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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

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. 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

- Review exercise 4 (chapter 11.4)
- Learn how to model the growth of bacteria (chapter 8.8)
- Know the most important transport and mixing processes in rivers and how to implement them in a model (6.1.2)
- Preview River Models (11.5-11.6)

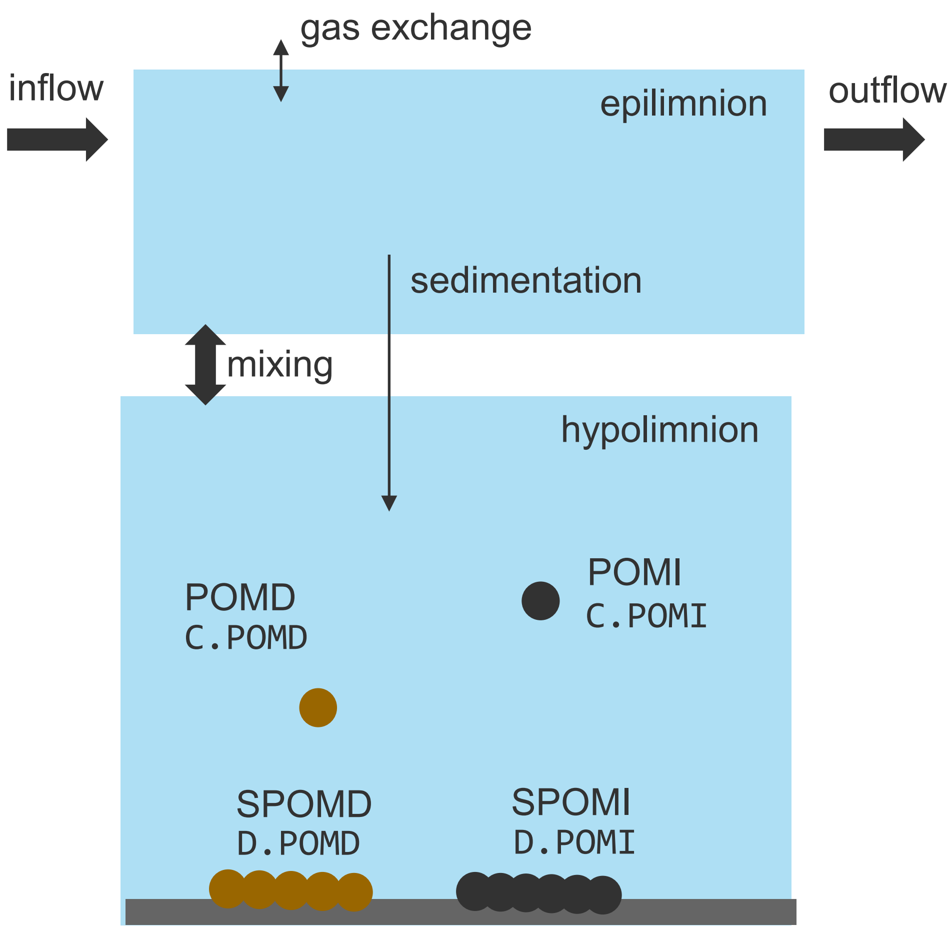
Base Model 11.4

State variables:

ALG, ZOO,

HPO_4^{2-}, NH_4^+, NO_3^-, O_2,

POM: inert/degradable,
suspended/sedimented



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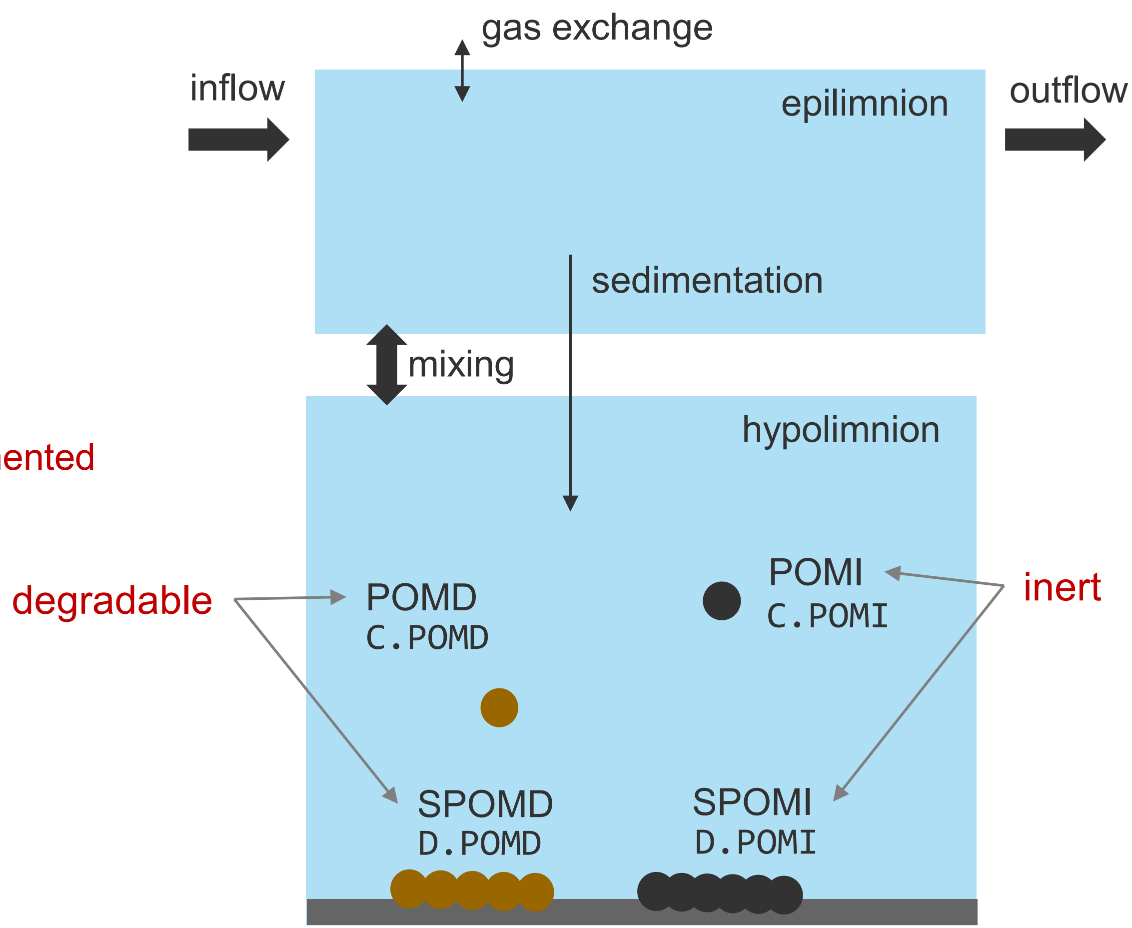

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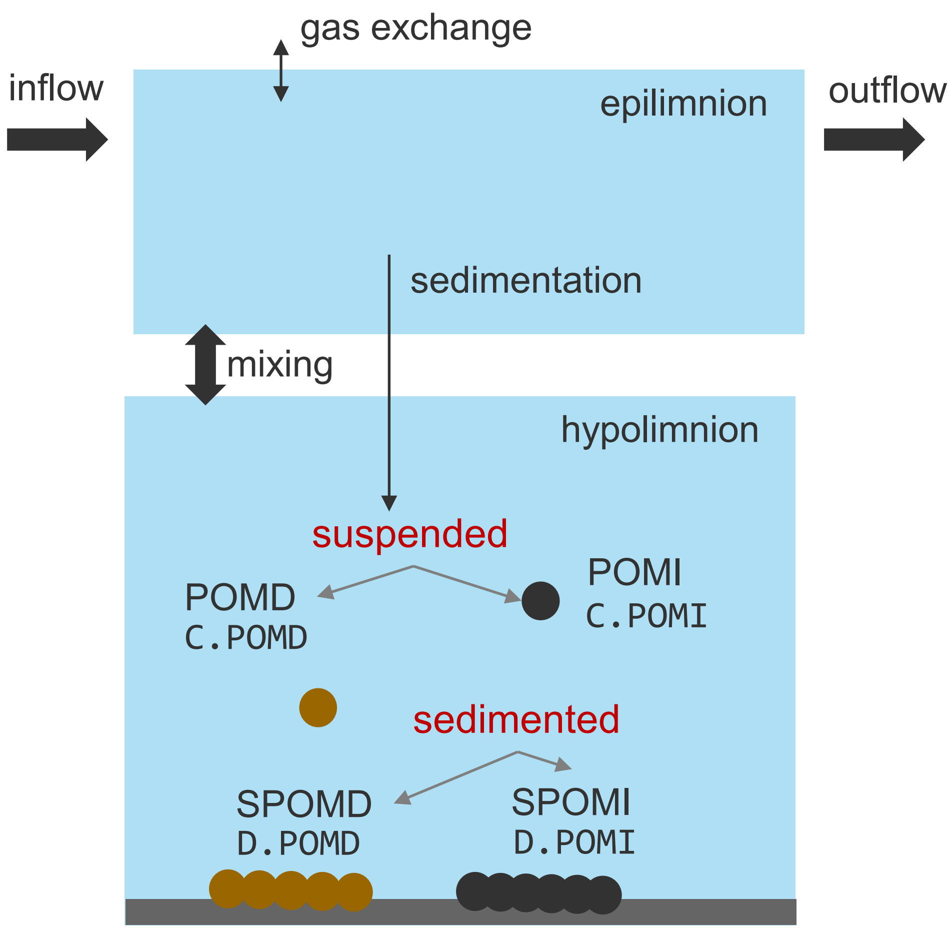
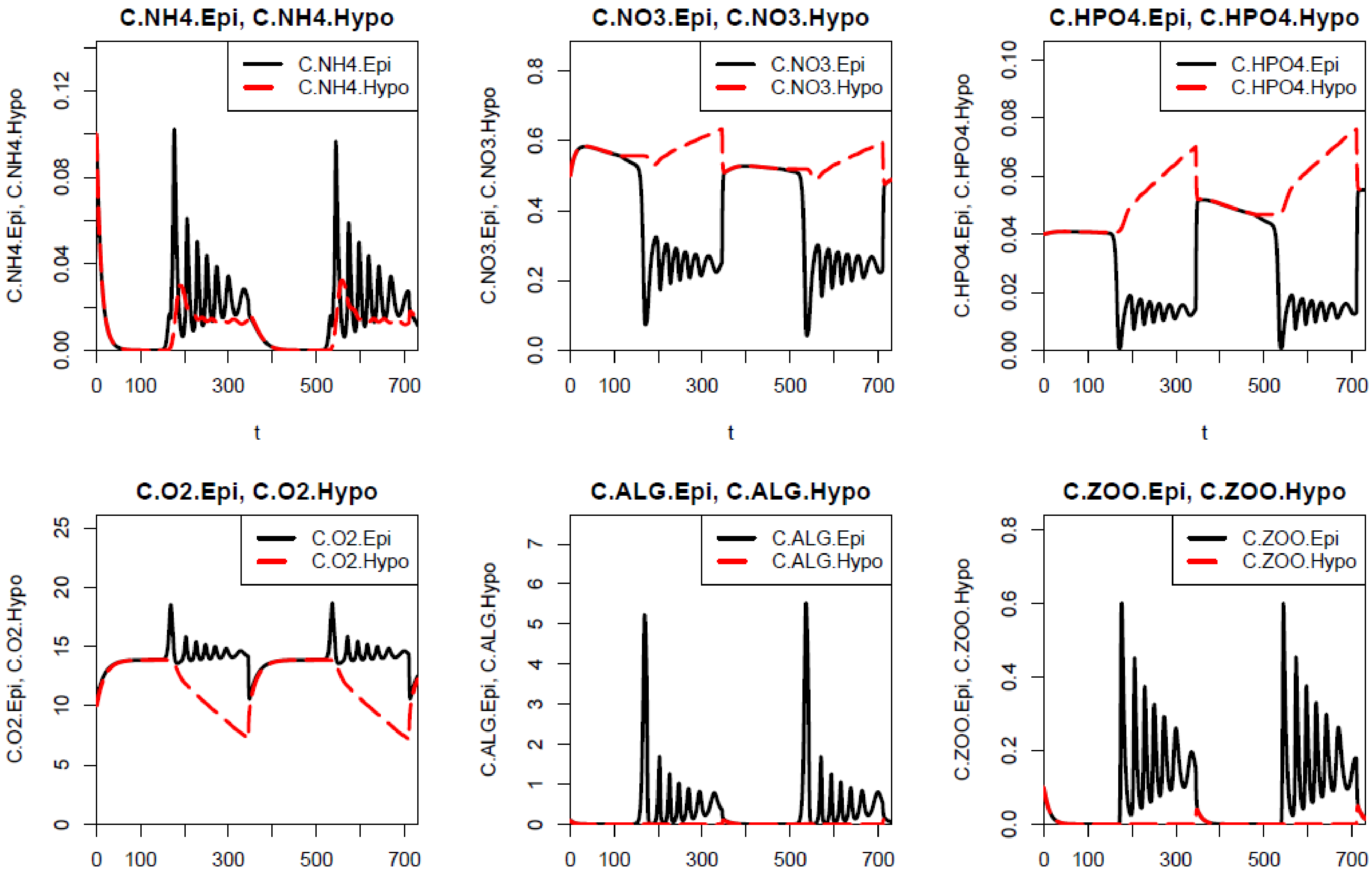


