Eawag:
Swiss Federal Institute of Aquatic
Science and Technology

Modelling Aquatic Ecosystems
Course 701-0426-00

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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

Today:

- learn how to formulate mass balances in multi-box (chapter 3.3) (and continuous, 3.4) systems
- get a basic understanding of mixing and transport processes in lakes (6.1.1), sedimentation (6.2) and gas exchange (6.3)
- introduction to the biogeochemical – ecological lake model (11.4)

Assignments of topics for own model

Assignments

There will be an **oral exam in the two weeks** after the semester
8.-12. June 25 (1.-5 June if needed).
It is your responsibility to register/deregister in time.

During the semester you will develop and implement your own model (in teams of two people), interpret simulation results and perform a sensitivity analysis. We will assign topics today.

Deadline for initial code submission: **07.05.26**

Deadline for submission of R-files, results and interpretation: **22.05.26**

This is mandatory for being admitted to the exam!
In the oral exam we will start with questions about your model before moving on to other topics.

Please use the time in the exercises to ask questions and get help!
Don't do it last minute.

Base Model 11.4

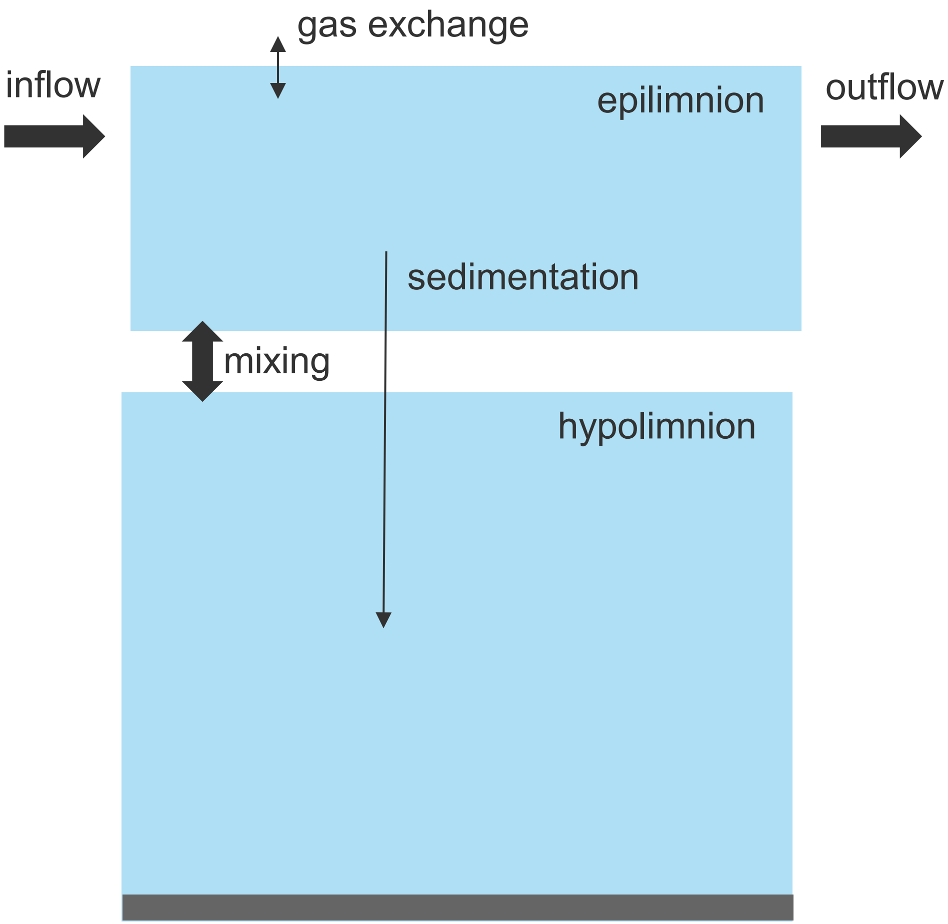
State variables:

ALG, ZOO,

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

POM: degradable/inert,

suspended/sedimented



(topic of today and next exercise)

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

Motivation

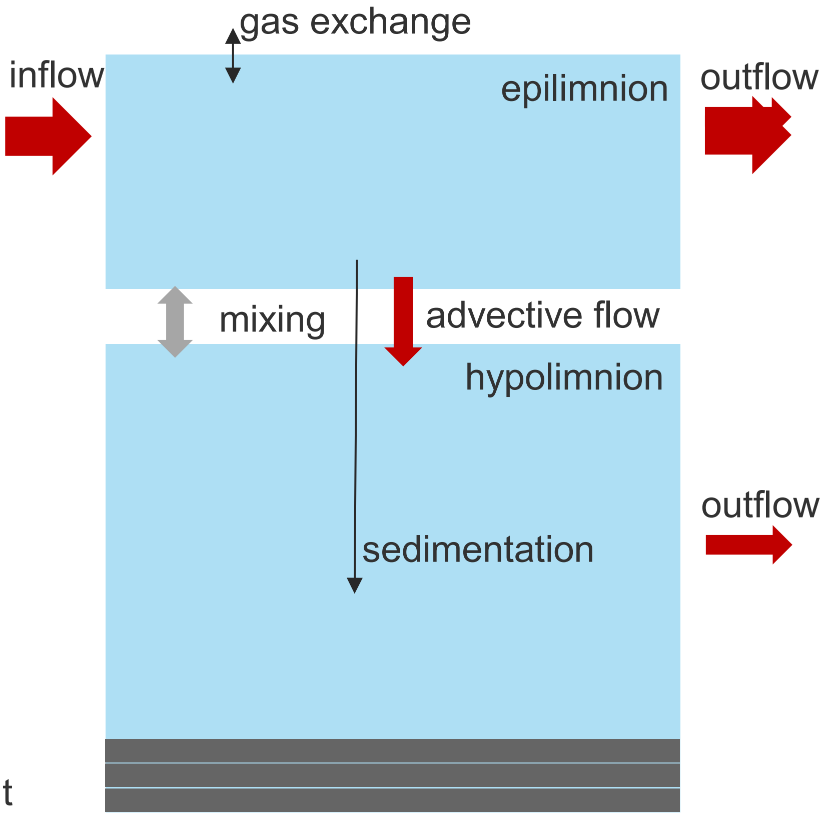
Assess management scenarios
to reduce eutrophication of a lake

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.

