4[nrow(res.11.4), "C.ALG.Hypo"])-
              (param$h.epi*res.11.4[1, "C.ALG.Epi"]+
               param$h.hypo*res.11.4[1, "C.ALG.Hypo"])),
            ZOO = param$A/1e6*param$alpha.P.ZOO*
            ((param$h.epi*res.11.4[nrow(res.11.4), "C.ZOO.Epi"]+
              param$h.hypo*res.11.4[nrow(res.11.4), "C.ZOO.Hypo"])-
              (param$h.epi*res.11.4[1, "C.ZOO.Epi"]+
               param$h.hypo*res.11.4[1, "C.ZOO.Hypo"])),
```



Run this part of the script to get the average mass fluxes of P and N (input, output and accumulation) (see Table 11.11)



Flux	Substances	Phosphorus (t/a)	Nitrogen (t/a)
Input	HPO ₄ ²⁻ , NO ₃ ⁻	12.6	158
Output	HPO ₄ ²⁻ , NO ₃ ⁻ , NH ₄ ⁺ ALG, ZOO, POMD, POMI	9.3 1.2	127 11.5
Accumulation	HPO ₄ ²⁻ , NO ₃ ⁻ , NH ₄ ⁺ ALG, ZOO, POMD, POMI SPOMD SPOMI	1.2 0.0 0.0 1.0	-7.4 0.1 0.2 8.6
Loss	Denitrification of NO ₃ ⁻	0.0	18.0

...

Work on your own model

- If you didn't tell us yet which model you chose, it's time to do it!
Team up with someone, choose a topic and inform us which one you picked.
- Read the assignment carefully and start thinking about how to modify today's model 11.4.
- Don't hesitate to ask questions !

Recap of today's exercise

- Simulate algae-zooplankton lake dynamics with a two-box model
- Introduce physical processes into the model (horizontal & vertical)
- Learn the seasonal variation in a lake with the two-box model

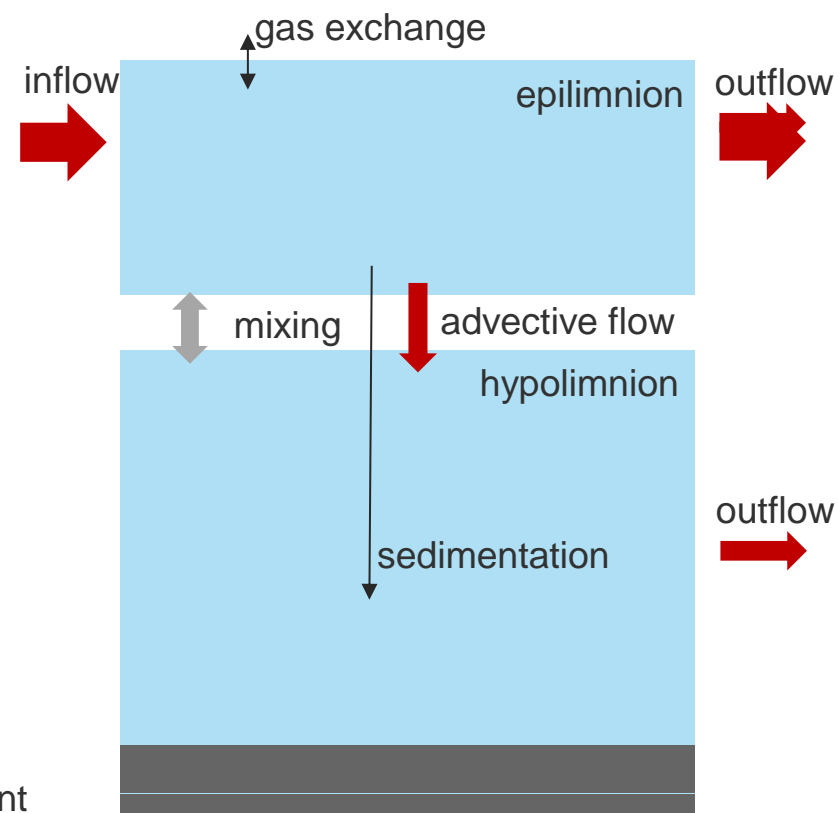
Topic 1: scenarios for phosphorus reduction in a lake: extraction of deep water and reduction of inflow

Motivation

Assess management scenarios to reduce eutrophication of a lake

Assignment

- Start from model 11.4
- Add a deep water extraction (outflow from hypolimnion)
- Investigate the following scenarios separately:
 1. Reduction of the inflow concentration of phosphorus by 50%
 2. deep water extraction: 50% of the inflow leaves the lake from hypolimnion (volume stays constant)
- Analyse the effect of both measures with a small or a large deposit of POMD in the sediment



Goal: Compare the effectiveness of different management scenarios for different sediment conditions and estimate how long it will take to see the effects.