Review Exercise 4

Process	Substances / Organisms									
	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					
Growth of algae NH_4^+	$-$	$-$		$+$	1					
Respiration of algae	$+$	$+$		$-$	-1					
Death of algae	$0/+$	$0/+$		$0/+$	-1		$(1-f_I)Y_{ALG,death}$	$f_I Y_{ALG,death}$		
Growth of zooplankton	$+$	$+$		$-$	$\frac{-1}{Y_{ZOO}}$	1	$\frac{(1-f_I)f_e}{Y_{ZOO}}$	$\frac{f_I f_e}{Y_{ZOO}}$		
Respiration of zoopl.	$+$	$+$		$-$		-1				
Death of zooplankton	$0/+$	$0/+$		$0/+$		-1	$(1-f_I)Y_{ZOO,death}$	$f_I Y_{ZOO,death}$		
Nitrification		-1	$+$	$-$						
Oxic mineral. of org. part.	$+$	$+$		$-$			-1			
Ox. min. of org. part. in sed.	$+$	$+$		$-$					-1	
Anox. min. of org. part. in sed.	$+$	$+$	$-$						-1	
Sed. of deg. org. part.							-1		1	
Sed. of inert org. part.								-1		1

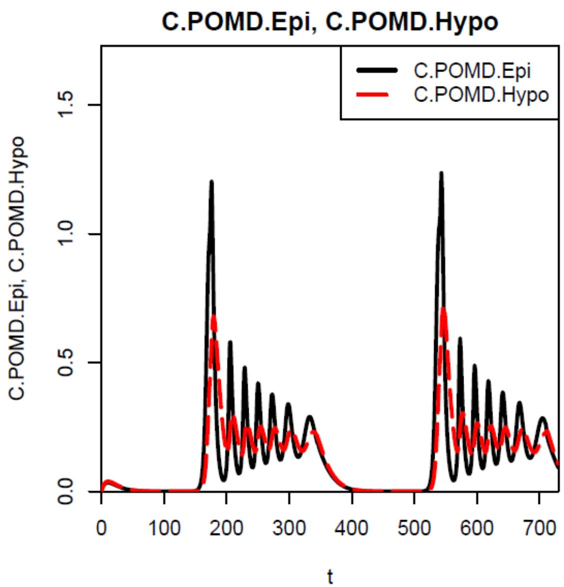
Review Exercise 4



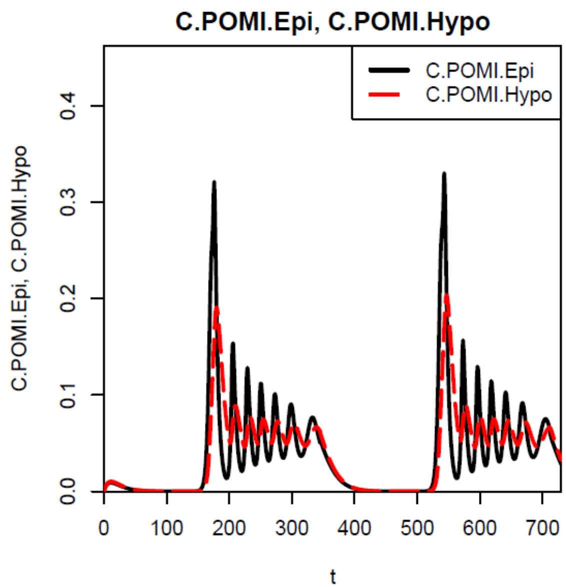
Review Exercise 4

suspended

degradable

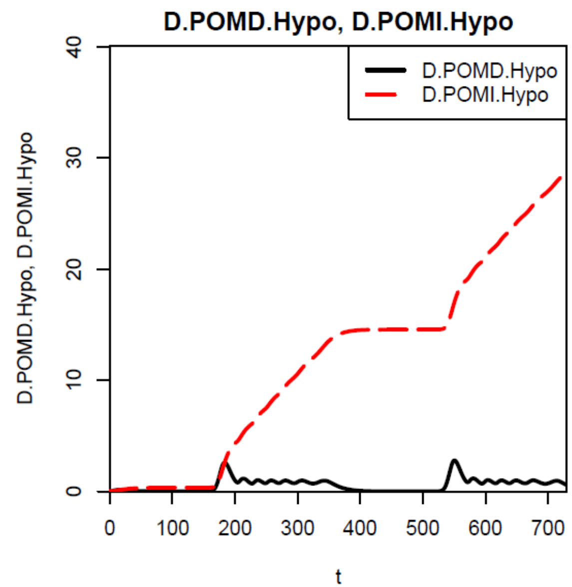


inert



sedimented

degradable / inert



Review Exercise 4

Questions to think about:

- Why is it important that some stoichiometric coefficients are defined as $0/+$?
- How is the metalimnion represented by the model?
- Look at the process rates of mineralization in the sediment. Why are they different than in chapter 8.5?

- Look at the mass balance for P and N. If there is a difference between input and output + accumulation, where does it come from?
Hint: Have a look at the stoichiometric coefficients for anoxic mineralization

Review Exercise 4

Questions to think about:

- How is the metalimnion represented by the model?

```
# 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))
```

Review Exercise 4

- Look at the process rates of mineralization in the sediment. Why are they different than in chapter 8.5?

see p. 186f

chapter 8.5

$$\rho_{\mathrm{miner,ox,POM}} = k_{\mathrm{miner,ox,POM},T_0} \cdot \exp\Big(\beta_{\mathrm{BAC}}(T - T_0)\Big) \cdot \frac{C_{\mathrm{O_2}}}{K_{\mathrm{O_2,miner}} + C_{\mathrm{O_2}}} \cdot C_{\mathrm{POM}}$$

$$\rho_{\mathrm{miner,anox,POM}} = k_{\mathrm{miner,anox,POM,T0}} \cdot \exp\Big(\beta_{\mathrm{BAC}}(T - T_0)\Big) \cdot \frac{K_{\mathrm{O_2,miner}}}{K_{\mathrm{O_2,miner}} + C_{\mathrm{O_2}}} \cdot \frac{C_{\mathrm{NO_3^-}}}{K_{\mathrm{NO_3^-,miner}} + C_{\mathrm{NO_3^-}}} \cdot C_{\mathrm{POM}}$$

Model 11.4

$$\begin{array}{l|l}
\rho_{\mathrm{miner,ox,SPOMD}} & k_{\mathrm{miner,ox,SPOMD},T_0} \cdot \exp\Big(\beta_{\mathrm{BAC}}(T - T_0)\Big) \cdot \dfrac{C_{\mathrm{O_2}}}{K_{\mathrm{O_2,miner}} + C_{\mathrm{O_2}}} \cdot \dfrac{D_{\mathrm{SPOMD}}}{K_{\mathrm{SPOM,miner,sed}} + D_{\mathrm{SPOMD}}} \\
\rho_{\mathrm{miner,anox,SPOMD}} & k_{\mathrm{miner,anox,SPOMD},T_0} \cdot \exp\Big(\beta_{\mathrm{BAC}}(T - T_0)\Big) \cdot \dfrac{C_{\mathrm{NO_3^-}}}{K_{\mathrm{NO_3^-,miner}} + C_{\mathrm{NO_3^-}}} \cdot \left(\dfrac{D_{\mathrm{SPOMD}}}{K_{\mathrm{SPOM,miner,sed}} + D_{\mathrm{SPOMD}}}\right)^2
\end{array}$$

Review Exercise 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?
  Hint: Have a look at the stoichiometric coefficients for anoxic mineralization

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**
difference in concentrations or densities between the end and start of the simulations	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**

Review Exercise 4

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- Look at the mass balance for P and N. If there is a difference between input and output + accumulation, where does it come from? *Hint*: Have a look at the stoichiometric coefficients for anoxic mineralization

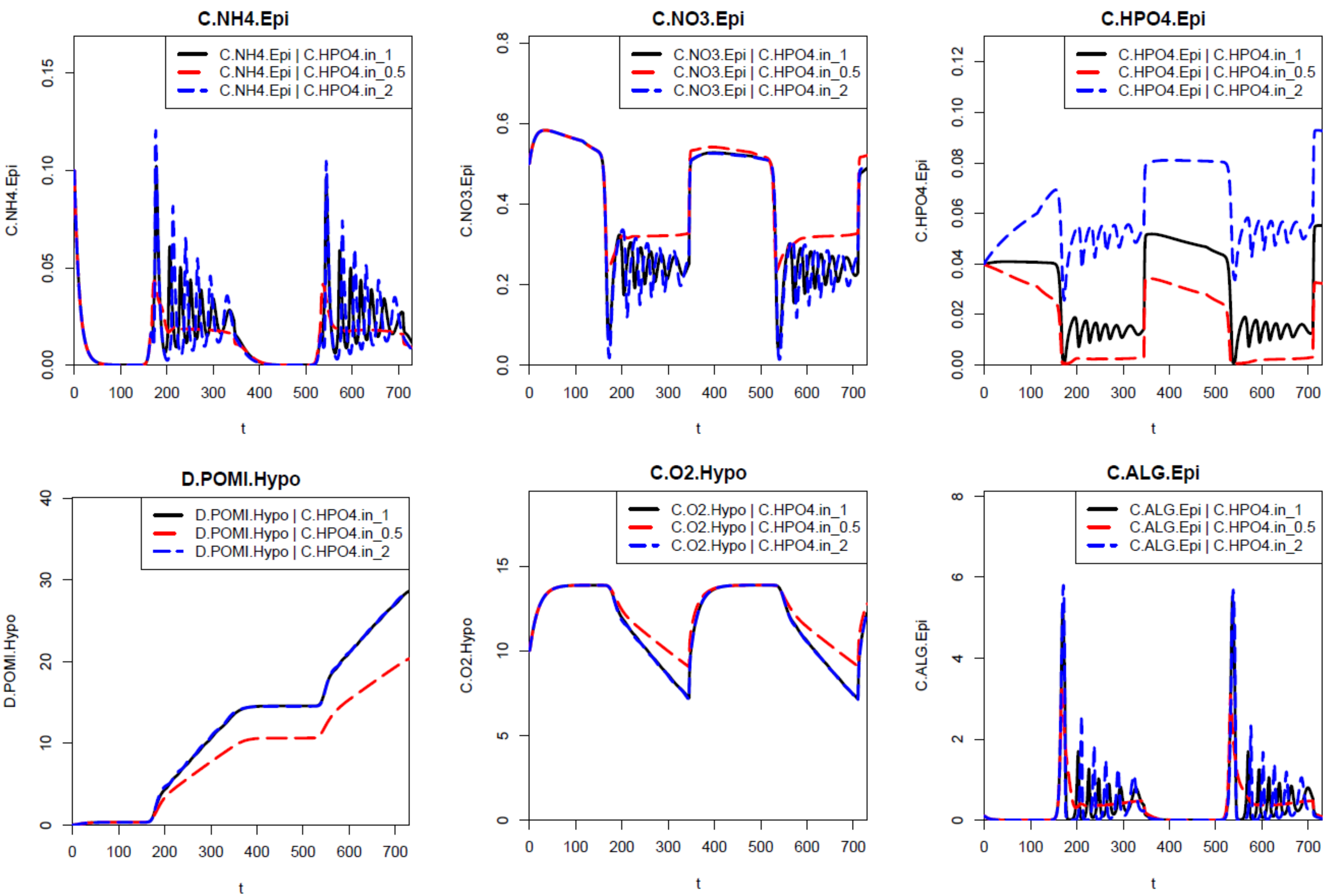
Process	Substances / Organisms								Rate
	NH_4^+	NO_3^-	N_2	HPO_4^{2-}	HCO_3^-	H^+	H_2O	POM	
	gN	gN	gN	gP	gC	mol	mol	gDM	
Anoxic miner.	+	−	+	+	+	?	?	−1	$\rho_{\text{miner,anox,POM}}$

Table 8.6: Process table of anoxic mineralization.