Topic 2: insecticide contamination and coexistence of two zooplankton groups

Motivation

Simulate effects of micropollutants

and analyze coexistence of multiple groups

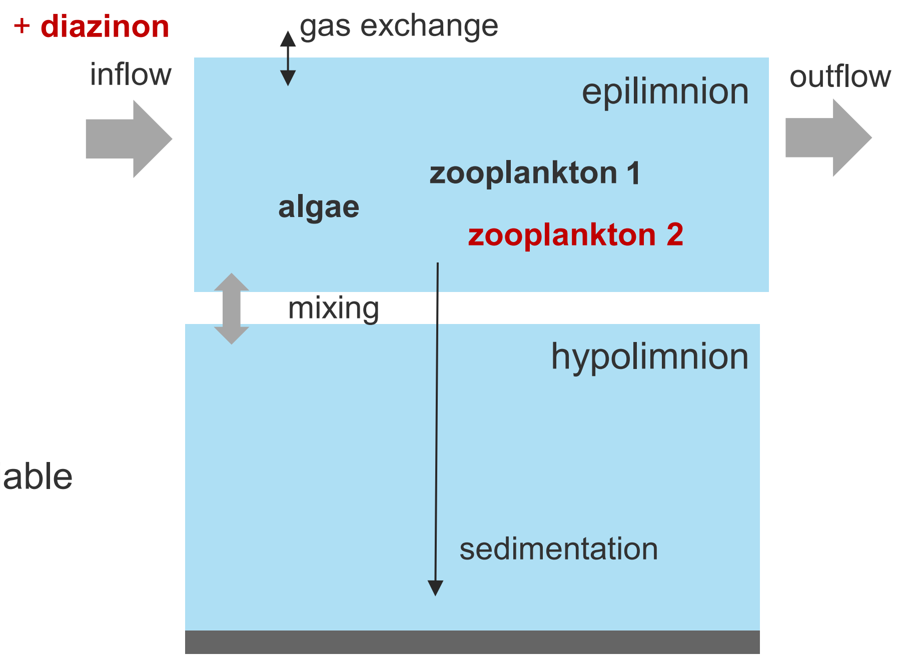
Assignment

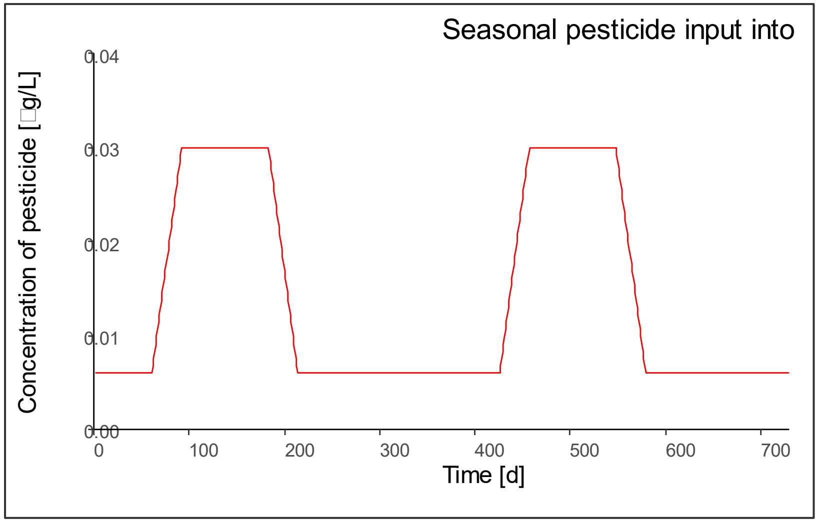
- start from model 11.4
- introduce an insecticide (diazinon) as state variable
- introduce two zooplankton groups differing in
  - half-saturation constant for food limitation
  - sensitivity towards insecticide

Goal: Try to achieve long-term coexistence

between the two zooplankton groups

by varying the parameters





Topic 3: simulation of temperature change scenarios

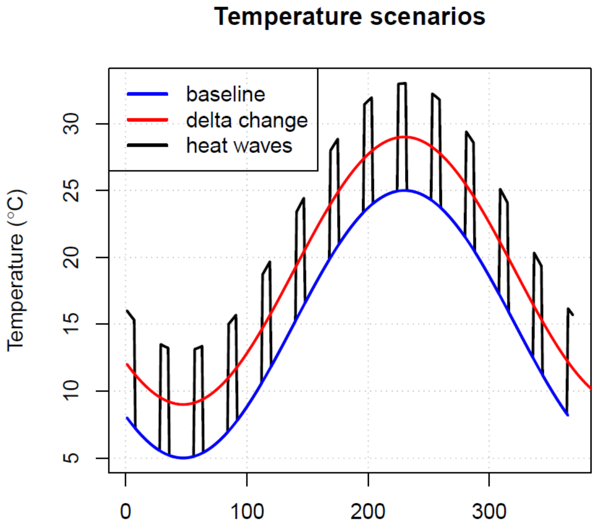
Motivation

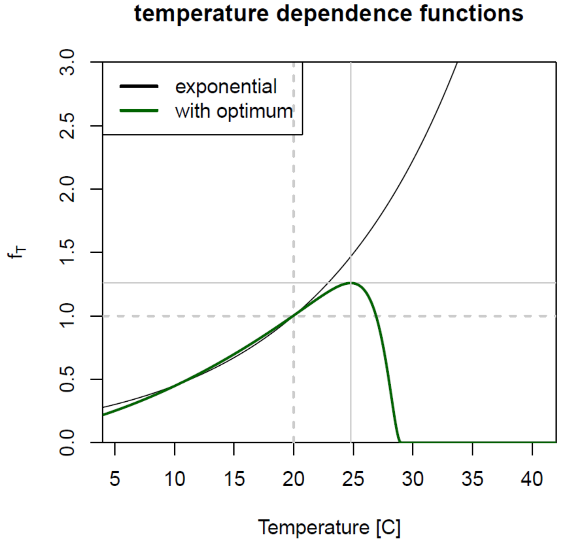
Simulate effects of temperature change scenarios.

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.


Temperature scenarios


temperature dependence functions

What do you already know about transport processes in aquatic systems?

Transport and Mixing in Lakes

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Transport processes

Advection: Transport of a substance by directed bulk motion of a fluid, in our case **transport with water flow**.

Sedimentation: Directed transport of particles in a fluid (water) caused by **gravitational forces** rather than by water flow.

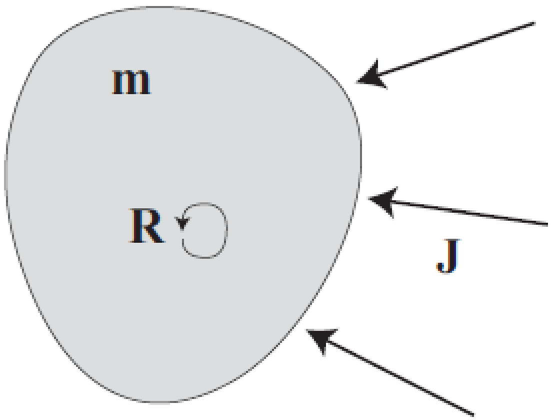
Diffusion: Undirected transport (mixing) due to molecular motion (**molecular diffusion**) or turbulent eddies (**turbulent diffusion**).

Dispersion: Mixing in flow direction due to transverse diffusion of particles between flow paths with different advective velocity ("shear flow dispersion", see transport and mixing in rivers).

Note that due to the large range of eddy sizes in turbulent flow, the distinction of "directed" (advection") and "undirected" flow may depend on the scale of a substance patch (see example on horizontal lake mixing)

Mass Balance Equations

General Principles and One Box Model



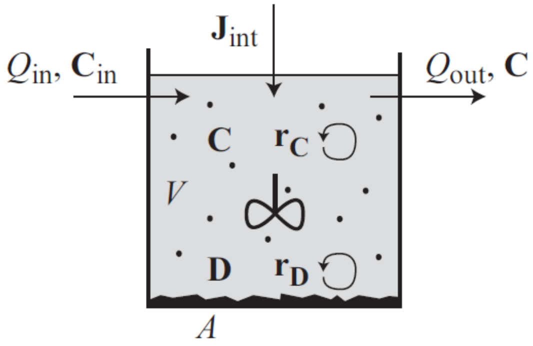
integral form:

$$\mathbf{m}(t_{\mathrm{end}}) = \mathbf{m}(t_{\mathrm{ini}}) + \int_{t_{\mathrm{ini}}}^{t_{\mathrm{end}}} \mathbf{J}(t)\,\mathrm{d}t + \int_{t_{\mathrm{ini}}}^{t_{\mathrm{end}}} \mathbf{R}(t)\,\mathrm{d}t$$

differential form:

$$\frac{\mathrm{d}\mathbf{m}}{\mathrm{d}t}(t) = \mathbf{J}(t) + \mathbf{R}(t)$$

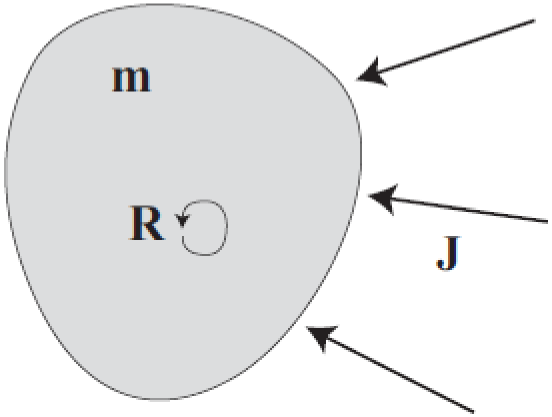
special case: one box



$$\mathbf{m} = \begin{pmatrix} V \\ VC_1 \\ VC_2 \\ \vdots \\ VC_{n_v} \\ AD_1 \\ AD_2 \\ \vdots \\ AD_{n_a} \end{pmatrix}, \quad \mathbf{J} = \begin{pmatrix} Q_{\mathrm{in}} - Q_{\mathrm{out}} \\ Q_{\mathrm{in}}C_{\mathrm{in},1} - Q_{\mathrm{out}}C_1 + J_{\mathrm{int},1} \\ Q_{\mathrm{in}}C_{\mathrm{in},2} - Q_{\mathrm{out}}C_2 + J_{\mathrm{int},2} \\ \vdots \\ Q_{\mathrm{in}}C_{\mathrm{in},n_v} - Q_{\mathrm{out}}C_{n_v} + J_{\mathrm{int},n_v} \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \quad \mathbf{R} = \begin{pmatrix} 0 \\ Vr_{C_1} \\ Vr_{C_2} \\ \vdots \\ Vr_{C_{n_v}} \\ Ar_{D_1} \\ Ar_{D_2} \\ \vdots \\ Ar_{D_{n_a}} \end{pmatrix}$$

