Exercise 4

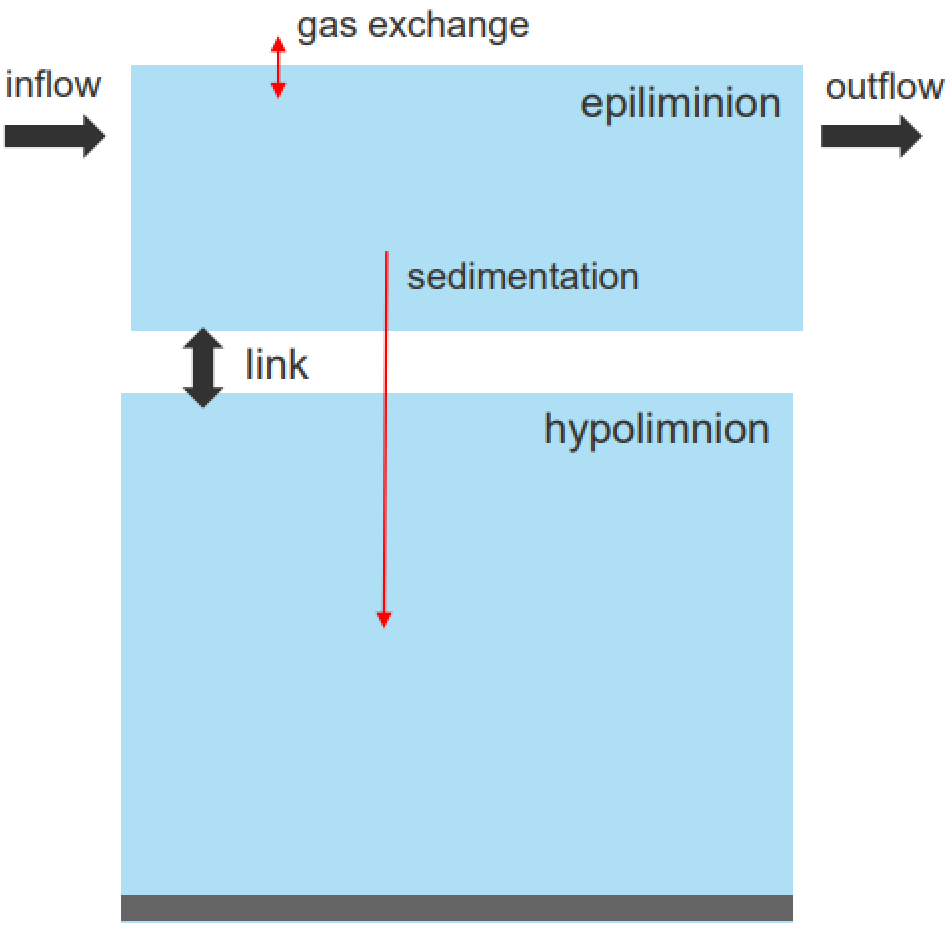
Modelling Aquatic Ecosystems FS25

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
  - Stratification
  - Horizontal mixing
  - 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