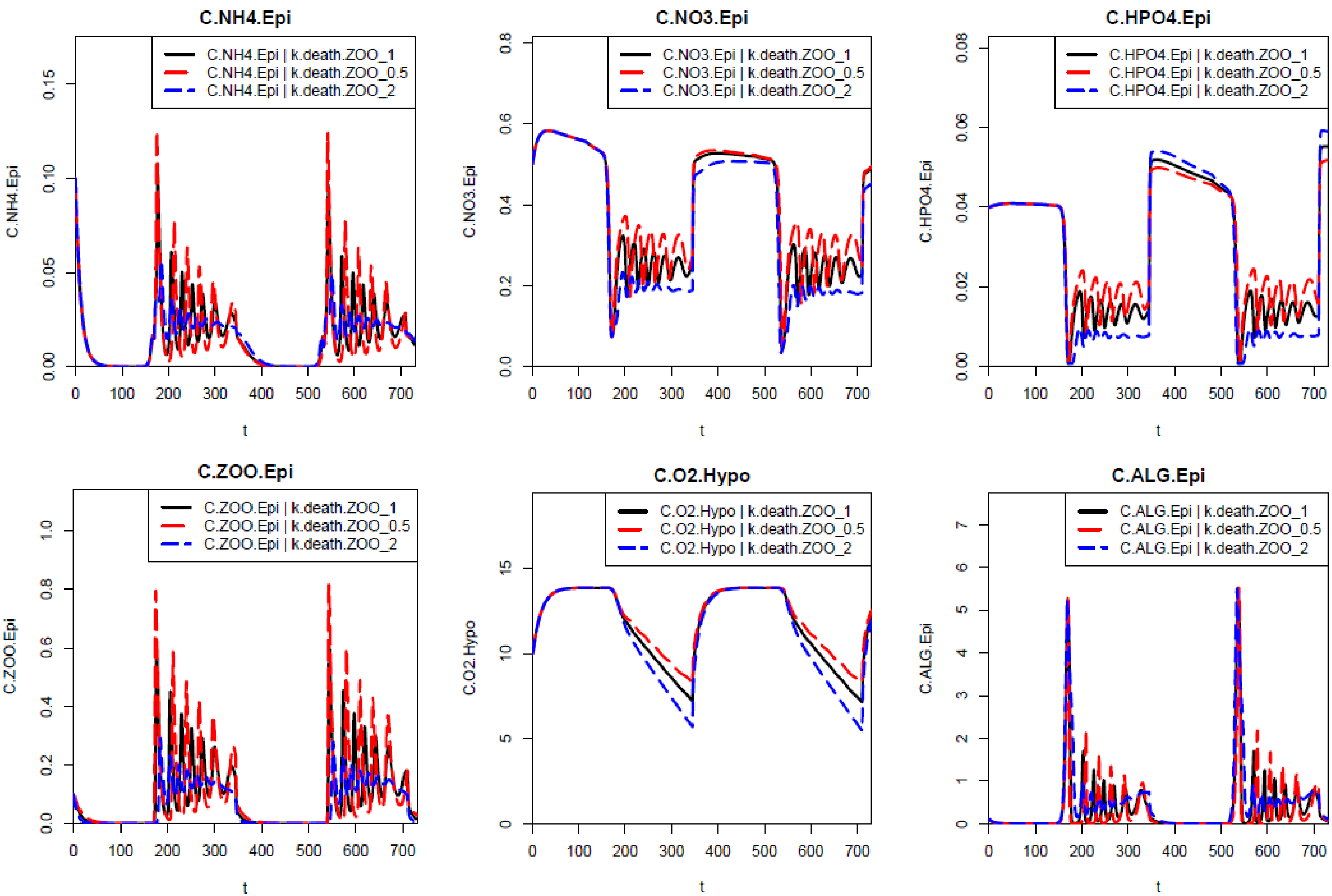
```
> print(round(nu,3))
```

	C.NH4	C.NO3	C.N2	C.HPO4	C.HCO3	C.O2	C.H	C.H2O	C.ALG	C.ZOO	C.POMD	D.POMD	C.POMI	D.POMI
gro.ALG.NH4	-0.060	0.000	0.000	-0.005	-0.365	0.937	-0.026	0.002	1	0	0.000	0	0.000	0
gro.ALG.NO3	0.000	-0.060	0.000	-0.005	-0.365	1.211	-0.035	-0.002	1	0	0.000	0	0.000	0
resp.ALG	0.060	0.000	0.000	0.005	0.365	-0.937	0.026	-0.002	-1	0	0.000	0	0.000	0
death.ALG	0.017	0.000	0.000	0.000	0.027	0.018	0.001	0.006	-1	0	0.571	0	0.143	0
gro.ZOO	0.180	0.000	0.000	0.008	0.992	-2.417	0.070	0.003	-5	1	0.800	0	0.200	0
resp.ZOO	0.060	0.000	0.000	0.010	0.360	-0.930	0.026	-0.002	0	-1	0.000	0	0.000	0
death.ZOO	0.014	0.000	0.000	0.005	0.000	0.088	-0.001	0.007	0	-1	0.609	0	0.152	0
nitri	-1.000	1.000	0.000	0.000	0.000	-4.571	0.143	0.071	0	0	0.000	0	0.000	0
miner.ox.POM	0.060	0.000	0.000	0.007	0.473	-1.338	0.036	-0.011	0	0	-1.000	0	0.000	0
miner.ox.POM.sed	0.060	0.000	0.000	0.007	0.473	-1.338	0.036	-0.011	0	0	0.000	-1	0.000	0
miner.anox.POM.sed	0.060	-0.468	0.468	0.007	0.473	0.000	0.002	0.006	0	0	0.000	-1	0.000	0
sed.POMD	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0	0	-1.000	1	0.000	0
sed.POMI	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0	0	0.000	0	-1.000	1

Sensitivity Analysis



Sensitivity Analysis



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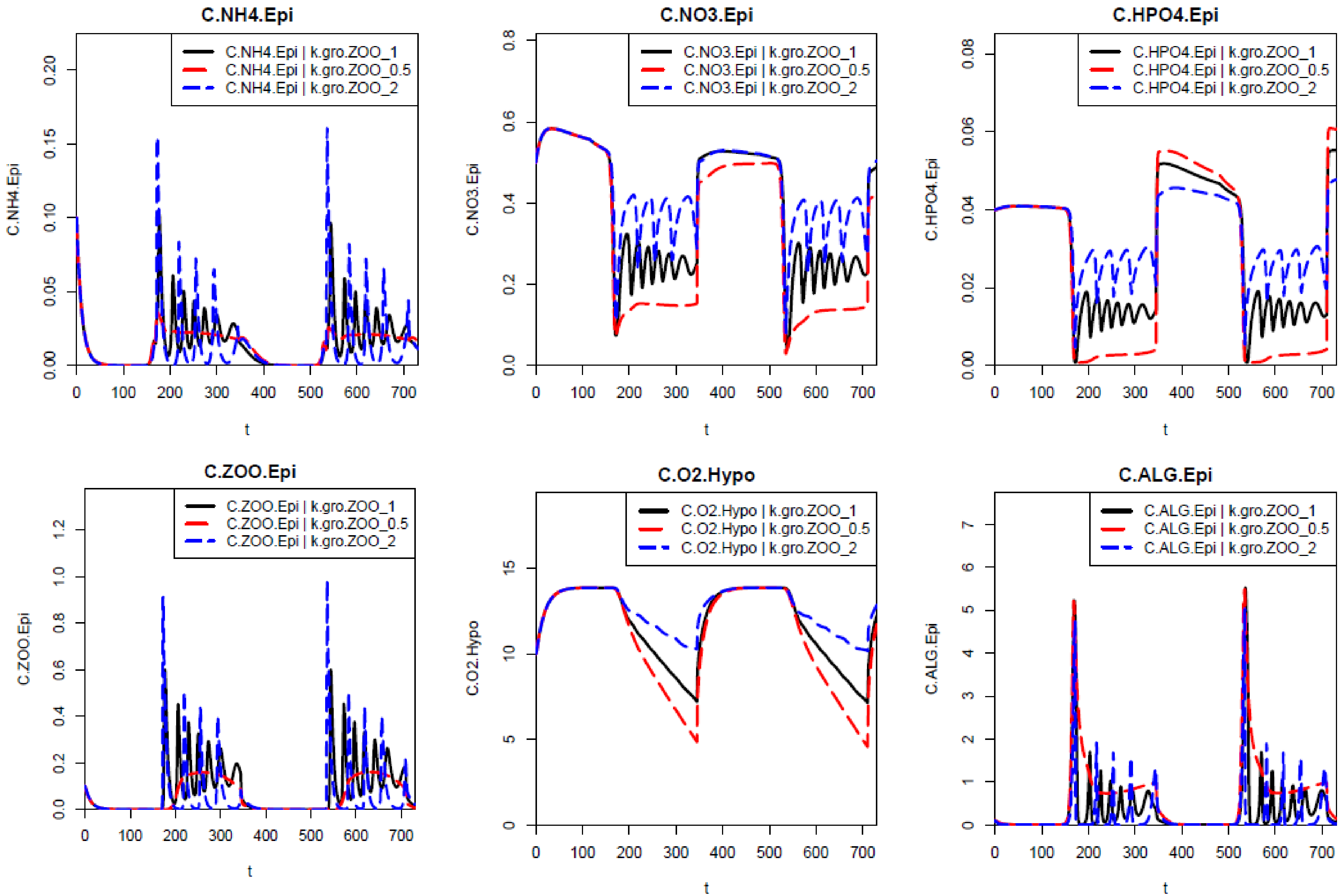


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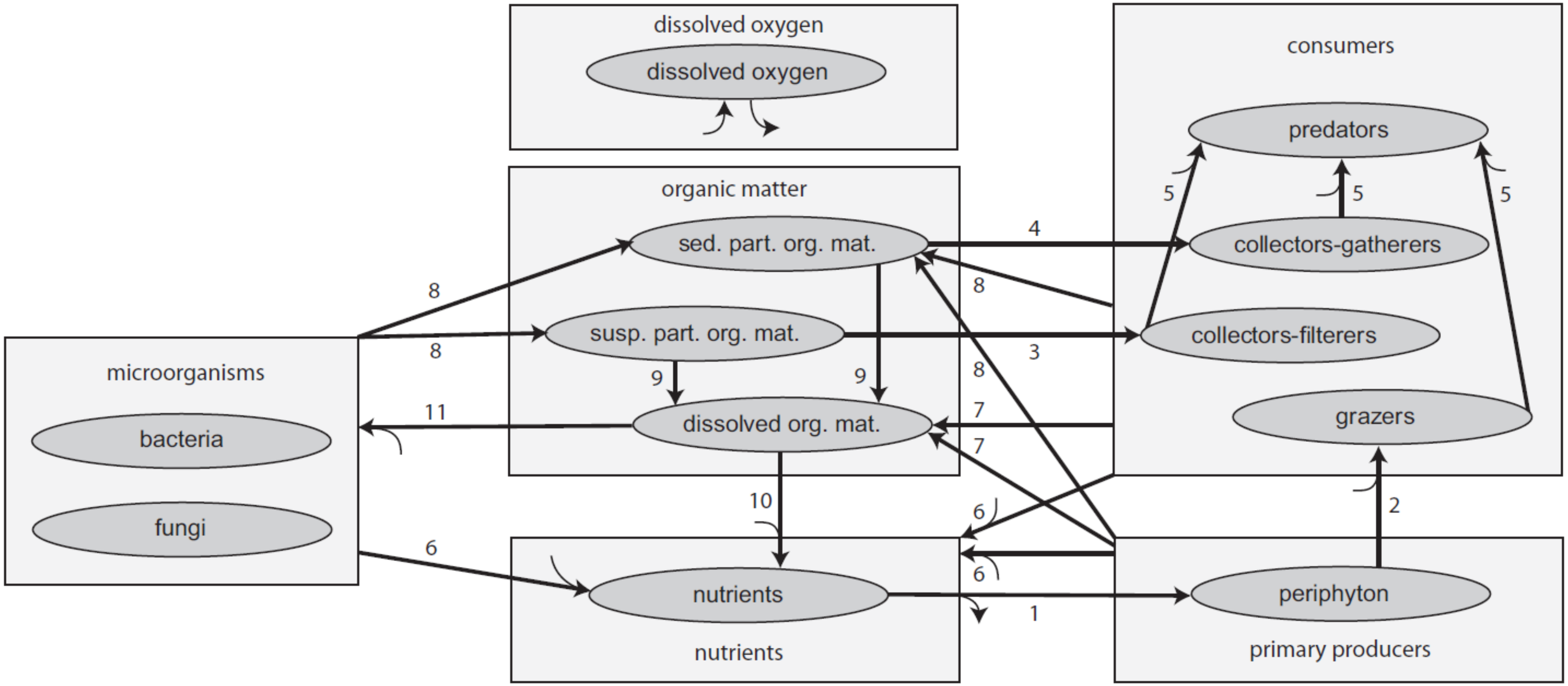
Benthic Foodweb