Mass Balance Equations

General Principles and One Box Model



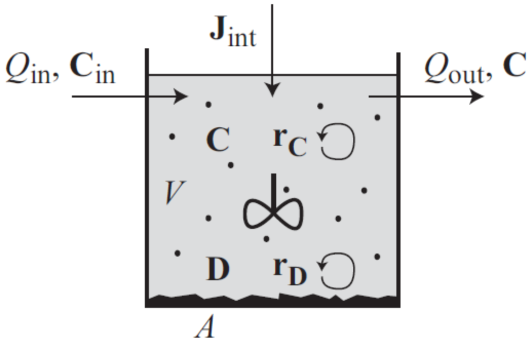
integral form:

$$\mathbf{m}(t_{\text{end}}) = \mathbf{m}(t_{\text{ini}}) + \int_{t_{\text{ini}}}^{t_{\text{end}}} \mathbf{J}(t)\,\mathrm{d}t + \int_{t_{\text{ini}}}^{t_{\text{end}}} \mathbf{R}(t)\,\mathrm{d}t$$

differential form:

$$\frac{\mathrm{d}\mathbf{m}}{\mathrm{d}t}(t) = \mathbf{J}(t) + \mathbf{R}(t)$$

special case: one box



volume change as difference of inflow - outflow

mass inflow – outflow caused by water flow (dissolved/suspended substances)

mass flow across interfaces not related to water flow (e.g. sedimentation, gas exchange)

$$\frac{\mathrm{d}V}{\mathrm{d}t} = \boxed{Q_{\text{in}} - Q_{\text{out}}}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(V\mathbf{C}\right) = \boxed{Q_{\text{in}}\mathbf{C}_{\text{in}} - Q_{\text{out}}\mathbf{C}} + \boxed{\mathbf{J}_{\text{int}}} + \boxed{V\mathbf{r}_{\mathbf{C}}}$$

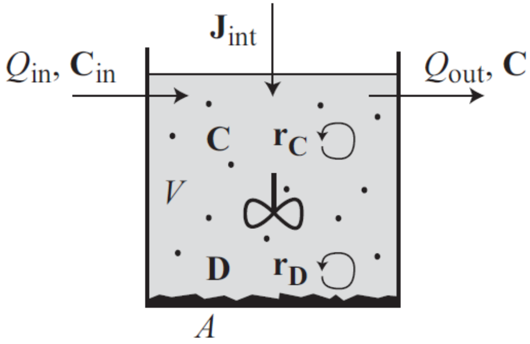
$$\frac{\mathrm{d}}{\mathrm{d}t}\left(A\mathbf{D}\right) = \boxed{A\mathbf{r}_{\mathbf{D}}}$$

effect of transformation processes

Mass Balance Equations Multiple Reactors

Multi-Reactor System

one box



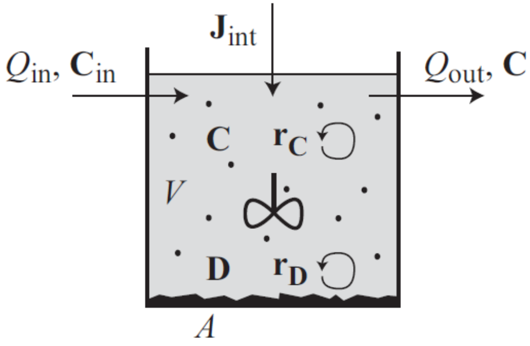
How would you discretize a lake into boxes?

How would you discretize a river into boxes?

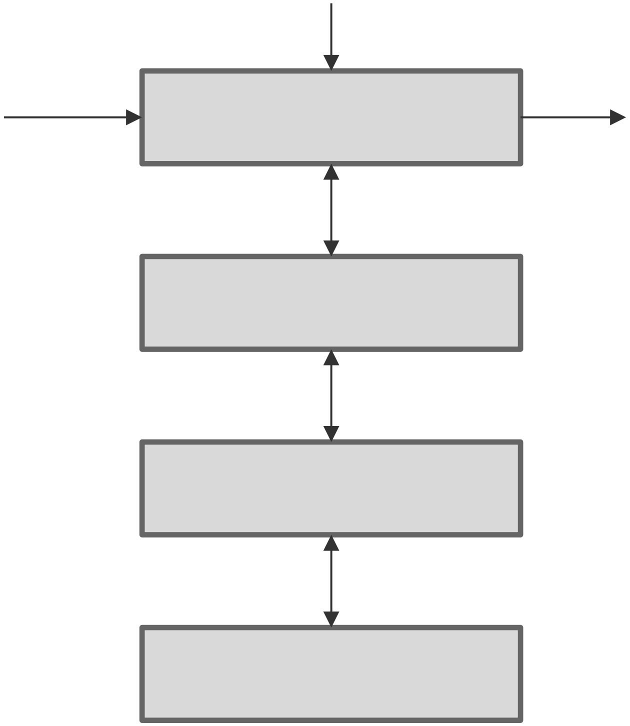
Mass Balance Equations Multiple Reactors

Multi-Reactor System

one box



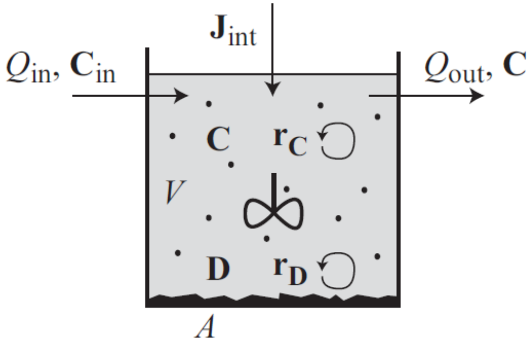
multiple boxes



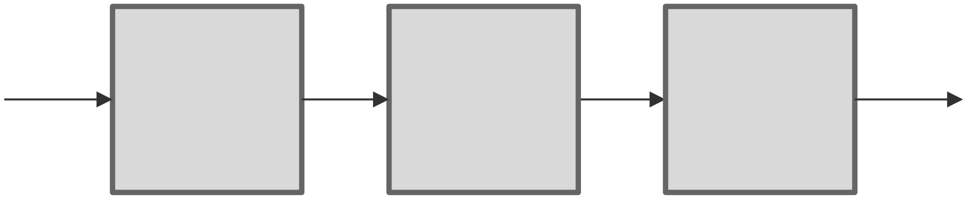
Mass Balance Equations Multiple Reactors

Multi-Reactor System

one box



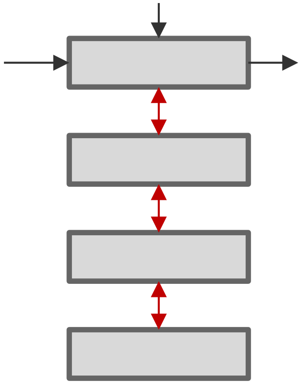
multiple boxes



Mass Balance Equations Multiple Reactors

chapter 3.4

New element: **links** between the reactors →



- need a definition of the logical flow direction (from box *x* to box *y*)
- the real flow direction depends if Q_{link}>0 or <0
- can include **advective transport** of substances with the water flow or **directed** transport such as sedimentation, where the flow depends only on the concentration in the originating box
- and **diffusive transport**, independent from the water flow, where the flow depends on concentration differences between the two boxes

Mass Balance Equations Multiple Reactors

directed mass flows

Transport proportional to the concentration of the originating reactor:

$$J_{l,j}^{\mathrm{adv}} = q_{l,j}^{\mathrm{adv}} \cdot C_j^{\mathrm{if}(q_{l,j}^{\mathrm{adv}}, k_l^{\mathrm{from}}, k_l^{\mathrm{to}})}$$

$$q_{l,j}^{\mathrm{adv}} = A\, v_{\mathrm{sed},j}$$

flow direction logical:
notation to choose concentration
from originating reactor

$$\mathrm{if}(Q, k_1, k_2) = \begin{cases} k_1 & \text{if } Q \geq 0 \\ k_2 & \text{if } Q < 0 \end{cases}$$

sedimentation:
proportionality coefficient [L^3/T]
equal to cross-sectional area *A*
times sedimentation velocity v_{sed}