One box model

5. Define the system
(one reactor-
Epilimnion)

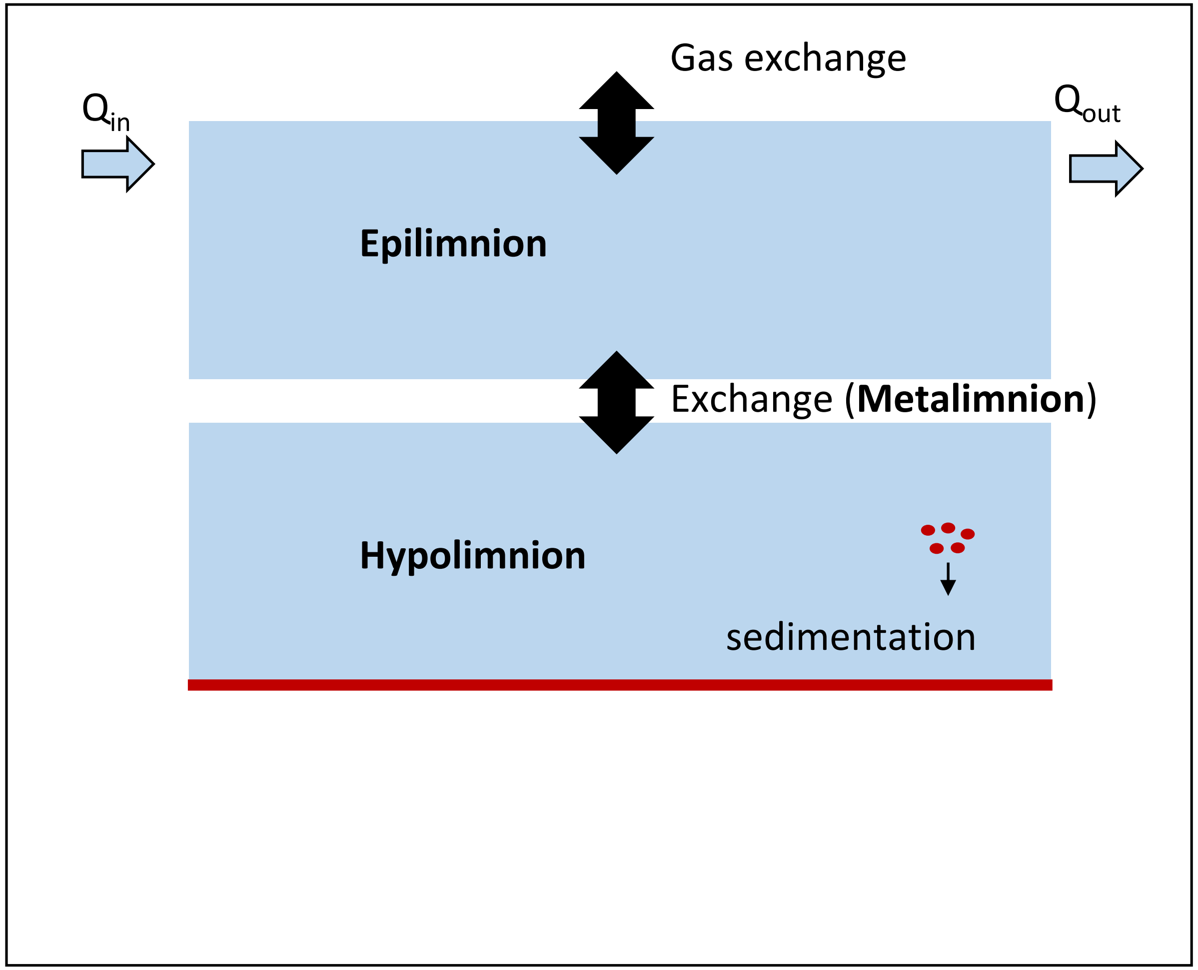
1. Define parameters
2. Calculate stoichiometric coefficients
3. Define processes
4. Define time-dependent conditions
6. Perform calculations

Two box model

5. Define the system
(two reactors
Epilimnion & Hypolimnion
+ one link
Metalimnion)

Two box biogeochemical-ecological lake model

Physical Representation



Biogeochem/ecological processes:

1. Growth, death, respiration: ALG, ZOO
2. Nitrification
3. Mineralization: oxic, anoxic
4. Sedimentation: degradable, inert

Consider the following env. factors:

1. Temperature
2. Light intensity
3. Seasonality of physical parameters; Exchange summer vs. winter

Process rate expressions

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						$\rho_{\mathrm{gro,ALG,NO_3^-}}$
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	$+$	$+$		$-$	$\frac{-1}{Y_{\mathrm{ZOO}}}$	1	$\frac{(1-f_{\mathrm{I}})f_{\mathrm{e}}}{Y_{\mathrm{ZOO}}}$	$\frac{f_{\mathrm{I}}f_{\mathrm{e}}}{Y_{\mathrm{ZOO}}}$			$\rho_{\mathrm{gro,ZOO}}$
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	$NH_4^+ + 2O_2 \rightarrow NO_3^- + 2H^+ + H_2O$										ρ_{nitri}
Oxic mineral. of org. part.	$POMD + O_2 \rightarrow NH_4^+ + HPO_4^{2-} + CO_2 + H_2O$										$\rho_{\mathrm{miner,ox,POMD}}$
Ox. min. of org. part. in sed.	$SPOMD + O_2 \rightarrow NH_4^+ + HPO_4^{2-} + CO_2 + H_2O$										$\rho_{\mathrm{miner,ox,SPOMD}}$
Anox. min. of org. part. in sed.	$SPOMD + NO_3^- \rightarrow NH_4^+ + HPO_4^{2-} + CO_2 + H_2O$										$\rho_{\mathrm{miner,anox,SPOMD}}$
Sed. of deg. org. part.	$POMD \rightarrow SPOMD$										$\rho_{\mathrm{sed,POMD}}$
Sed. of inert org. part.	$POMI \rightarrow SPOMI$										$\rho_{\mathrm{sed,POMI}}$