Benthic Foodweb

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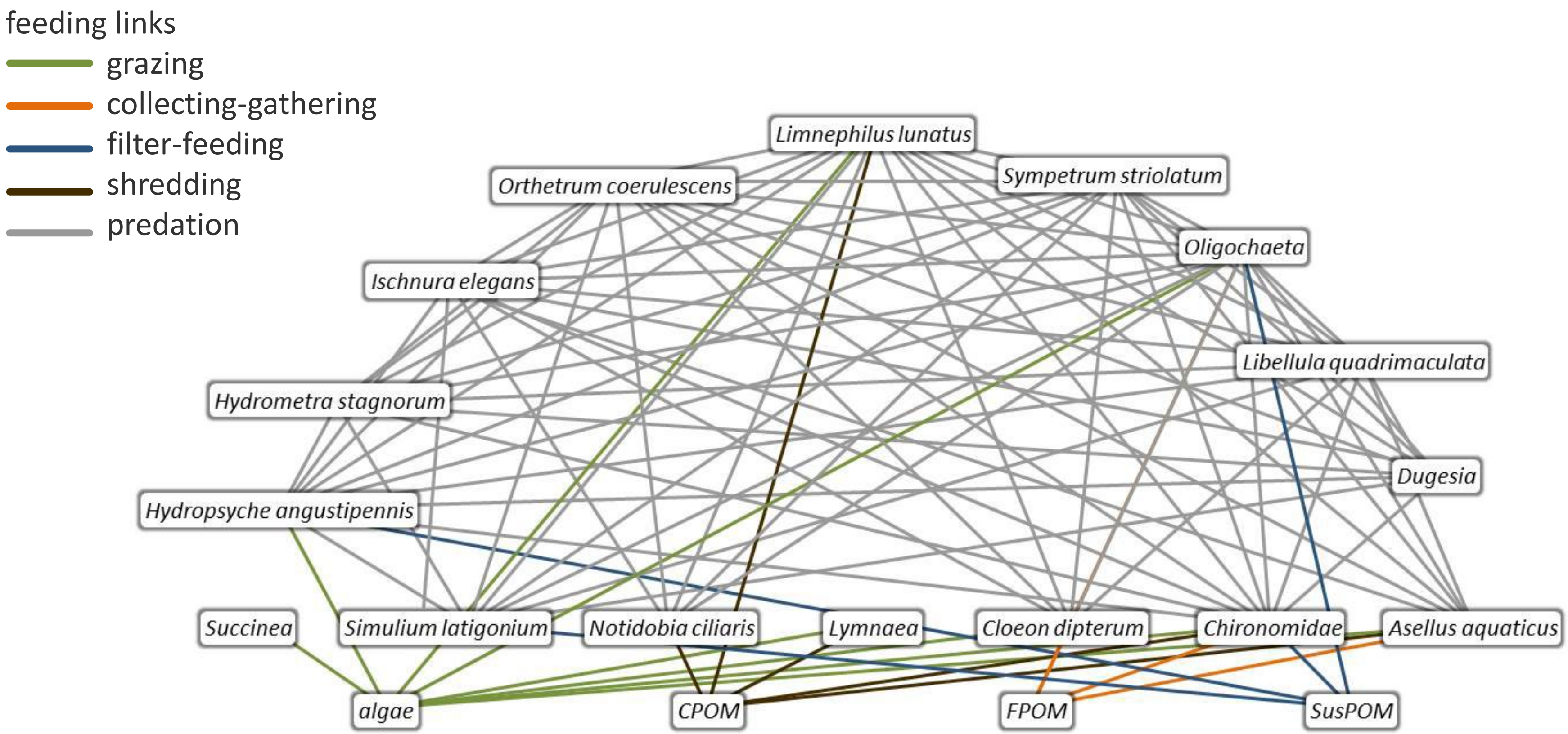
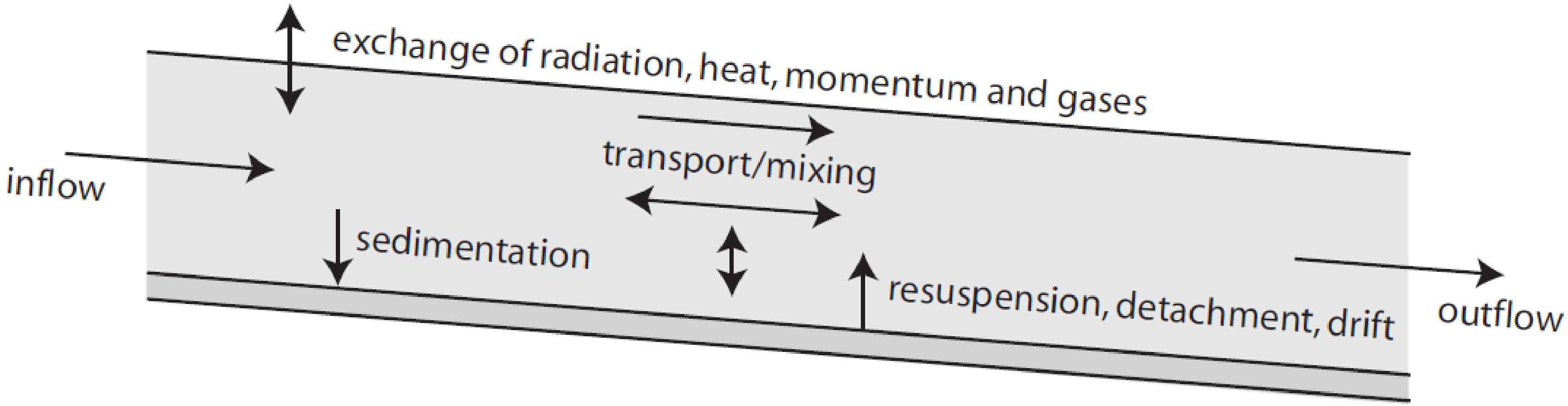


Kattwinkel et al. 2016 *ES&T*

Transport Processes in a River



Decomposition of Organic Material

Heterotrophic organisms, such as bacteria and fungi are responsible for the decomposition of organic material.

So far, this was only considered implicitly when modelling mineralization.

We will now describe the overall process of mineralization of organic particles as **hydrolysis** of the particles to dissolved organic matter, **growth of heterotrophic bacteria**, and finally **death and respiration of the bacteria**.

Classification of Growth Processes

energy source		electron donor		carbon source	
light:	**photo-**	organic comp.:	**organo-**	organic comp.:	**hetero-**
redox proc.:	**chemo-**	inorg. comp.:	**litho-**	inorg. comp.:	**auto-**

Algae and macrophytes: *photolithoautotrophic*

Heterophic bacteria: *chemoorganoheterotrophic*

Nitrifiers: *chemolithoautotrophic*

You: ?

Also mixotrophic organisms exist:

ciliates

sea slug

carnivorous plants

spotted salamander

Growth of Heterotrophic Bacteria

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Stoichiometry:

Process	NH_4^+ gN	NO_3^- gN	N_2 gN	HPO_4^{2-} gP	HCO_3^- gC	O_2 gO	H^+ mol	H_2O mol	DOM g	HET gDM	Rate
Oxgro. HET NH4	?			?	+	−	?	?	$-\frac{1}{Y_H}$	1	$\rho_{\text{gro,HET,ox,NH4}}$
Oxgro. HET NO3		?		?	+	−	?	?	$-\frac{1}{Y_H}$	1	$\rho_{\text{gro,HET,ox,NO3}}$
Anoxgro. HET		−	+	?	+		?	?	$-\frac{1}{Y_H}$	1	$\rho_{\text{gro,HET,anox}}$

Constraints:

$$\nu_{\text{gro,HET,ox,NH4 HET}} + \nu_{\text{gro,HET,ox,NH4 DOM}} Y_{\text{HET}} = 0$$

$$\nu_{\text{gro,HET,ox,NO3 HET}} + \nu_{\text{gro,HET,ox,NO3 DOM}} Y_{\text{HET}} = 0$$

$$\nu_{\text{gro,HET,anox,NH4 HET}} + \nu_{\text{gro,HET,anox,NH4 DOM}} Y_{\text{HET}} = 0$$

Growth of Heterotrophic Bacteria

Process rates for oxic growth:

$$
\begin{aligned}
\rho_{\mathrm{gro,HET,ox,NH4}} =& k_{\mathrm{gro,HET,ox}} \cdot \exp\Big(\beta_{\mathrm{BAC}}(T-T_0)\Big)\left[\cdot \frac{p_{\mathrm{NH4,HET}}C_{\mathrm{NH4}}}{p_{\mathrm{NH4,HET}}C_{\mathrm{NH4}}+C_{\mathrm{NO3}}}\right] \\
&\cdot \min\left(\frac{C_{\mathrm{DOM}}}{K_{\mathrm{DOM,HET}}+C_{\mathrm{DOM}}}, \frac{C_{\mathrm{O2}}}{K_{\mathrm{O2,HET}}+C_{\mathrm{O2}}},\right. \\
&\left.\left[\frac{C_{\mathrm{HPO4}}}{K_{\mathrm{HPO4,HET}}+C_{\mathrm{HPO4}}}\right], \left[\frac{C_{\mathrm{NH4}}+C_{\mathrm{NO3}}}{K_{\mathrm{N,HET}}+C_{\mathrm{NH4}}+C_{\mathrm{NO3}}}\right]\right) \cdot C_{\mathrm{HET}}
\end{aligned}
$$

$$
\begin{aligned}
\rho_{\mathrm{gro,HET,ox,NO3}} =& k_{\mathrm{gro,HET,ox}} \cdot \exp\Big(\beta_{\mathrm{BAC}}(T-T_0)\Big)\left[\cdot \frac{C_{\mathrm{NO3}}}{p_{\mathrm{NH4,HET}}C_{\mathrm{NH4}}+C_{\mathrm{NO3}}}\right] \\
&\cdot \min\left(\frac{C_{\mathrm{DOM}}}{K_{\mathrm{DOM,HET}}+C_{\mathrm{DOM}}}, \frac{C_{\mathrm{O2}}}{K_{\mathrm{O2,HET}}+C_{\mathrm{O2}}},\right. \\
&\left.\left[\frac{C_{\mathrm{HPO4}}}{K_{\mathrm{HPO4,HET}}+C_{\mathrm{HPO4}}}\right], \left[\frac{C_{\mathrm{NH4}}+C_{\mathrm{NO3}}}{K_{\mathrm{N,HET}}+C_{\mathrm{NH4}}+C_{\mathrm{NO3}}}\right]\right) \cdot C_{\mathrm{HET}}
\end{aligned}
$$

[...] if the corresponding stoichiometric coefficients are negative

Growth of Heterotrophic Bacteria

Process rates for anoxic growth:

$$\rho_{\mathrm{gro,HET,anox}} = k_{\mathrm{gro,HET,anox}} \cdot \exp\Big(\beta_{\mathrm{BAC}}(T - T_0)\Big) \cdot \frac{K_{\mathrm{O2,HET}}}{K_{\mathrm{O2,HET}} + C_{\mathrm{O2}}}$$

$$\cdot \min\left(\frac{C_{\mathrm{DOM}}}{K_{\mathrm{DOM,HET}} + C_{\mathrm{DOM}}}, \frac{C_{\mathrm{NO3}}}{K_{\mathrm{NO3,HET}} + C_{\mathrm{NO3}}}, \left[\frac{C_{\mathrm{HPO4}}}{K_{\mathrm{HPO4,HET}} + C_{\mathrm{HPO4}}}\right]\right) \cdot C_{\mathrm{HET}}$$

Growth of Nitrifying Bacteria

Nitrification is mediated by nitrifying bacteria.

Different organisms are responsible for the two steps of nitrification:

- N1: First step of nitrification from ammonium to nitrite (e.g. *Nitrosomonas*)
- N2: Second step of nitrification from nitrite to nitrate (e.g. *Nitrobacter*)

Growth of Nitrifying Bacteria

Stoichiometry:

Process	NH_4^+ gN	NO_2^- gN	NO_3^- gN	HPO_4^{2-} gP	HCO_3^- gC	O_2 gO	H^+ mol	H_2O mol	N1 gDM	N2 gDM	Rate
Growth of N1	$-\frac{1}{Y_{\mathrm{N1}}}$	$+$		$-$	$-$	$-$	?	?	1		$\rho_{\mathrm{gro,N1}}$
Growth of N2		$-\frac{1}{Y_{\mathrm{N2}}}$	$+$	$-$	$-$	$-$	?	?		1	$\rho_{\mathrm{gro,N2}}$

Rates:

$$\rho_{\mathrm{gro,N1}} = k_{\mathrm{gro,N1},T_0} \cdot \exp\Big(\beta_{\mathrm{N1}}(T-T_0)\Big) \cdot \min\left(\frac{C_{\mathrm{NH4}}}{K_{\mathrm{NH4,nitri}}+C_{\mathrm{NH4}}}, \frac{C_{\mathrm{O2}}}{K_{\mathrm{O2,nitri}}+C_{\mathrm{O2}}}, \frac{C_{\mathrm{HPO4}}}{K_{\mathrm{HPO4,nitri}}+C_{\mathrm{HPO4}}}\right) \cdot C_{\mathrm{N1}}$$

$$\rho_{\mathrm{gro,N2}} = k_{\mathrm{gro,N2},T_0} \cdot \exp\Big(\beta_{\mathrm{N2}}(T-T_0)\Big) \cdot \min\left(\frac{C_{\mathrm{NO2}}}{K_{\mathrm{NO2,nitri}}+C_{\mathrm{NO2}}}, \frac{C_{\mathrm{O2}}}{K_{\mathrm{O2,nitri}}+C_{\mathrm{O2}}}, \frac{C_{\mathrm{HPO4}}}{K_{\mathrm{HPO4,nitri}}+C_{\mathrm{HPO4}}}\right) \cdot C_{\mathrm{N2}}$$

Question to think about

What are advantages and disadvantages of modelling heterotrophic and nitrifying bacteria explicitly?