Mass Balance Equations Multiple Reactors

diffusive mass flows

Diffusive exchange leads to a flux proportional to the concentration difference across the interface:

$$J_{l,j}^{\mathrm{diff}} = q_{l,j}^{\mathrm{diff}} \cdot \left(C_j^{k_l^{\mathrm{from}}} - C_j^{k_l^{\mathrm{to}}}\right) \qquad q_{l,j}^{\mathrm{diff}} = A\,\frac{D_j}{L_{\mathrm{diff}}}$$

q^{diff}: proportionality coefficient [L^3/T] equal to the cross-sectional area A [L^2] times the diffusion coefficient D [L^2/T] divided by the thickness of the diffusive layer L_{diff} [L]

Mass Balance Equations Multiple Reactors

water flow from reactor k into other reactors

water flow from other reactors into reactor k

$$\frac{\mathrm{d}V^k}{\mathrm{d}t} = \boxed{Q^k_{\mathrm{in}} - Q^k_{\mathrm{out}}} - \boxed{\sum_{l \text{ with } k_l^{\mathrm{from}}=k} Q_l} + \boxed{\sum_{l \text{ with } k_l^{\mathrm{to}}=k} Q_l}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(V^k\mathbf{C}^k\right) = \boxed{Q^k_{\mathrm{in}}\mathbf{C}^k_{\mathrm{in}} - Q^k_{\mathrm{out}}\mathbf{C}^k + \mathbf{J}^k_{\mathrm{int}} + V^k\mathbf{r}^k_{\mathbf{C}}}$$

$$\boxed{-\sum_{l \text{ with } k_l^{\mathrm{from}}=k}\left(Q_l\mathbf{C}^{\mathrm{if}(Q_l,k_l^{\mathrm{from}},k_l^{\mathrm{to}})} + \mathbf{J}_l\right)}$$

mass flow from reactor k into other reactors

$$\boxed{+\sum_{l \text{ with } k_l^{\mathrm{to}}=k}\left(Q_l\mathbf{C}^{\mathrm{if}(Q_l,k_l^{\mathrm{from}},k_l^{\mathrm{to}})} + \mathbf{J}_l\right)}$$

mass flow from other reactors into reactor k

equations for each reactor k as in the 1 box case

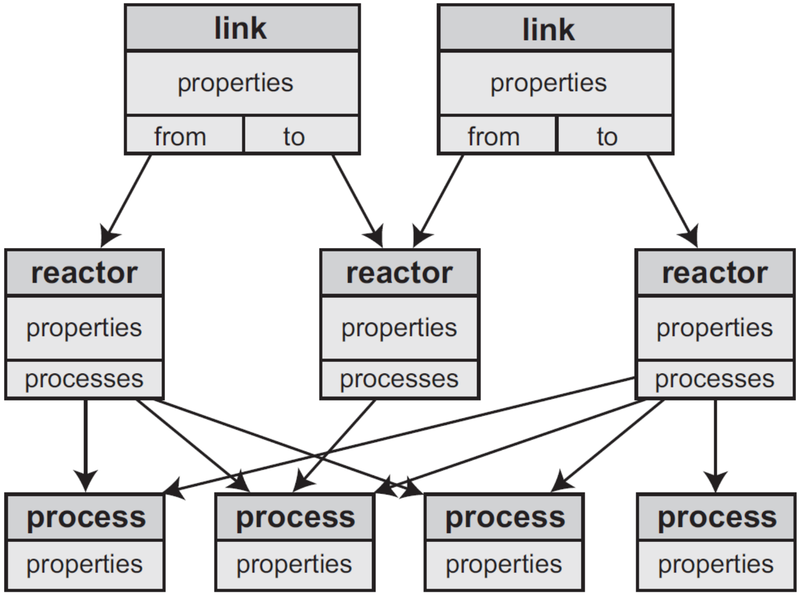
$$\frac{\mathrm{d}}{\mathrm{d}t}\left(A^k\mathbf{D}^k\right) = \boxed{A^k\mathbf{r}^k_{\mathbf{D}}}$$

$$\mathrm{if}(Q,k_1,k_2) = \begin{cases} k_1 & \text{if } Q \geq 0 \\ k_2 & \text{if } Q < 0 \end{cases}$$

flow direct. logical: notation to choose concentration from originating reactor

Mass Balance Equations

Multi-Reactor System



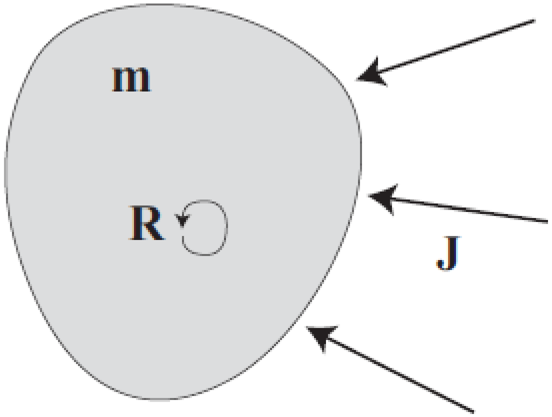
Implementation in Ecosim:

```
link <-
   new(Class       = "link",
       name        = "Metalimnion",
       from        = "Epi",
       to          = "Hypo",
       flow        = 0,
       qadv.gen    = 0,
       qadv.spec   = list(C.POMD = expression(v.sed.POM*A),
                          C.POMI = expression(v.sed.POM*A)),
       qdiff.gen   = expression(A/h.meta*Kz),
       qdiff.spec = 0)
```

Mass Balance Equations

Continuous System in Three Dimensions

chapter 3.4

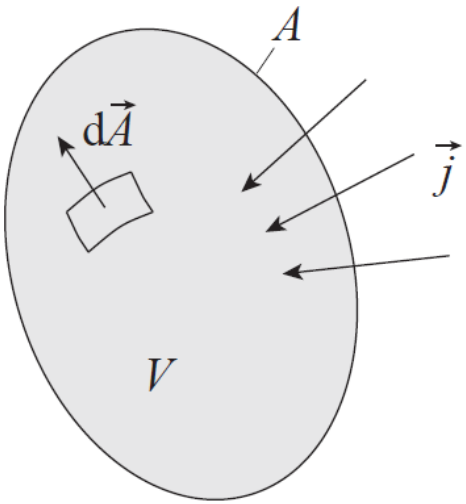


integral form:

$$\mathbf{m}(t_{\text{end}}) = \mathbf{m}(t_{\text{ini}}) + \int_{t_{\text{ini}}}^{t_{\text{end}}} \mathbf{J}(t)\,\mathrm{d}t + \int_{t_{\text{ini}}}^{t_{\text{end}}} \mathbf{R}(t)\,\mathrm{d}t$$

differential form:

$$\frac{\mathrm{d}\mathbf{m}}{\mathrm{d}t}(t) = \mathbf{J}(t) + \mathbf{R}(t)$$



$$\mathbf{m}(t) = \int_V \boldsymbol{\rho}(\vec{x},t)\,\mathrm{d}V$$

total mass = volume integral of mass density (mass per volume)

$$\mathbf{J}(t) = -\int_A \vec{\mathbf{j}}(\vec{x},t)\cdot\mathrm{d}\vec{A}$$

net total flux = surface integral of flux density

$$\mathbf{R}(t) = \int_V \mathbf{r}(\vec{x},t)\,\mathrm{d}V$$

net transformation rate = volume integral of transformation rate per volume

Mass Balance Equations

Continuous System in Three Dimensions

3D - Advection-Diffusion-Reaction equation

$$\frac{\partial C}{\partial t} + \overbrace{\frac{\partial (v_x C)}{\partial x} + \frac{\partial (v_y C)}{\partial y} + \frac{\partial (v_z C)}{\partial z}}^{\text{advection}}$$