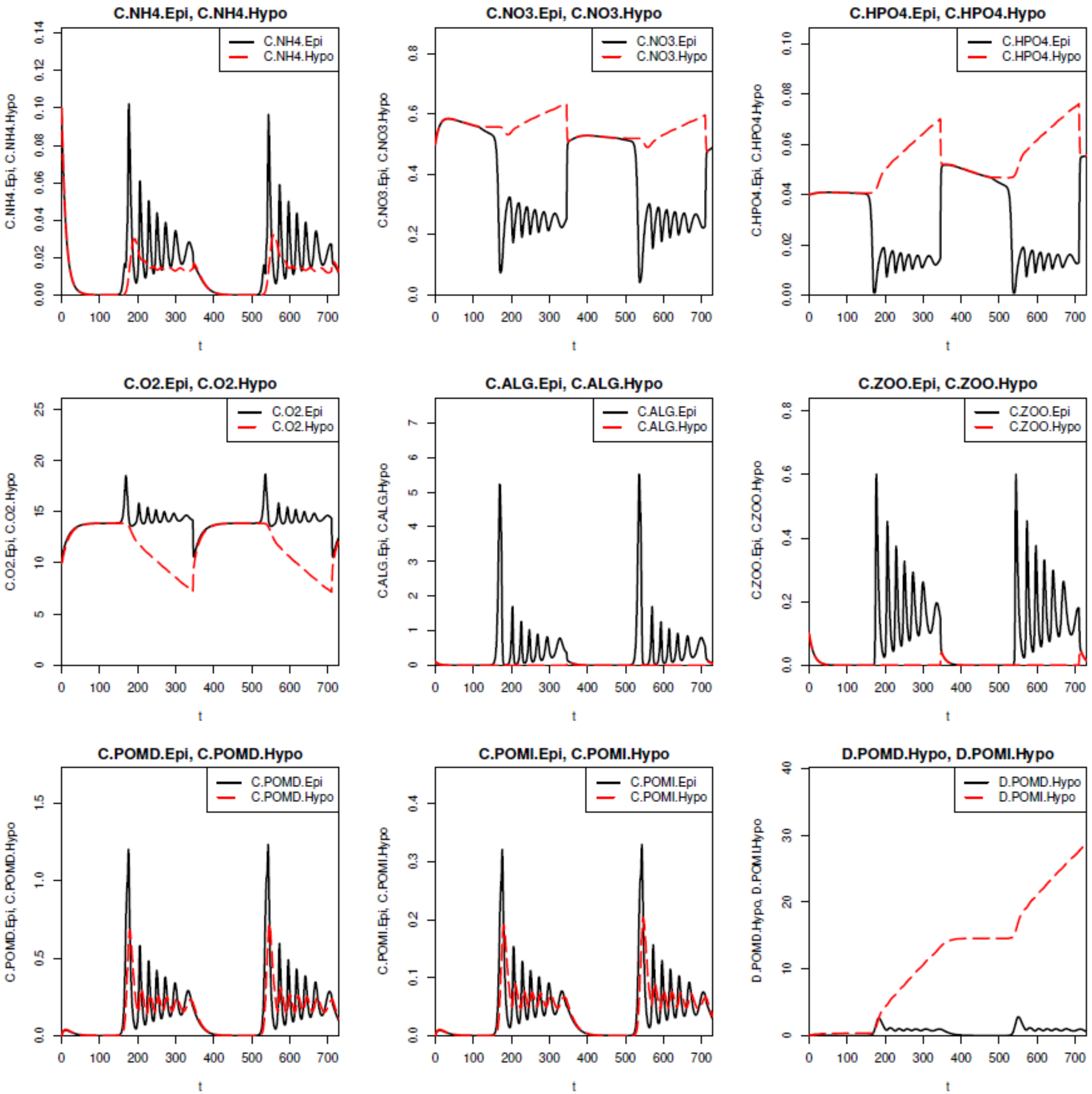
Rate	Rate expression
$\rho_{\mathrm{gro,ALG,NH_4^+}}$	$k_{\mathrm{gro,ALG},T_0}\cdot\exp\left(\beta_{\mathrm{ALG}}(T-T_0)\right)\cdot\frac{1}{\lambda h}\log\left(\frac{K_I+I_0}{K_I+I_0\exp(-\lambda h)}\right)\cdot\min\left(\frac{C_{\mathrm{HPO_4^{2-}}}}{K_{\mathrm{HPO_4^{2-},ALG}}+C_{\mathrm{HPO_4^{2-}}}},\frac{C_{\mathrm{NH_4^+}}+C_{\mathrm{NO_3^-}}}{K_{\mathrm{N,ALG}}+C_{\mathrm{NH_4^+}}+C_{\mathrm{NO_3^-}}}\right)\cdot\frac{p_{\mathrm{NH_4^+}}C_{\mathrm{NH_4^+}}}{p_{\mathrm{NH_4^+}}C_{\mathrm{NH_4^+}}+C_{\mathrm{NO_3^-}}}\cdot C_{\mathrm{ALG}}$
$\rho_{\mathrm{gro,ALG,NO_3^-}}$	$k_{\mathrm{gro,ALG},T_0}\cdot\exp\left(\beta_{\mathrm{ALG}}(T-T_0)\right)\cdot\frac{1}{\lambda h}\log\left(\frac{K_I+I_0}{K_I+I_0\exp(-\lambda h)}\right)\cdot\min\left(\frac{C_{\mathrm{HPO_4^{2-}}}}{K_{\mathrm{HPO_4^{2-},ALG}}+C_{\mathrm{HPO_4^{2-}}}},\frac{C_{\mathrm{NH_4^+}}+C_{\mathrm{NO_3^-}}}{K_{\mathrm{N,ALG}}+C_{\mathrm{NH_4^+}}+C_{\mathrm{NO_3^-}}}\right)\cdot\frac{C_{\mathrm{NO_3^-}}}{p_{\mathrm{NH_4^+}}C_{\mathrm{NH_4^+}}+C_{\mathrm{NO_3^-}}}\cdot C_{\mathrm{ALG}}$
$\rho_{\mathrm{resp,ALG}}$	$k_{\mathrm{resp,ALG},T_0}\cdot\exp\left(\beta_{\mathrm{ALG}}(T-T_0)\right)\cdot\frac{C_{\mathrm{O_2}}}{K_{\mathrm{O_2,ALG}}+C_{\mathrm{O_2}}}\cdot C_{\mathrm{ALG}}$
$\rho_{\mathrm{death,ALG}}$	$k_{\mathrm{death,ALG}}\cdot C_{\mathrm{ALG}}$
$\rho_{\mathrm{gro,ZOO}}$	$k_{\mathrm{gro,ZOO},T_0}\cdot\exp\left(\beta_{\mathrm{ZOO}}(T-T_0)\right)\cdot\frac{C_{\mathrm{O_2}}}{K_{\mathrm{O_2,ZOO}}+C_{\mathrm{O_2}}}\cdot C_{\mathrm{ALG}}\cdot C_{\mathrm{ZOO}}$