Overview of substance transport and mixing processes in rivers under steady-state hydraulic conditions:

- the estimation of average flow velocity and water depth
- vertical mixing
- lateral mixing
- longitudinal transport and dispersion

We often know the geometry and discharge of a river,

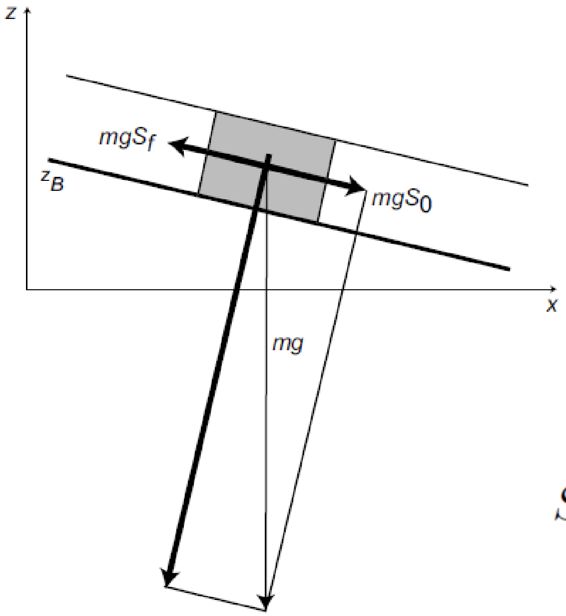
but we have to estimate the average **flow velocity** and **water depth**

What do you think:

What affects the flow velocity in a river?

What affects the water depth?

Steady-state hydraulics: average flow velocity v and water depth h depend on discharge Q and the geometry of the river bed.



$$S_0 = -\frac{\mathrm{d}z_\mathrm{B}}{\mathrm{d}x}$$

z_B: vertical coordinate of the river bed, x: distance along the river, S_f: non-dimensional friction force, S_0: slope of the river bed, m: mass, g: gravitational acceleration

Friction is caused by surface roughness and irregularities of the river bed, by irregularities in channel geometry, obstructions, vegetation and curves.

All these causes generate **dissipation** (loss of kinetic energy in the open system due to conversion into heat).

This is a very complex process that cannot be accounted for mechanistically in simple, one-dimensional models.

To estimate the friction force, we use a simple parameterization as a function of averaged flow quantities, geometry of the riverbed and surface roughness.

Friction force made non-dimensional by division through the gravitational force of the fluid, formulation after Darcy-Weisbach and Manning-Strickler.

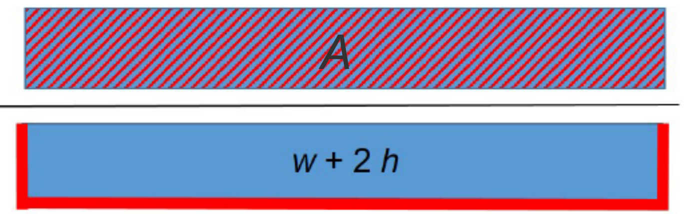
Darcy-Weisbach | Strickler | Manning

$$S_\mathrm{f} = \frac{f}{8g}\frac{1}{R}\frac{Q^2}{A^2}\,, \qquad S_\mathrm{f} = \frac{1}{K_\mathrm{st}^2}\frac{1}{R^{4/3}}\frac{Q^2}{A^2} = n^2\frac{1}{R^{4/3}}\frac{Q^2}{A^2}\,, \qquad n = \frac{1}{K_\mathrm{st}}$$

f: non-dimensional friction-factor, Q: discharge, A: wetted cross-sectional area, R: hydraulic radius (A divided by wetted perimeter), K_st: Friction coefficient according to Strickler, n: friction coefficient according to Manning

Transport and Mixing in Rivers

hydraulic radius R = cross-sectional area A / wetted perimeter P



for a wide rectangular river bed: $P = w + 2h \approx w$ $\quad R = \dfrac{A}{P} \approx \dfrac{A}{w}$

Assumption: prismatic river reach, constant friction, no backwater:

$$S_f = S_0$$

Transport and Mixing in Rivers

$$S_f = \frac{1}{{K_{st}}^2} \frac{1}{R^{4/3}} \frac{Q^2}{A^2}$$

substituting: $S_f = S_0$; $\quad R = \frac{A}{P} \approx \frac{A}{w}$; $\quad A = \frac{Q}{v}$

$$S_0 = \frac{1}{{K_{st}}^2} \frac{1}{\left(\frac{\frac{Q}{v}}{w}\right)^{4/3}} \frac{Q^2}{\left(\frac{Q}{v}\right)^2}$$

solving for v :

$$v = \left(K_{st}\sqrt{S_0}\right)^{\frac{3}{5}} \left(\frac{Q}{w}\right)^{\frac{2}{5}}$$

with
non-dimensional friction force S_f
Strickler coefficient K_{st},
hydraulic radius R,
discharge Q,
cross sectional area A,
wetted perimeter P,
river width w,
flow velocity v,
slope S_0

similar for Darcy-Weissbach and Manning equation:

$$v = \left(\frac{8g}{f} S_0 \frac{Q}{w} \right)^{\frac{1}{3}} \text{ (Darcy-Weissbach)}$$

$$v = \left(K_{\mathbf{st}} \sqrt{S_0} \right)^{\frac{3}{5}} \left(\frac{Q}{w} \right)^{\frac{2}{5}} = \left(\frac{\sqrt{S_0}}{n} \right)^{\frac{3}{5}} \left(\frac{Q}{w} \right)^{\frac{2}{5}} \text{ (Strickler-Manning)}$$

$K_{st}=1/n$

$$h = \frac{Q}{wv}$$

Estimation of the Manning coefficient:

Category	Property	Contribution to friction		
Surface material of the river bed	earth	$n_1 =$	0.020	$\mathrm{s/m^{1/3}}$
	fine gravel		0.024	$\mathrm{s/m^{1/3}}$
	coarse gravel		0.028	$\mathrm{s/m^{1/3}}$
Irregularities of the river bed	smooth	$n_2 =$	0.000	$\mathrm{s/m^{1/3}}$
	minor		0.005	$\mathrm{s/m^{1/3}}$
	moderate		0.010	$\mathrm{s/m^{1/3}}$
	severe		0.020	$\mathrm{s/m^{1/3}}$
Variation of shape of the cross-section	gradual	$n_3 =$	0.000	$\mathrm{s/m^{1/3}}$
	occasional		0.005	$\mathrm{s/m^{1/3}}$
	frequent		0.010 - 0.015	$\mathrm{s/m^{1/3}}$
Obstructions in the river bed	negligible	$n_4 =$	0.000	$\mathrm{s/m^{1/3}}$
	minor		0.010 - 0.015	$\mathrm{s/m^{1/3}}$
	appreciable		0.020 - 0.030	$\mathrm{s/m^{1/3}}$
	severe		0.040 - 0.060	$\mathrm{s/m^{1/3}}$
Vegetation	none	$n_5 =$	0.000	$\mathrm{s/m^{1/3}}$
	low		0.005 - 0.010	$\mathrm{s/m^{1/3}}$
	medium		0.010 - 0.025	$\mathrm{s/m^{1/3}}$
	high		0.025 - 0.050	$\mathrm{s/m^{1/3}}$
	very high		0.050 - 0.100	$\mathrm{s/m^{1/3}}$
Effect of curves	minor	$n_6 =$	0.000	$\mathrm{s/m^{1/3}}$
	appreciable		$0.15 \sum_{i=1}^{5} n_i$	
	severe		$0.30 \sum_{i=1}^{5} n_i$	

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River Glatt

With a mean width of about 16 m, a slope of 0.34 % and a discharge of 4 m^3/s we get the following values for mean flow velocity and mean depth:

winter				summer			
n_1	=	0.028	$s/m^{1/3}$	n_1	=	0.028	$s/m^{1/3}$
n_2	=	0.005	$s/m^{1/3}$	n_2	=	0.005	$s/m^{1/3}$
n_3	=	0.000	$s/m^{1/3}$	n_3	=	0.000	$s/m^{1/3}$
n_4	=	0.000	$s/m^{1/3}$	n_4	=	0.000	$s/m^{1/3}$
n_5	=	0.010	$s/m^{1/3}$	n_5	=	0.050	$s/m^{1/3}$
n_6	=	0.000	$s/m^{1/3}$	n_6	=	0.000	$s/m^{1/3}$
n	=	0.043	$s/m^{1/3}$	n	=	0.083	$s/m^{1/3}$
K_{st}	=	23	$m^{1/3}/s$	K_{st}	=	12	$m^{1/3}/s$

winter				summer			
v	=	?	m/s	v	=	?	m/s
h	=	?	m	h	=	?	m

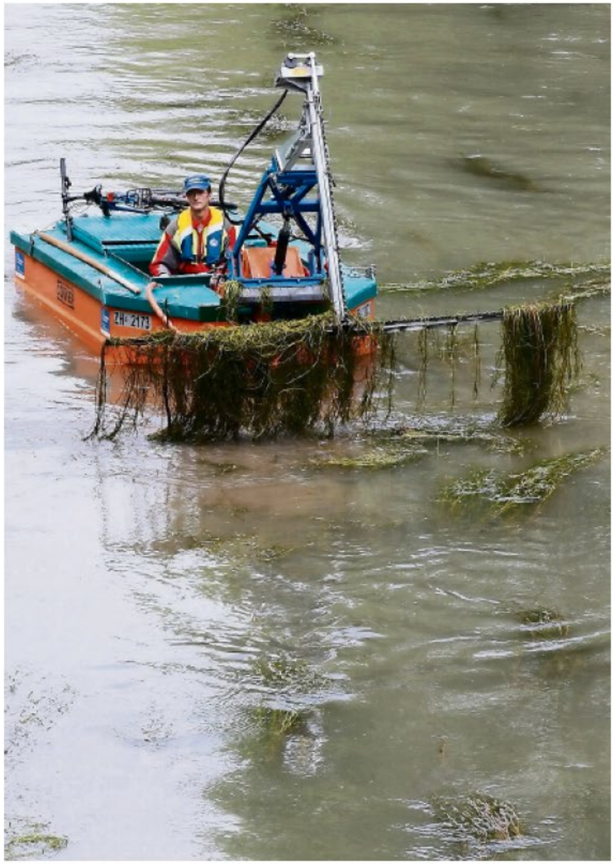
River Glatt

With a mean width of about 16 m, a slope of 0.34 % and a discharge of 4 m^3/s we get the following values for mean flow velocity and mean depth:

winter				summer			
n_1	$=$	0.028	$s/m^{1/3}$	n_1	$=$	0.028	$s/m^{1/3}$
n_2	$=$	0.005	$s/m^{1/3}$	n_2	$=$	0.005	$s/m^{1/3}$
n_3	$=$	0.000	$s/m^{1/3}$	n_3	$=$	0.000	$s/m^{1/3}$
n_4	$=$	0.000	$s/m^{1/3}$	n_4	$=$	0.000	$s/m^{1/3}$
n_5	$=$	0.010	$s/m^{1/3}$	n_5	$=$	0.050	$s/m^{1/3}$
n_6	$=$	0.000	$s/m^{1/3}$	n_6	$=$	0.000	$s/m^{1/3}$
n	$=$	0.043	$s/m^{1/3}$	n	$=$	0.083	$s/m^{1/3}$
K_{st}	$=$	23	$m^{1/3}/s$	K_{st}	$=$	12	$m^{1/3}/s$

winter				summer			
v	$=$	0.68	m/s	v	$=$	0.46	m/s
h	$=$	0.36	m	h	$=$	0.54	m

Zürcher Unterland



Das Mähboot kommt aus Holland, der Bootsführer braucht dafür eine Extraprüfung.