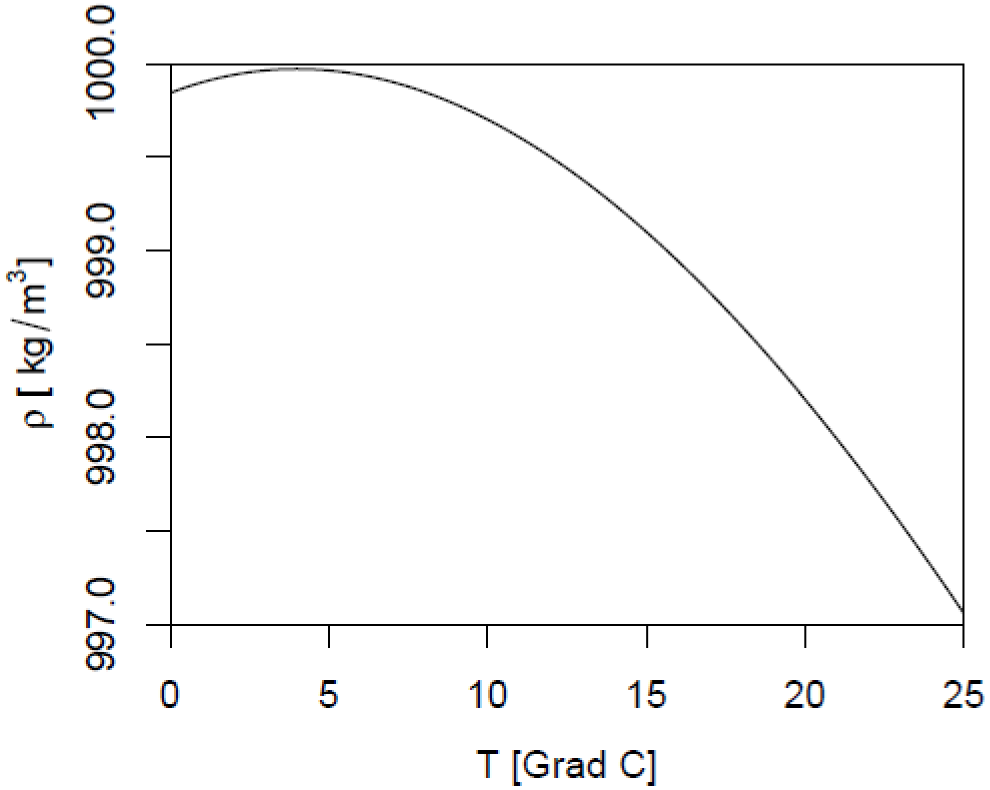
$$= \underbrace{\frac{\partial}{\partial x}\left(D_x \frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_y \frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial z}\left(D_z \frac{\partial C}{\partial z}\right)}_{\text{diffusion}} + \underset{\text{reaction}}{r}$$

Transport and Mixing in Lakes

Density of Water

chapter 6.1.1

The density of water is temperature dependent with a maximum at 4°C



Despite the weakness of this dependence, it has a very high effect on aquatic ecosystems.

Transport and Mixing in Lakes

Density Stratification of Water in a Lake

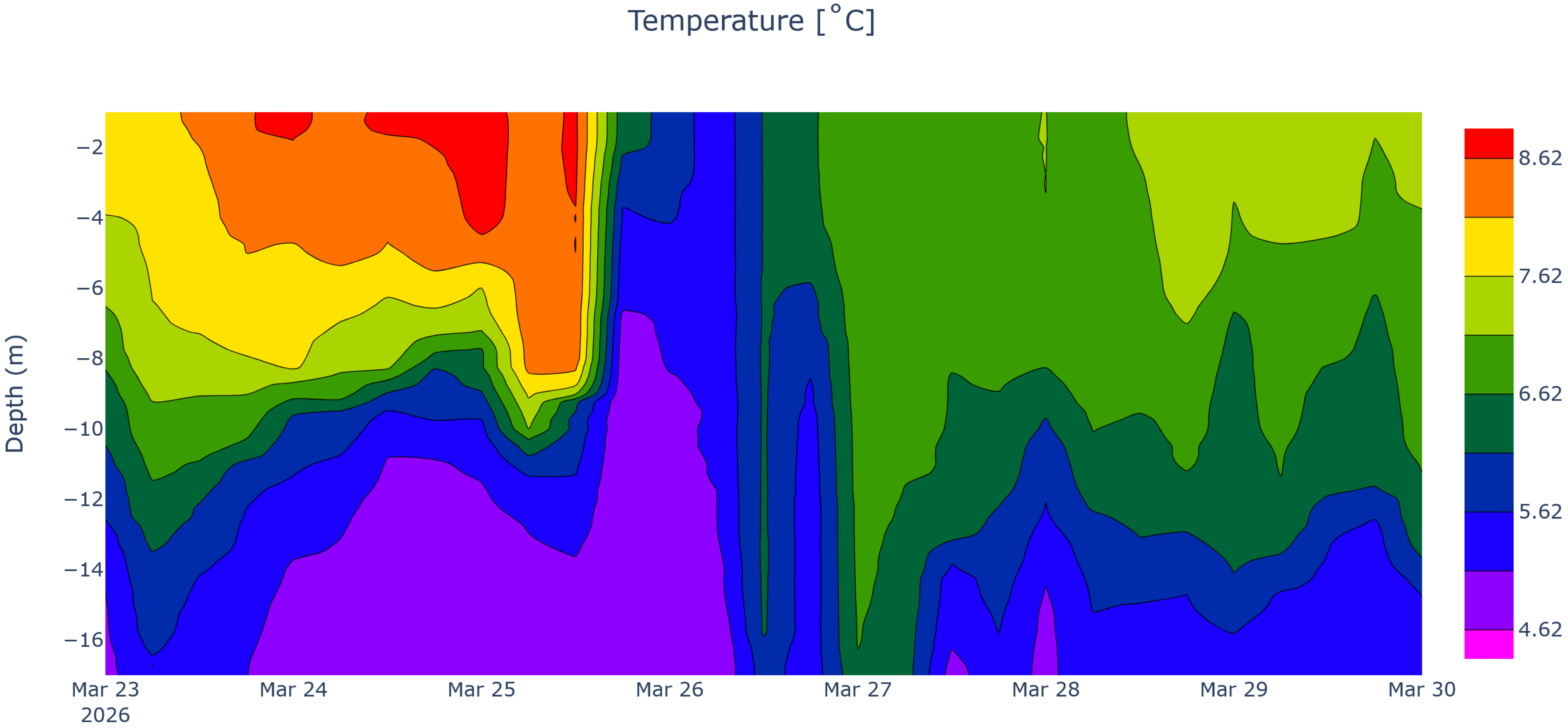
Spring/summer: Heating from the top leads to strong stratification of the water column:

- **Epilimnion**: The top 5-15 m of the lake contains warm water with stratification of the top layer during the day. However, wind and cooling during the night leads to a relatively well-mixed surface layer.
- **Hypolimnion**: The deep water zone in the lake is shielded from warming by the top layer.
- **Metalimnion**: In deep lakes, relatively thin zone with a very strong temperature gradient between epilimnion and metalimnion.

Autumn/winter: Cooling from the top and wind-induced turbulence often destroy stratification (partially or completely, depending on wind and depth). With climate change this happens less often in larger Swiss lakes! (e.g. Lake Zug)