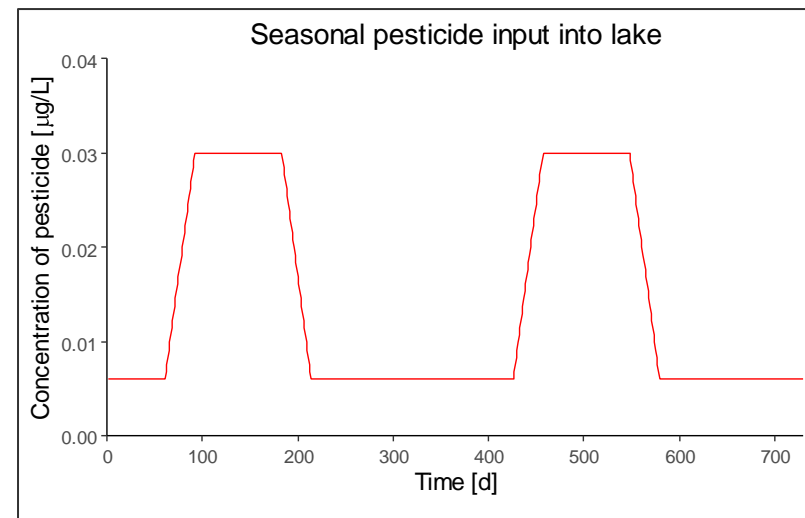
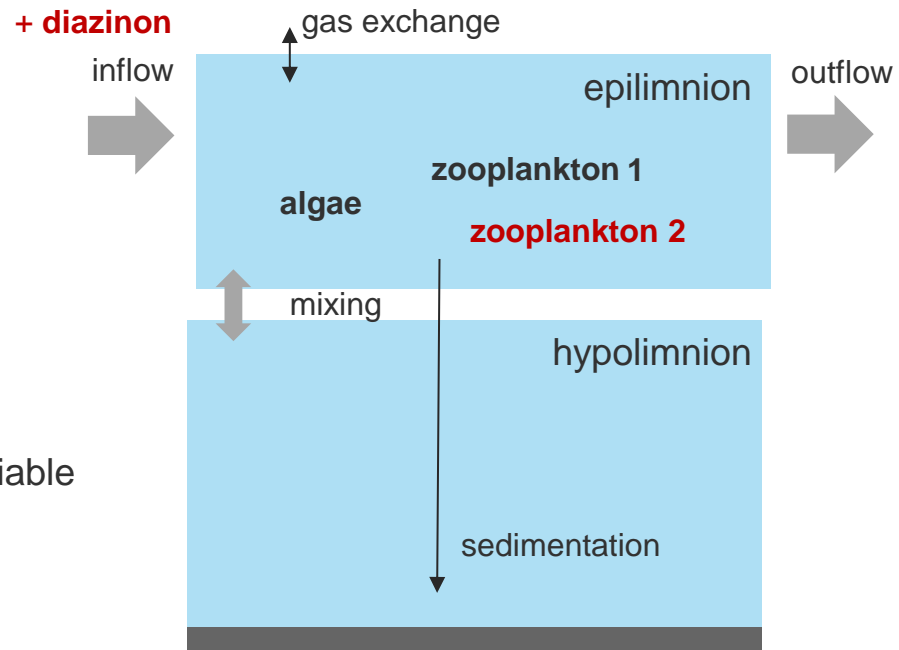
Motivation

Simulate effects of micropollutants
and analyze coexistence of multiple groups

Assignment

- start from model 11.4
- introduce an insecticide (diazinon) as state variable
- introduce two zooplankton groups differing in
 - half-saturation constant for food limitation
 - sensitivity towards insecticide

Goal: Try to achieve long-term coexistence
between the two zooplankton groups
by varying the parameters



Motivation

Simulate effects of temperature change scenarios.

Assignment

- start from model 11.4
- implement three different temperature scenarios
- change the temperature dependence of the growth rate of zoo plankton

Goal: Analyze the effects of the scenarios on zooplankton and the other state variables and reflect about how realistic the results are.