Stundenlang stehen die Männer mit ihren Sensen im Wasser. Fotos: Sibylle Meier

Mit Boot und Sensen die Glatt mähen

Dieses Jahr ist der Wasserhahnenfuss besonders stark gewachsen. Zwölf Arbeiter stutzen nun bei Opfikon das Gras, um Hochwasser zu verhindern.

Von Andreas Frei

Opfikon – In grossen Ballen treibt der abgemähte Wasserhahnenfuss die Glatt hinunter in Richtung Flughafen. Auf der Höhe des Opfiker Werkhofs wird das Gras mit einer Maschine auf eine Flussseite in ein aufgestelltes Gitter getrieben. Dort holt Hermann Meier, Betriebsleiter Gewässerunterhalt in Oberglatt, die Pflanzenteile mit einer riesigen Greifzange aus dem Nass.

vom Hahnenfuss befreien. Sie sind beim Amt für Abfall, Wasser, Energie und Luft (Awel) des Kantons angestellt. Für die Hahnenfussentfernung arbeiten sie mit den Opfikern zusammen.

Sechs Meter langes Gras

Ein paar Hundert Meter vom Auffanggitter entfernt mäht Albert Spühler das Gras mit einem Spezialboot, das am Bug einen drei Meter breiten, T-förmi-

Bei einem Wasserfall neben der abgebrannten Holzbrücke kommt das Boot nicht mehr weiter. Auch dort staut sich der Hahnenfuss bereits in grossen Mengen und muss später mit einem Spezialkran entfernt werden.

Flussaufwärts mähen drei weitere Werkarbeiter. Ruedi Meier, Remo Bosshard und Andreas Perren stehen mitten in der Glatt und rücken dem Hahnenfuss nur mit ihren Sensen zu Leibe.

wir es vorziehen mussten.» Weshalb das so ist, sei nicht klar. «Temperatur, Wasserhöhe und Licht haben einen Einfluss. Wieso es jetzt aber bei etwa gleichen Voraussetzungen viel mehr Gras als letztes Jahr hat, können wir nicht erklären.»

Hahnenfuss

Hochwassergefahr durch Pflanze

Transport Processes

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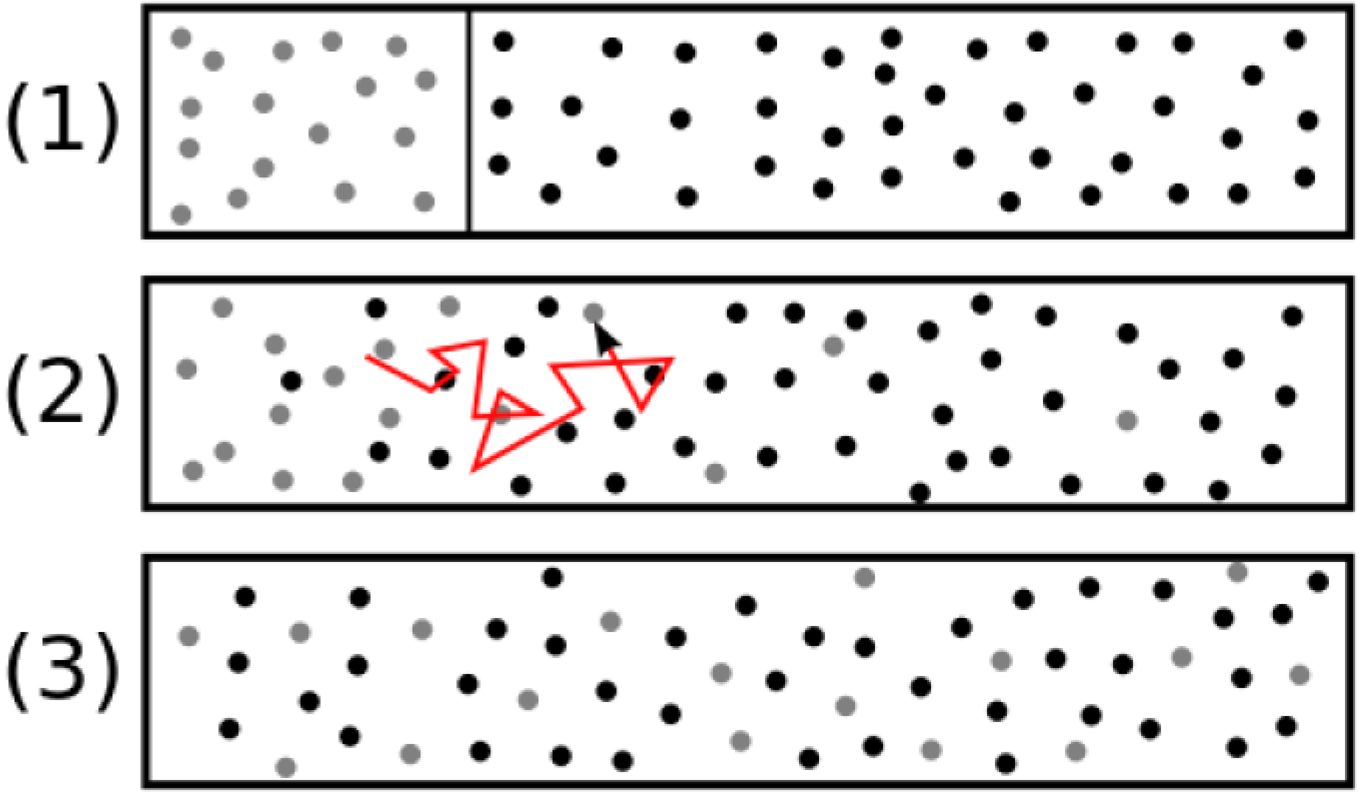
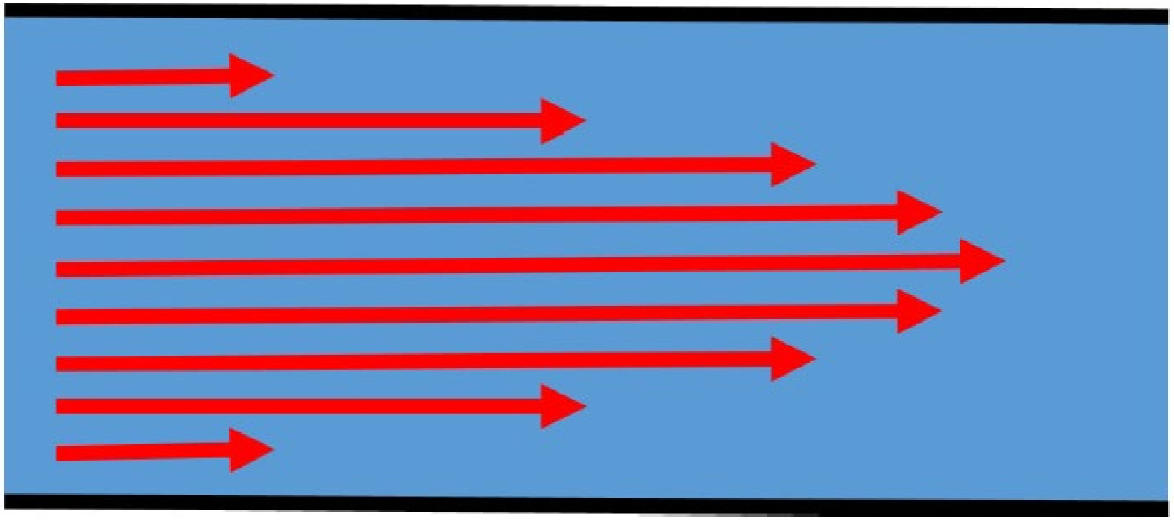
- **Advection**: directional transport with the water flow
- **Diffusion**: spreading of mass from highly concentrated areas to less concentrated areas due to undirectional motion;
  Molecular diffusion (caused by Brownian motion)
  Turbulent diffusion (caused by turbulence eddies)
- **Dispersion**: spreading of mass from highly concentrated areas to less concentrated areas due to differences in flow velocity at different flow paths and mixing between the flow paths by diffusion

Molecular Diffusion



Dispersion



Transport and Mixing in Rivers

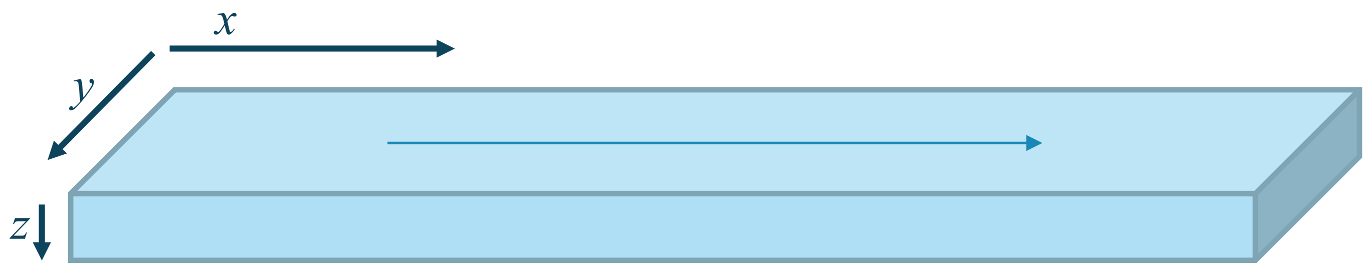
Simple estimate of dispersal of a substance transported in a river using analytical solutions of the transport equation.

Simplifying assumptions:

- constant flow velocity v in time and across river cross-section
- constant vertical turbulent diffusion coefficient K_z
- constant lateral diffusion and dispersion coefficient e_y

Transport equation:

$$\frac{\partial C}{\partial t} = -v\frac{\partial C}{\partial x} + e_y\frac{\partial^2 C}{\partial y^2} + K_z\frac{\partial^2 C}{\partial z^2}$$



Vertical mixing

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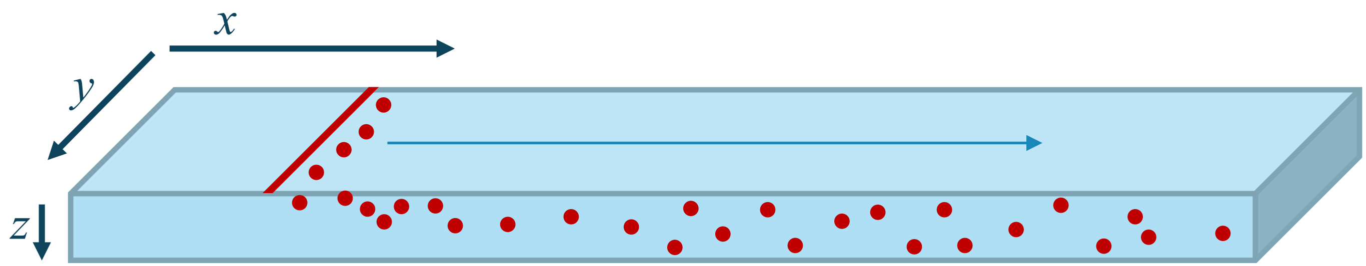
Assumption: Substance enters the river homogeneously spread over the river width, lateral dimension can be omitted:

$$v\frac{\partial C}{\partial x} = K_z \frac{\partial^2 C}{\partial z^2}$$

Analytical solution for a substance entering the river at the water surface and no considerable concentration reaching the river bed:

$$C(x,y,z) = \frac{J}{w}\frac{1}{v}\frac{2}{\sqrt{2\pi}}\frac{1}{\sigma_z(x)}\exp\left(-\frac{(z-z_0)^2}{2\sigma_z(x)^2}\right) \quad , \quad \sigma_z(x) = \sqrt{2K_z\frac{x}{v}}$$

J: mass flux of the substance entering the river at its surface, w: river width, z_0: z-coordinate of the river surface.



Vertical mixing

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For longer distances along the river, this solution must be extended to

$$C(x,y,z) = \frac{J}{w}\frac{1}{v}\frac{2}{\sqrt{2\pi}}\frac{1}{\sigma_z(x)}\sum_{n=-\infty}^{\infty}\exp\left(-\frac{(z-z_0-2\cdot nh)^2}{2\sigma_z(x)^2}\right)$$

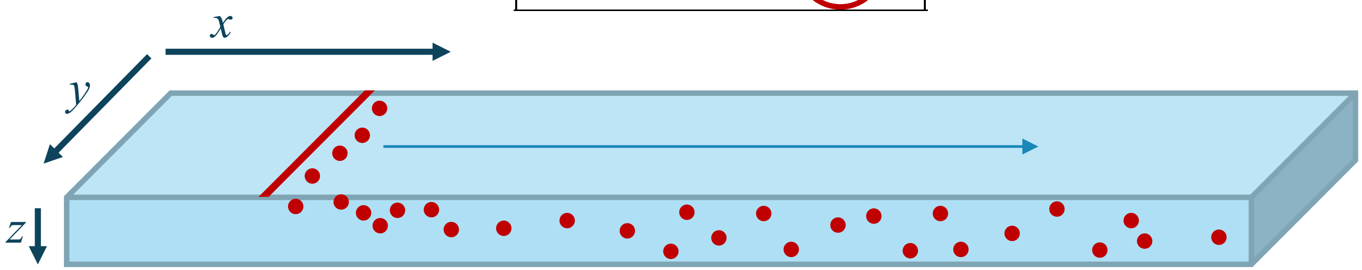
Consideration of the increase in concentration due to the no-flux boundary condition at the river bed. Because of the quick decrease of the exponential function, in most situations only a small number of terms must be considered in this sum.