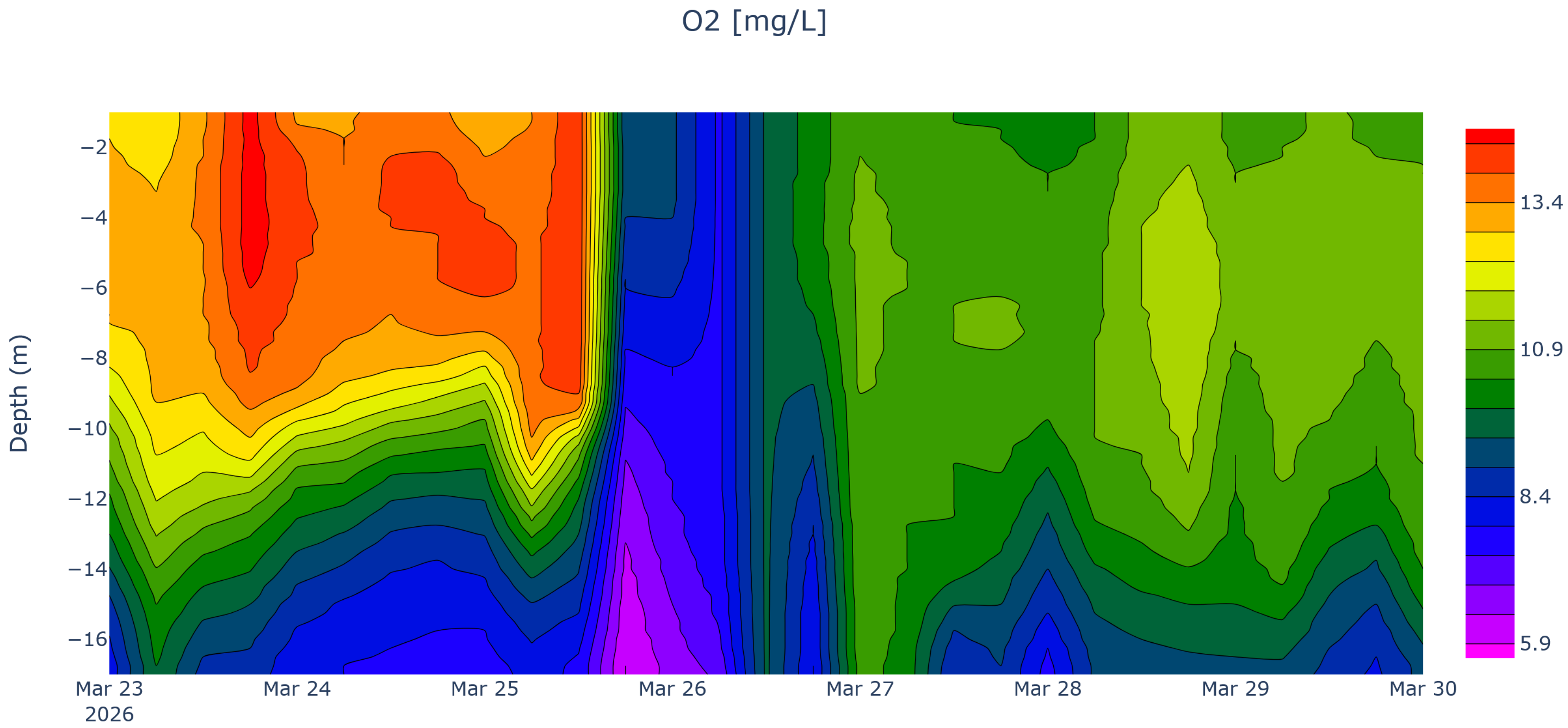
Transport and Mixing in Lakes

Eawag - Greifensee Monitoring



https://sensors-eawag.ch/greifensee/add_to_html.php?head=head&nav=nav&dst=Temperature_Profile.html

Eawag - Greifensee Monitoring



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Transport and Mixing in Lakes

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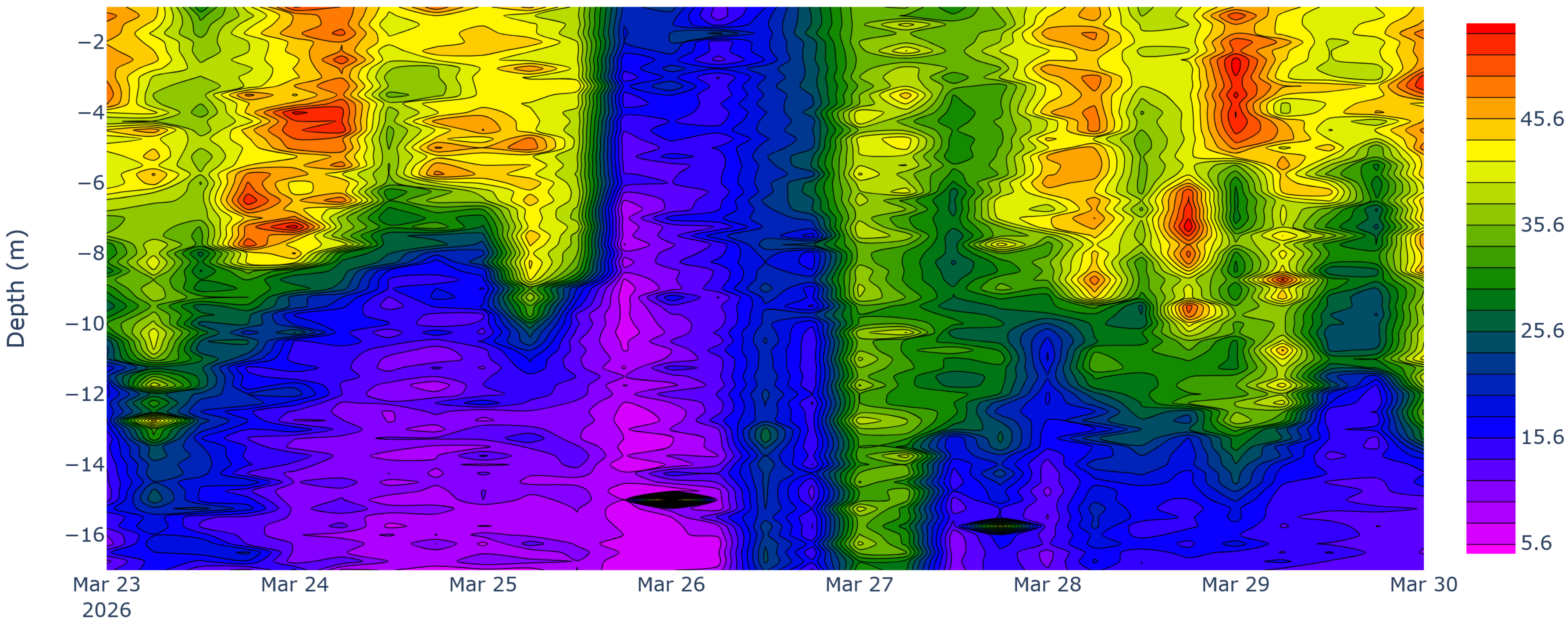
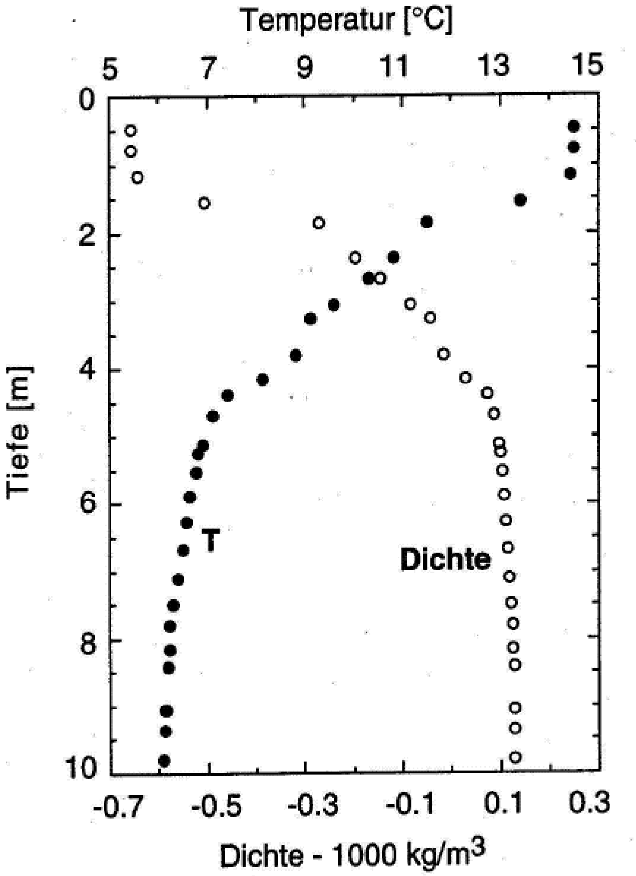
Chl-a [µg/L]



Transport and Mixing in Lakes

Stratification of Lakes



Typical temperature and density profile in spring (Lake Hallwil, spring 1992)