$\rho_{\mathrm{resp,ZOO}}$	$k_{\mathrm{resp,ZOO},T_0}\cdot\exp\left(\beta_{\mathrm{ZOO}}(T-T_0)\right)\cdot\frac{C_{\mathrm{O_2}}}{K_{\mathrm{O_2,ZOO}}+C_{\mathrm{O_2}}}\cdot C_{\mathrm{ZOO}}$
$\rho_{\mathrm{death,ZOO}}$	$k_{\mathrm{death,ZOO}}\cdot C_{\mathrm{ZOO}}$
ρ_{nitri}	$k_{\mathrm{nitri},T_0}\cdot\exp\left(\beta_{\mathrm{BAC}}(T-T_0)\right)\cdot\min\left(\frac{C_{\mathrm{NH_4^+}}}{K_{\mathrm{NH_4^+,nitri}}+C_{\mathrm{NH_4^+}}},\frac{C_{\mathrm{O_2}}}{K_{\mathrm{O_2,nitri}}+C_{\mathrm{O_2}}}\right)$
$\rho_{\mathrm{miner,ox,POMD}}$	$k_{\mathrm{miner,ox,POMD},T_0}\cdot\exp\left(\beta_{\mathrm{BAC}}(T-T_0)\right)\cdot\frac{C_{\mathrm{O_2}}}{K_{\mathrm{O_2,miner}}+C_{\mathrm{O_2}}}\cdot C_{\mathrm{POMD}}$
$\rho_{\mathrm{miner,ox,SPOMD}}$	$k_{\mathrm{miner,ox,SPOMD},T_0}\cdot\exp\left(\beta_{\mathrm{BAC}}(T-T_0)\right)\cdot\frac{C_{\mathrm{O_2}}}{K_{\mathrm{O_2,miner}}+C_{\mathrm{O_2}}}\cdot\frac{D_{\mathrm{SPOMD}}}{K_{\mathrm{SPOM,miner,sed}}+D_{\mathrm{SPOMD}}}$
$\rho_{\mathrm{miner,anox,SPOMD}}$	$k_{\mathrm{miner,anox,SPOMD},T_0}\cdot\exp\left(\beta_{\mathrm{BAC}}(T-T_0)\right)\cdot\frac{C_{\mathrm{NO_3^-}}}{K_{\mathrm{NO_3^-,miner}}+C_{\mathrm{NO_3^-}}}\cdot\left(\frac{D_{\mathrm{SPOMD}}}{K_{\mathrm{SPOM,miner,sed}}+D_{\mathrm{SPOMD}}}\right)^2$
$\rho_{\mathrm{sed,POMD}}$	$\frac{v_{\mathrm{sed,POM}}}{h_{\mathrm{hypo}}}\cdot C_{\mathrm{POMD}}$
$\rho_{\mathrm{sed,POMI}}$	$\frac{v_{\mathrm{sed,POM}}}{h_{\mathrm{hypo}}}\cdot C_{\mathrm{POMI}}$