Mixing distance:

Horizontal distance, after which the substance is nearly homogenously mixed over the depth of the river

Definition: distance, after which the standard deviation $\sigma_z(x)$ of the vertical substance distribution is equal to the depth of the river.

$$\boxed{s_{\text{mix},z} \approx \frac{h^2}{2K_z}v}$$



Vertical mixing

Estimation of the coefficient of vertical turbulent diffusion, K_z:

$$\tau_0 \approx \rho g h S_0$$

$$u^* = \sqrt{\frac{\tau_0}{\rho}} \quad , \quad u^* \approx \sqrt{g h S_0}$$

$$\boxed{K_z \approx \frac{1}{6}\kappa u^* h \approx 0.07 u^* h}$$

τ_0: bottom shear stress, ρ: density of the flowing medium,
g: graviational acceleration, h: water depth, S_0: river slope,
u^*: shear velocity, $\kappa \approx 0.4$: Karman constant

Vertical mixing

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River Glatt

With a mean width of about 16 m, a slope of 0.34 % and a discharge of 4 m^3/s

winter				summer			
v	=	0.68	m/s	v	=	0.46	m/s
h	=	0.36	m	h	=	0.54	m
K_z	=	?	m^2/s	K_z	=	?	m^2/s
$s_{\mathrm{mix},z}$	=	?	m	$s_{\mathrm{mix},z}$	=	?	m

Similar result for $s_{\mathrm{mix},z}$: difference in mixing coefficient partly compensated by difference in water depth.

$$K_z \approx \frac{1}{6} * 0.4 * \sqrt{ghS_0} * h \qquad s_{mix,z} \approx \frac{h^2}{2K_z} v \qquad \text{with } g = 9.8067\ \mathrm{m/s^2}$$

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River Glatt

With a mean width of about 16 m, a slope of 0.34 % and a discharge of 4 m^3/s

winter				summer			
v	=	0.68	m/s	v	=	0.46	m/s
h	=	0.36	m	h	=	0.54	m
K_z	=	0.0028	m^2/s	K_z	=	0.0051	m^2/s
$s_{\mathrm{mix},z}$	=	17	m	$s_{\mathrm{mix},z}$	=	14	m

Similar result for $s_{\mathrm{mix},z}$: difference in mixing coefficient partly compensated by difference in water depth.

$$K_z \approx \frac{1}{6} * 0.4 * \sqrt{ghS_0} * h \qquad s_{mix,z} \approx \frac{h^2}{2K_z} v \qquad \text{with } g = 9.8067 \text{ m/s}^2$$

Lateral mixing

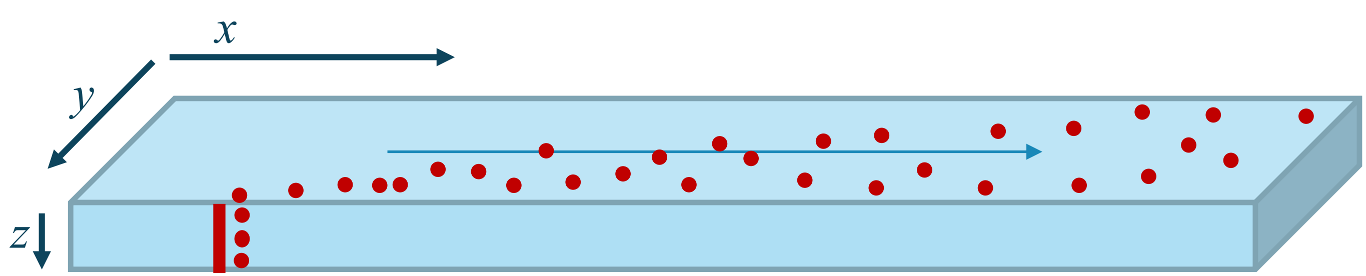
Assumption: Substance enters the river well mixed over the river depth, vertical dimension and time dependence can be ignored:

$$v\frac{\partial C}{\partial x} = e_y \frac{\partial^2 C}{\partial y^2}$$

Analytical solution for a substance entering the river at its bank and no considerable concentration reaching the other bank:

$$C(x,y,z) = \frac{J}{h}\frac{1}{v}\frac{2}{\sqrt{2\pi}}\frac{1}{\sigma_y(x)}\exp\left(-\frac{(y-y_0)^2}{2\sigma_y(x)^2}\right) \quad , \quad \sigma_y(x) = \sqrt{2e_y\frac{x}{v}}$$

J: mass flux of the substance entering the river at its bank, h: water depth, y_0: y-coordinate of this bank



Lateral mixing

For longer flow distances along the river, the no-flow boundary condition at the other bank must be taken into account and the solution must be extended:

$$C(x,y,z) = \frac{J}{h}\frac{1}{v}\frac{2}{\sqrt{2\pi}}\frac{1}{\sigma_y(x)}\sum_{n=-\infty}^{\infty}\exp\left(-\frac{(y-y_0-2\cdot nw)^2}{2\sigma_y(x)^2}\right)$$

Due to the fast decrease of the exponential function, in most cases only a small number of terms must be considered in this sum.

Lateral mixing

Estimation of the lateral extension of the substance distribution (close to the point of entrance into the river):

$$L_y \approx 2\sigma_y(x) = 2\sqrt{2e_y \frac{x}{v}}$$

Estimation of the maximum concentration with a rectangular distribution with half of this width:

$$C_{\max} \approx \frac{J}{hv} \frac{1}{\min(\sigma_y(x), w)} = \frac{J}{hv} \frac{1}{\min\left(\sqrt{2e_y \frac{x}{v}}, w\right)}$$

Far from the input site, the maximum concentration is equal to the concentration after complete mixing across the cross-sectional area.

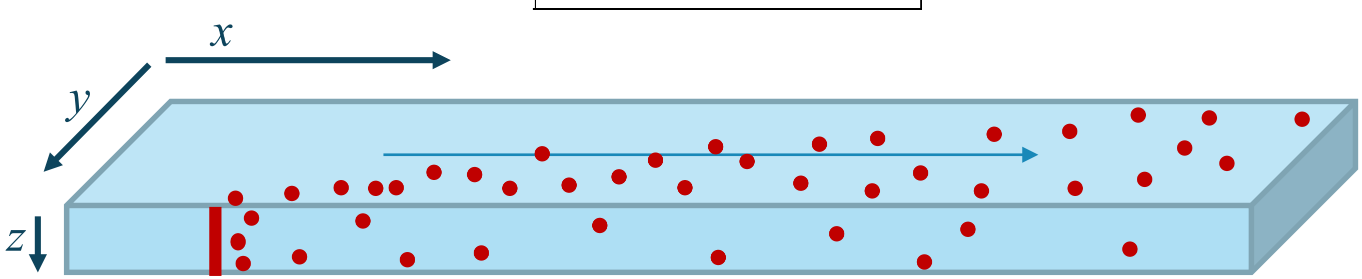
Lateral mixing

Lateral mixing distance:

Distance along the river, after which the substance is nearly homogeneously mixed in lateral direction

Definition: distance, after which the standard deviation $\sigma_y(x)$ of the lateral substance distribution is equal to the river width.

$$\boxed{s_{\mathrm{mix},y} \approx \frac{w^2}{2e_y} v}$$



Lateral mixing

For longer flow distances along the river, the no-flow boundary condition at the other bank must be taken into account and the solution must be extended:

$$C(x,y,z) = \frac{J}{h}\frac{1}{v}\frac{2}{\sqrt{2\pi}}\frac{1}{\sigma_y(x)}\sum_{n=-\infty}^{\infty}\exp\left(-\frac{(y-y_0-2\cdot nw)^2}{2\sigma_y(x)^2}\right)$$

Due to the fast decrease of the exponential function, in most cases only a small number of terms must be considered in this sum.

Lateral mixing

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Estimation of the coefficient of lateral turbulent diffusion plus dispersion e_y:

$$\tau_0 \approx \rho g h S_0 \quad , \quad u^* = \sqrt{\frac{\tau_0}{\rho}} \quad , \quad u^* \approx \sqrt{g h S_0}$$

$$K_x \approx K_y \approx \theta_K u^* h \quad , \quad \theta_K \approx 0.15$$

$$\boxed{e_y \approx \theta_e u^* h} \quad , \quad \theta_e \approx 0.6$$

K_x: coefficient of horizontal turbulent diffusion, K_y: coefficient of lateral turbulent diffusion, θ_K: proportionality factor for lateral turbulent diffusion, u^*: shear velocity, h: water depth, θe: proportionality factor for lateral turbulent diffusion plus dispersion

Lateral mixing

River Glatt

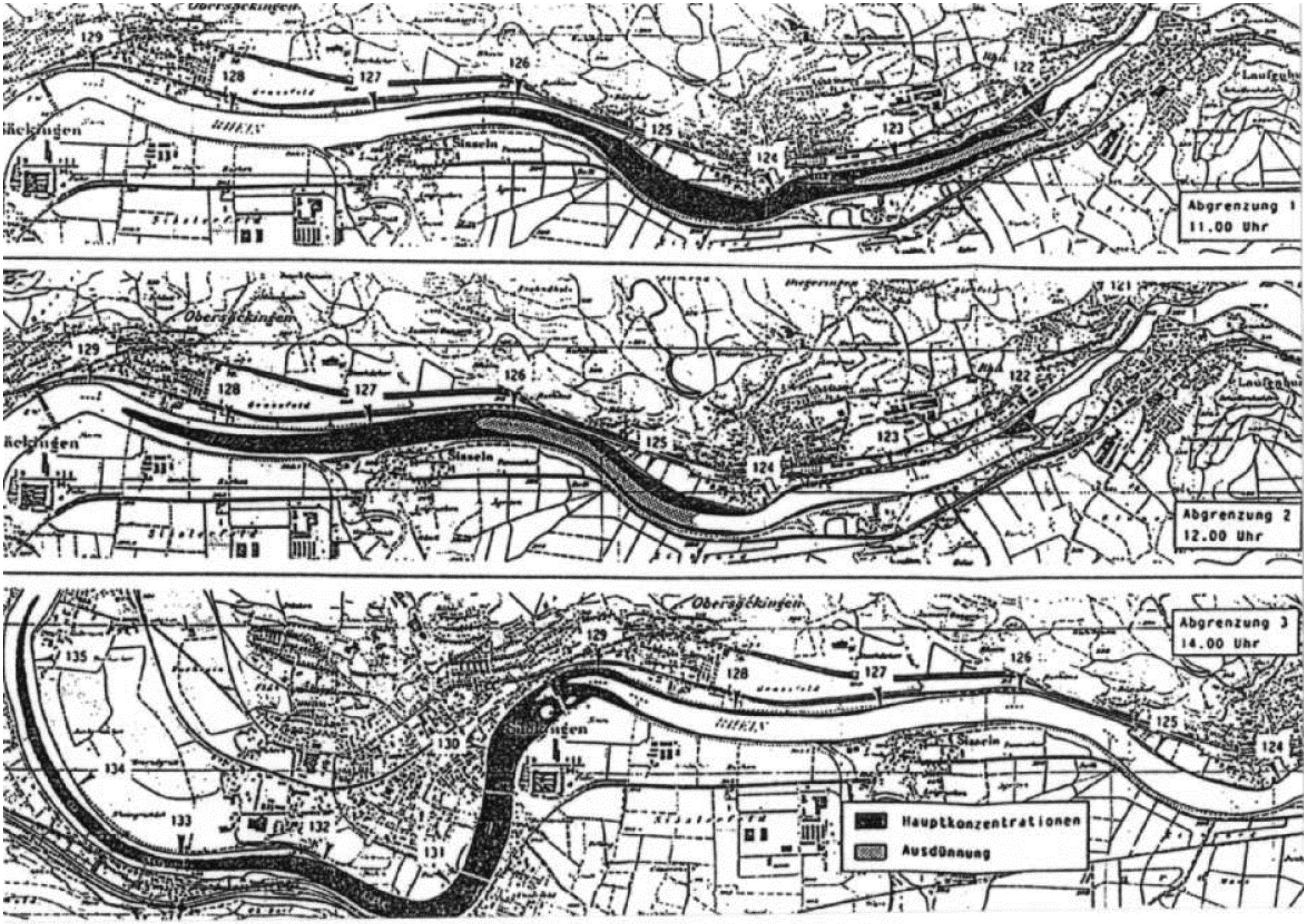
With a mean width of about 16 m, a slope of 0.34 % and a discharge of 4 m^3/s

winter				summer			
e_y	=	0.024	m^2/s	e_y	=	0.043	m^2/s
$s_{\mathrm{mix},y}$	=	3600	m	$s_{\mathrm{mix},y}$	=	1400	m

Note that mixing distances in a river with a width of 16 m can already be of considerable length. This must be considered when taking water samples downstream of tributaries or pollutant discharge sites.