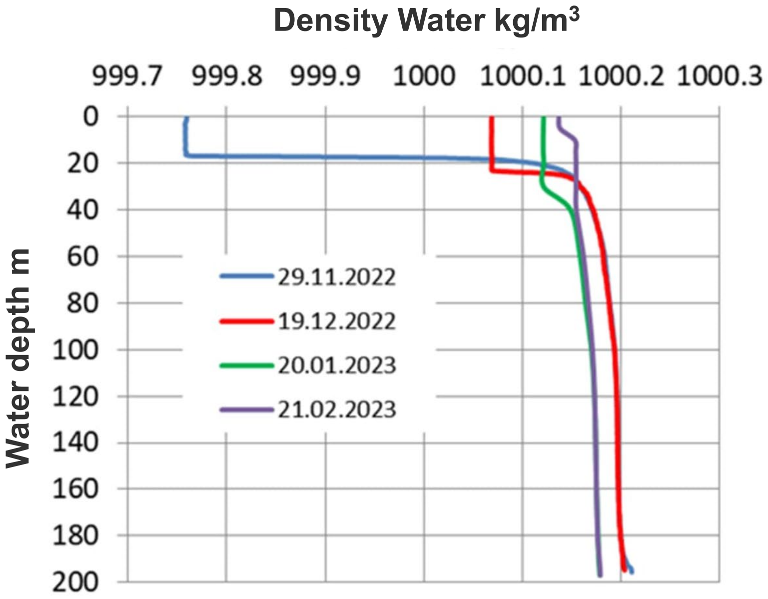


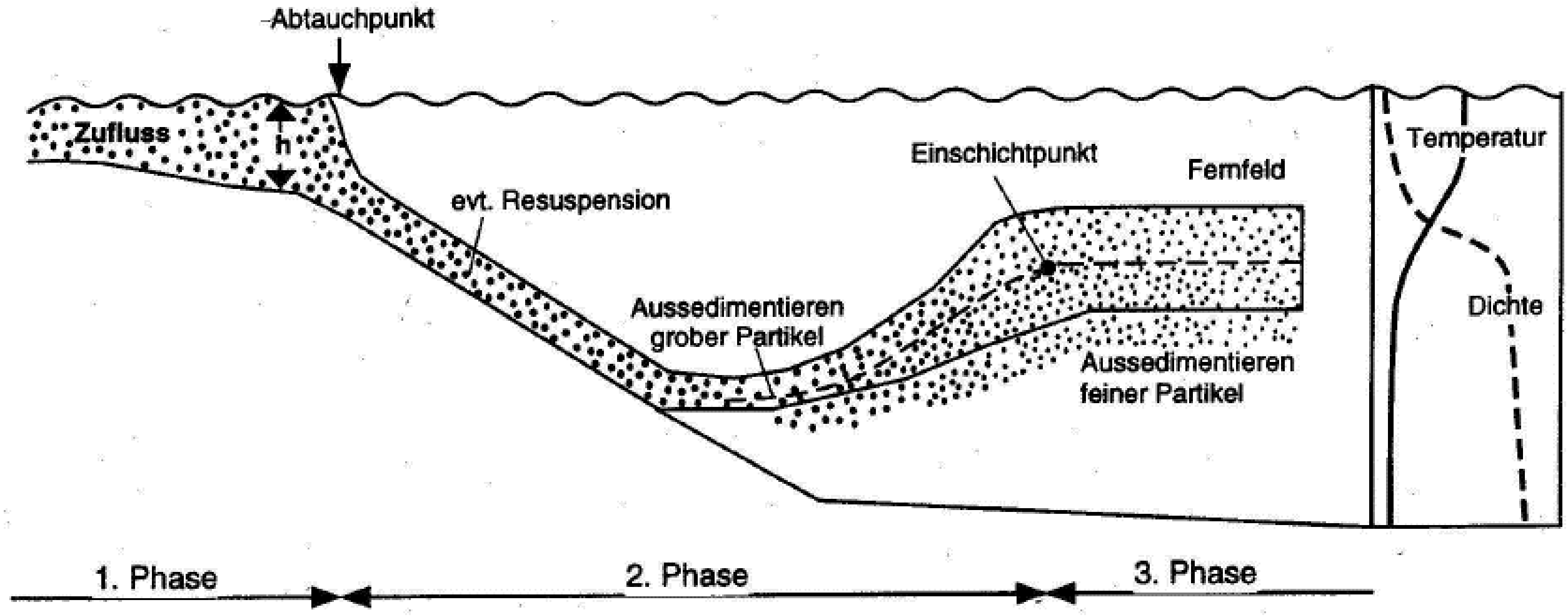
Abbildung 5: Dichteprofile des Zugersees in der Winterperiode 2022/23

https://zg.ch/dam/jcr:ba95d3d3-eabd-4694-8a71-0e9a85475748/20230821_TB%20Vorprojekt_Zirkulationsunterst%C3%BCtzung_v2.1_ohne%20Anhang.pdf

Transport and Mixing in Lakes

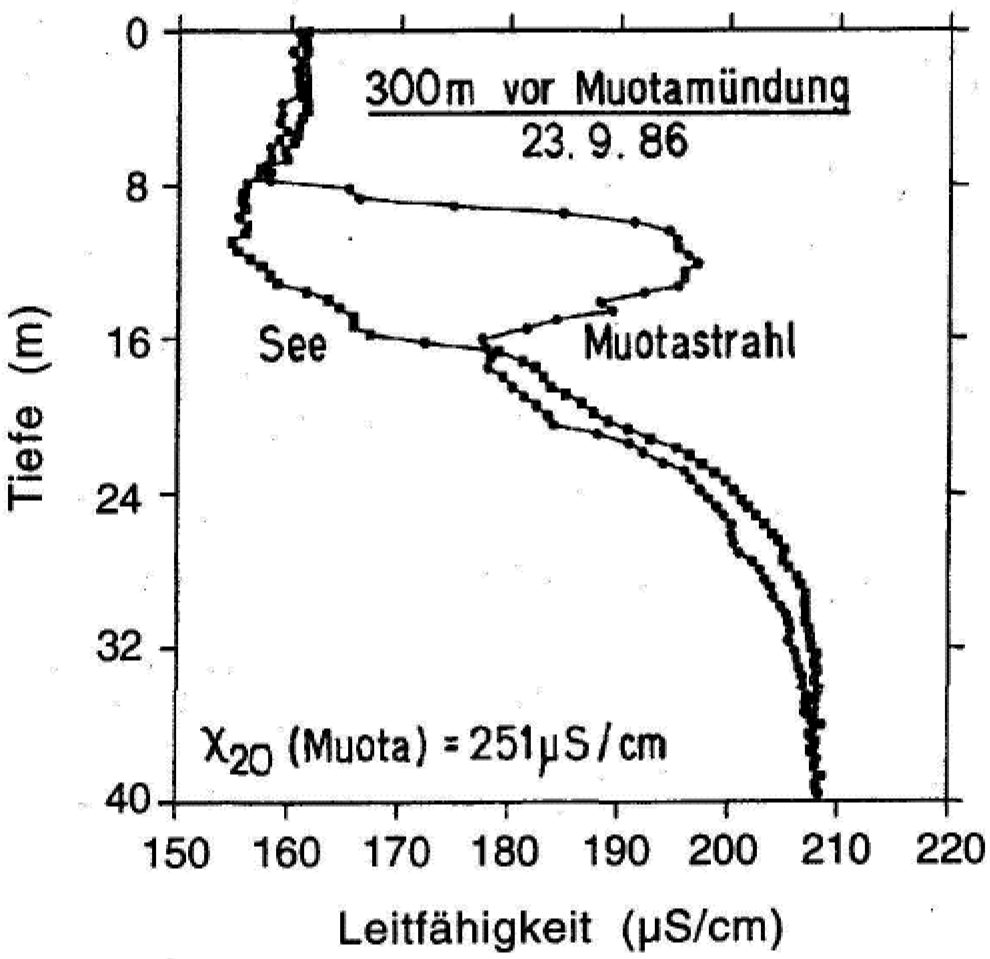
Plunging of Inflows

Illustration of plunging process of inflow into a stratified water body (Wüest):



Plunging of Inflows

Conductivity signal of a plunging inflow (of Muota into lake Lucerne):



Transport and Mixing in Lakes

Plunging of Inflows

Another illustration of a plunging inflow (Seez into Walensee near Walenstadt):

Don't go swimming close to the inflow into a lake!

Horizontal Mixing

The diffusion part of the advection-diffusion-reaction equation reduced to two dimensions provides an approximate description of horizontal mixing:

$$\frac{\partial C}{\partial t} = K_{xy} \left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} \right)$$

coefficient of horizontal turbulent diffusion

The solution of this equation for a substance point source of mass m, distributed over a depth h at time $t = 0$ is given by a normal distribution with linearly increasing variance in time:

$$C(x, y, t) = \frac{m}{h} \frac{1}{2\pi} \frac{1}{\sigma_{xy}(t)^2} \exp\left(-\frac{(x - x_0)^2 + (y - y_0)^2}{2\sigma_{xy}(t)^2} \right)$$

$$\sigma_{xy}(t) = \sqrt{2K_{xy}t}$$

Horizontal Mixing

The width of the substance distribution can roughly be estimated by 4 times the standard deviation and thus also increases with the square root of time:

$$L_{xy}(t) \approx 4\sigma_{xy}(t) = 4\sqrt{2K_{xy}t}$$

The maximum concentrations decreases with 1/time:

$$C_{\max} \approx \frac{m}{h}\frac{1}{4\sigma_{xy}(t)^2} = \frac{m}{h}\frac{1}{8K_{xy}t}$$