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

Time to work on Exercise 4

Discuss the results

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	+	+		−	$\frac{-1}{Y_{\mathrm{ZOO}}}$	1	$\frac{(1-f_\mathrm{I})f_\mathrm{e}}{Y_{\mathrm{ZOO}}}$	$\frac{f_\mathrm{I}f_\mathrm{e}}{Y_{\mathrm{ZOO}}}$			$\rho_{\mathrm{gro,ZOO}}$
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	$\rho_{\mathrm{sed,POMI}}$



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)	$\nu = 0$	All organic matter goes to detritus.
	$\nu > 0$	A portion of organic matter is mineralized.
	$\nu < 0$	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 advective flow with sedimentation from epi. to hypo.

Vertical diffusive flow expression

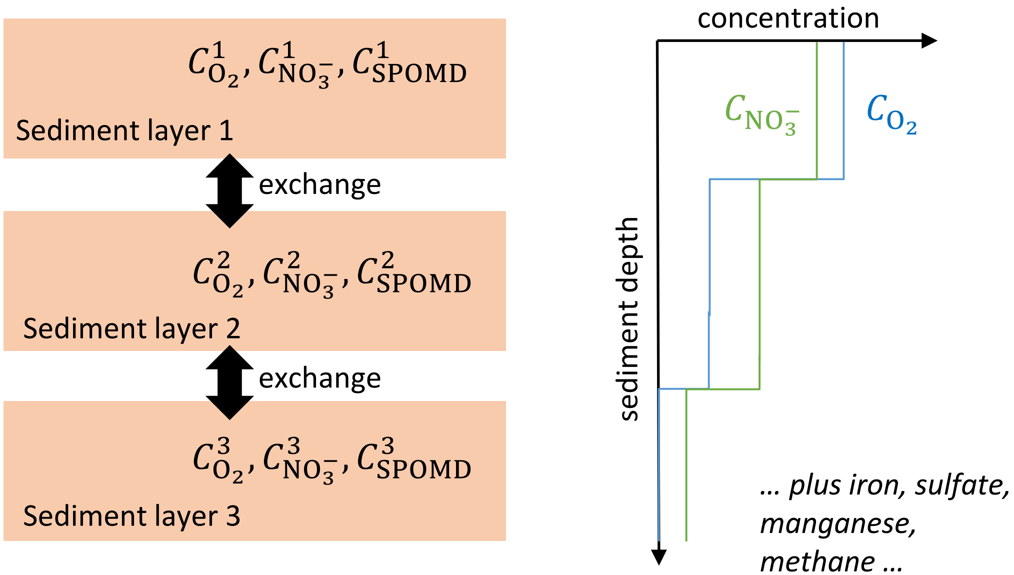
3. How and why do we differentiate oxic and anoxic mineralization ?

In a more realistic model

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

$$\rho_{\text{miner,ox,SPOMD}} = k_{\text{miner,ox}} \cdot f_{\text{temp}}(T) \cdot f_{\text{lim}}(C_{O_2}) \cdot C_{\text{SPOMD}}$$

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

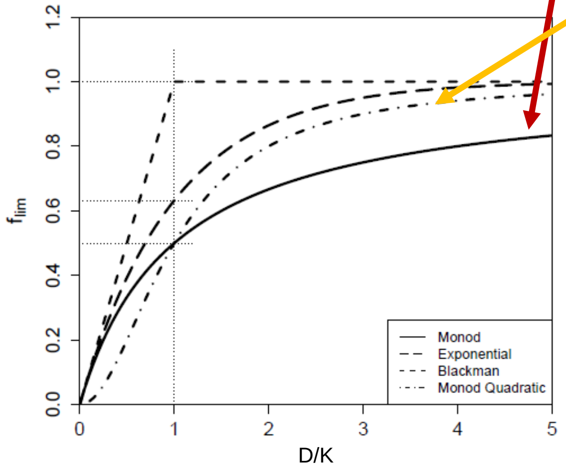


In our two-box model

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

$$\rho_{\text{miner,ox,SPOMD}} = k_{\text{miner,ox}} \cdot f_{\text{temp}}(T) \cdot f_{\text{lim}}(C_{O_2}) \cdot \boxed{\frac{D_{\text{SPOMD}}}{K_{\text{SPOMD,miner}} + D_{\text{SPOMD}}}}$$

$$\rho_{\text{miner,anox,SPOMD}} = k_{\text{miner,anox}} \cdot f_{\text{temp}}(T) \cdot f_{\text{lim}}(C_{NO_3^-}) \cdot \boxed{\frac{D^2_{\text{SPOMD}}}{K^2_{\text{SPOMD},mner} + D^2_{\text{SPOMD}}}}$$



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^+	**9.3**	**127**
	ALG, ZOO, POMD, POMI	1.2	11.5
Accumulation	HPO_4^{2-}, NO_3^-, NH_4^+	**1.2**	**-7.4**
	ALG, ZOO, POMD, POMI	0.0	0.1
	SPOMD	0.0	0.2
	SPOMI	1.0	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 !