Lateral mixing

Transport and longitudinal dispersion



Transport and longitudinal dispersion

Simple estimate of longitudinal dispersal of a substance transported in a river using analytical solutions of the one-dimensional transport (advections-dispersion) equation.

$$\frac{\partial C}{\partial t} = -v\frac{\partial C}{\partial x} + E_x\frac{\partial^2 C}{\partial x^2}$$

E_x: coefficient of longitudinal dispersion, v: mean flow velocity

Transport and longitudinal dispersion

Solution of the transport equation for a pulse input of mass m:

$$C(x,t) = \frac{m}{hw}\frac{1}{\sqrt{2\pi}}\frac{1}{\sigma_x(t)}\exp\left(-\frac{(x-vt)^2}{2\sigma_x(t)^2}\right) \quad , \quad \sigma_x(t) = \sqrt{2E_x t}$$

w: width of the river, h: mean water depth, v: mean flow velocity,
E_x: longitudinal dispersion coefficient

Transport and longitudinal dispersion

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Estimation of the longitudinal dispersion coefficient E_x

$$\boxed{E_x \approx c_f \frac{w^2 v^2}{u^* h}} \quad , \quad c_f \approx 0.011$$

- Dispersion increases with increasing velocity differences across the river
- Dispersion increases with increasing width of the river, because of decreasing lateral mixing
- Dispersion decreases with lateral turbulent diffusivity $(u^* h)$, as this increases mixing across the river

w: width of the river, v: mean flow velocity, u^*: shear velocity, h: mean water depth, c_f: non-dimensional proportionality factor

Transport and longitudinal dispersion

Estimation of the position of the pulse:

$$\boxed{s_x \approx vt}$$

Estimation of the length of the pulse

$$\boxed{L_x \approx 4\sigma_x(t) = 4\sqrt{2E_x t}}$$

Estimation of the maximum concentration (rectangular pulse with half of this length)

$$\boxed{C_{\max} \approx \frac{m}{hw}\frac{1}{2\sigma_x(t)} = \frac{m}{hw}\frac{1}{2\sqrt{2E_x t}}}$$

River Glatt

winter				summer			
E_x	$=$	33	$\mathrm{m^2/s}$	E_x	$=$	8	$\mathrm{m^2/s}$

The significantly stronger mixing across the width of the river reduces longitudinal dispersion considerably in summer compared to the winter situation. Note that the length of the pulse depends only on the square root of E_x.

Transport and longitudial dispersion in a box model:

Many simple models of rivers approximate the river by a sequence of mixed reactors. The distance along the river is divided into sections of length Δx. The volume V of the reactors can be described by:

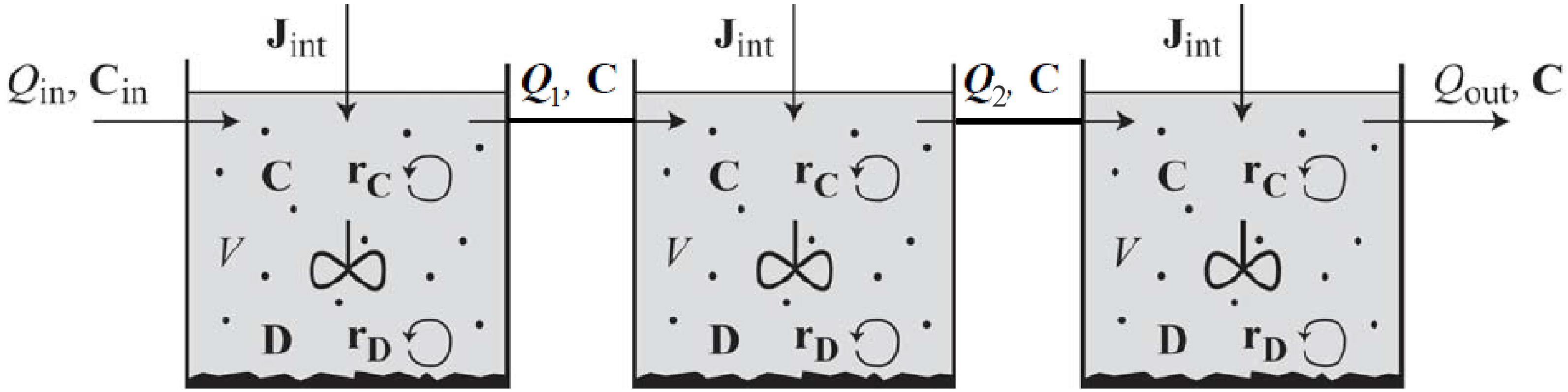
$$V = wh\Delta x$$

Mixing within these boxes results in longitudinal dispersion with an equivalent dispersion coefficient given by:

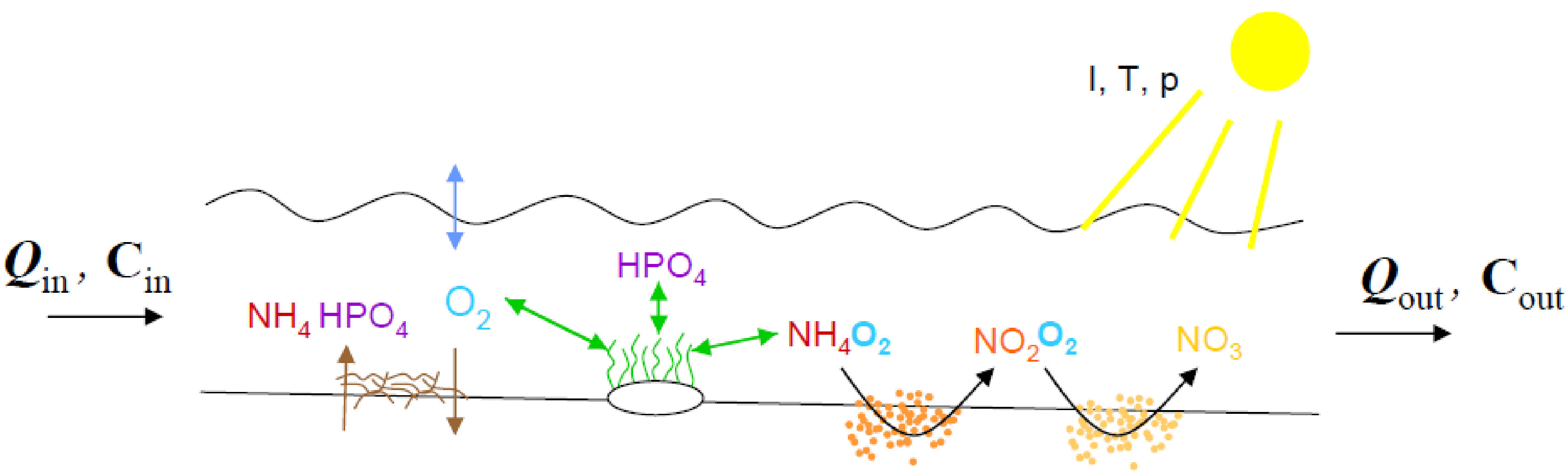
$$\boxed{E_x = \frac{v\Delta x}{2} = \frac{Q\Delta x}{2wh}}$$

This effect is called "numerical diffusion".

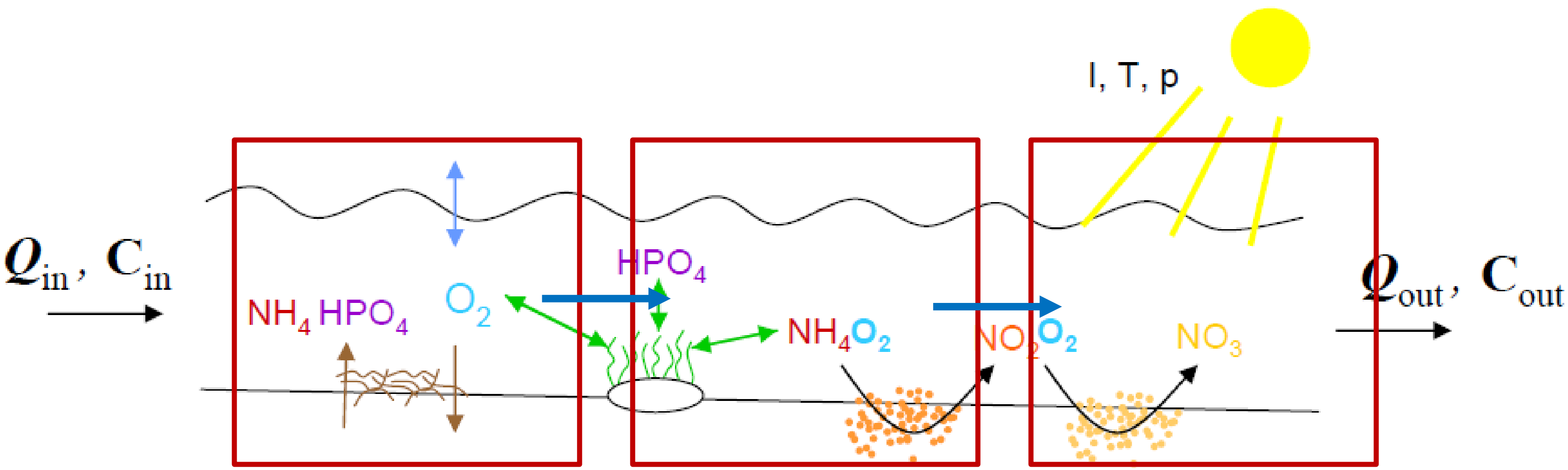
Benthic Population, O, N, P in a River



Benthic Population, O, N, P in a River



Benthic Population, O, N, P in a River



Benthic Population, O, N, P in a River

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	Process	Substances / Organisms											Rate
		HPO_4^{2-} gP	NH_4^+ gN	NO_2^- gN	NO_3^- gN	O_2 gO	DOM g	SALG gDM	SHET gDM	SN1 gDM	SN2 gDM	SPOM gDM	
Algae	Growth of alg. NH4	$-$	$-$			$+$		1					$\rho_{\mathrm{gro,SALG,NH4}}$
	Growth of alg. NO3	$-$			$-$	$+$		1					$\rho_{\mathrm{gro,SALG,NO3}}$
	Respiration of algae	$+$	$+$			$-$		-1					$\rho_{\mathrm{resp,SALG}}$
	Death of algae	$0/+$	$0/+$			$0/+$		-1				$Y_{\mathrm{ALG,death}}$	$\rho_{\mathrm{death,SALG}}$
Het. Bac	Growth het. b. NH4	?	?			$-$	$\frac{-1}{Y_{\mathrm{HET}}}$		1				$\rho_{\mathrm{gro,SHET,NH4}}$
	Growth het. b. NO3	?			?	$-$	$\frac{-1}{Y_{\mathrm{HET}}}$		1				$\rho_{\mathrm{gro,SHET,NO3}}$
	Resp. of het. bact.	$+$	$+$			$-$			-1				$\rho_{\mathrm{resp,SHET}}$
	Death of het. bact.	$0/+$	$0/+$			$0/+$			-1			$Y_{\mathrm{HET,death}}$	$\rho_{\mathrm{death,SHET}}$
N1	Growth of N1	$-$	$\frac{-1}{Y_{\mathrm{N1}}}$	$+$		$-$				1			$\rho_{\mathrm{gro,SN1}}$
	Resp. of N1	$+$	$+$			$-$				-1			$\rho_{\mathrm{resp,SN1}}$
	Death of N1	$0/+$	$0/+$			$0/+$				-1		$Y_{\mathrm{N1,death}}$	$\rho_{\mathrm{death,SN1}}$
N2	Growth of N2	$-$		$\frac{-1}{Y_{\mathrm{N2}}}$	$+$	$-$					1		$\rho_{\mathrm{gro,SN2}}$
	Resp. of N2	$+$	$+$			$-$					-1		$\rho_{\mathrm{resp,SN2}}$
	Death of N2	$0/+$	$0/+$			$0/+$					-1	$Y_{\mathrm{N2,death}}$	$\rho_{\mathrm{death,SN2}}$
	Hydrolysis	$0/+$	$0/+$			$0/+$	Y_{hyd}					-1	ρ_{hyd}

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. 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

Homework

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- Read Chapters 11.5 and 11.6 about the river model
- Think about your questions regarding this lecture