A typical range for the coefficient of horizontal turbulent diffusion is:

$$K_{xy} \approx 10^4 - 10^6 \ \mathrm{m^2/d}$$

Transport and Mixing in Lakes

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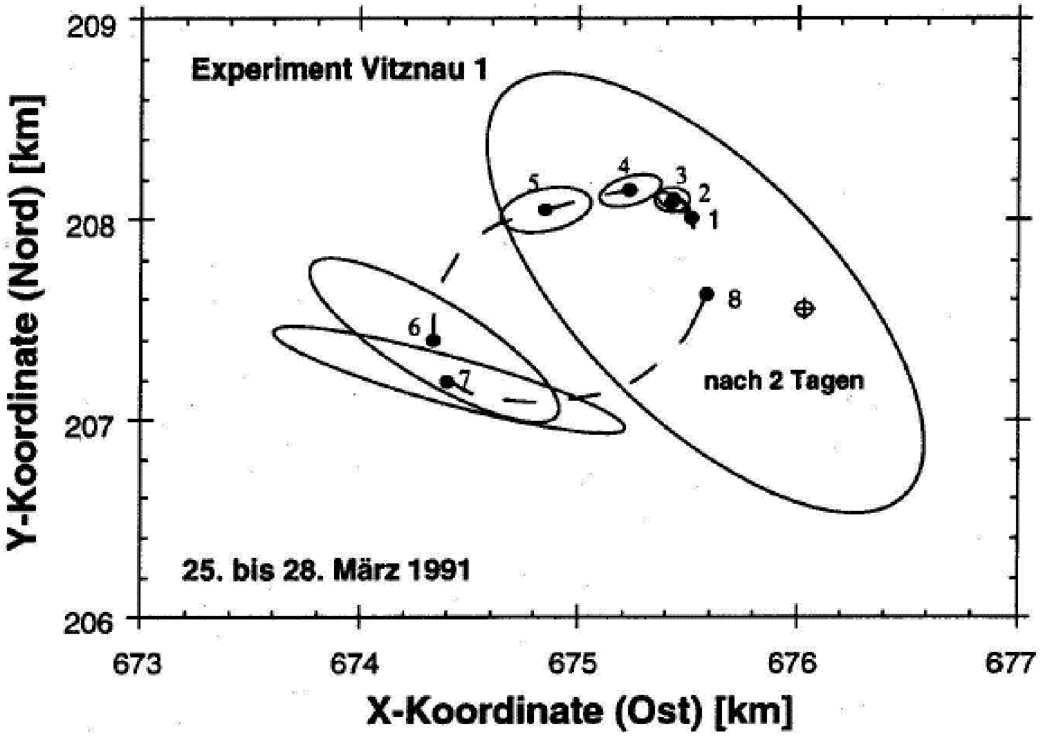
Horizontal Mixing

An example of horizontal transport and mixing of an artificial tracer cloud:



Note that large eddies initially move the whole tracer cloud while when it becomes larger, they contribute to enlarging it. This leads to an increase of the apparent coefficient of turbulent diffusion with the size of the tracer cloud.

Transport and Mixing in Lakes

Vertical Mixing

The diffusion part of the advection-diffusion-reaction equation reduced to the vertical dimension provides an approximate description of vertical mixing:

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

coefficient of vertical turbulent diffusion

The solution of this equation for a substance point source of mass m, distributed over the cross-sectional area A at time t = 0 is given by a normal distribution with linearly increasing variance in time:

$$C(z,t) = \frac{m}{A} \frac{1}{\sqrt{2\pi}} \frac{1}{\sigma_z(t)} \exp\left(-\frac{(z-z_0)^2}{2\sigma_z(t)^2} \right)$$

$$\sigma_z(t) = \sqrt{2K_z t}$$

Transport and Mixing in Lakes

Vertical Mixing

The overall size of the distribution can roughly be estimated by 4 times the standard deviation and thus also increases with the square root of time:

$$L_z(t) \approx 4\sigma_z(t) = 4\sqrt{2K_z t}$$

The maximum concentrations decreases with 1/time:

$$C_{\text{max}} \approx \frac{m}{A}\frac{1}{2\sigma_z(t)} = \frac{m}{A}\frac{1}{2\sqrt{2K_z t}}$$

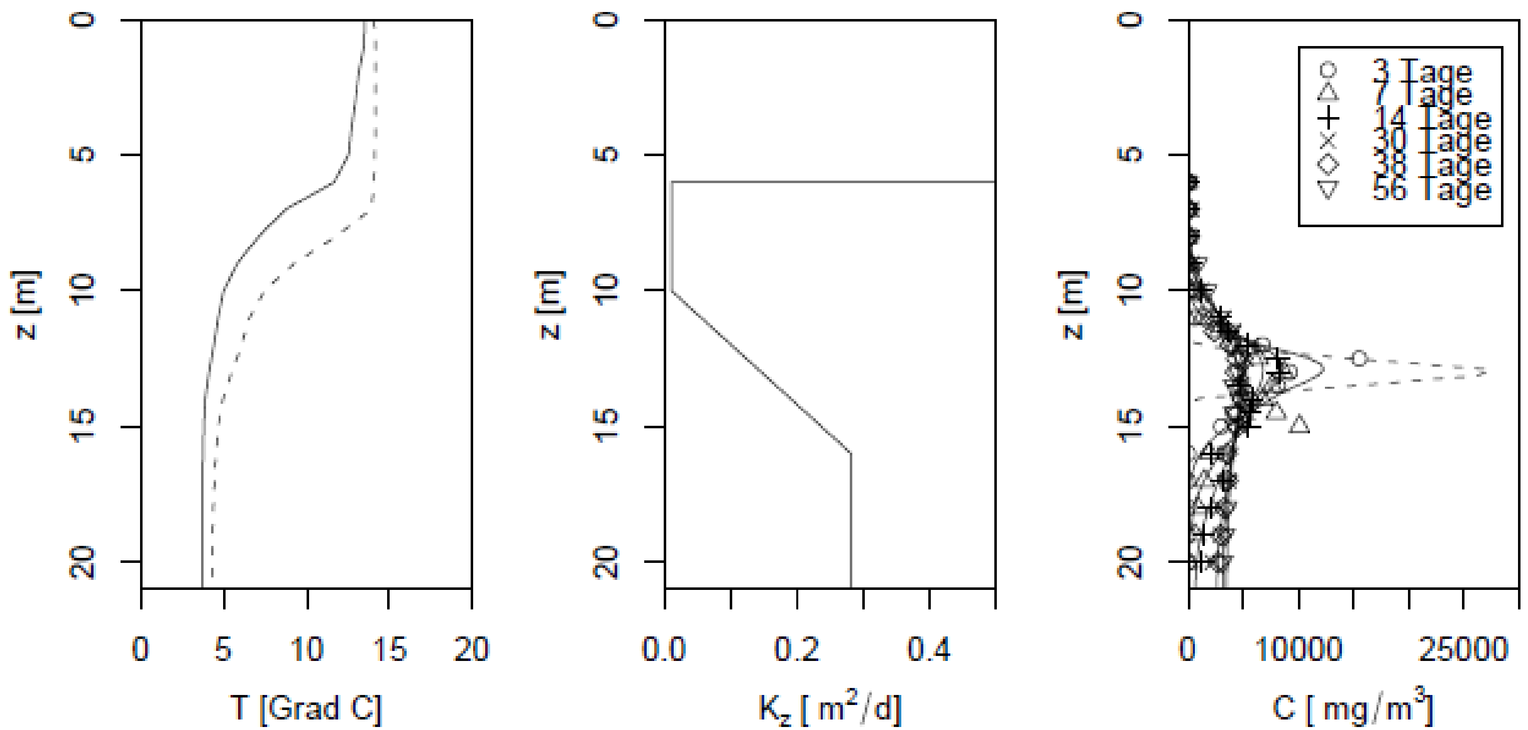
Typical ranges for the coefficient of vertical turbulent diffusion are:

$$\begin{aligned} K_{z,\text{epi}} &\approx 100\ \text{m}^2/\text{d} && \approx \text{complete mixing} \\ K_{z,\text{meta}} &\approx 0.01 - 0.1\ \text{m}^2/\text{d} && \left.\right\} \\ K_{z,\text{hypo}} &\approx 0.1 - 10\ \text{m}^2/\text{d} && \left.\right\} \text{during stratification} \end{aligned}$$

Transport and Mixing in Lakes

Vertical Mixing

The figure below demonstrates vertical diffusion of a tracer in lake Cadagno. The strong density gradient induced by the temperature gradient in the metalimnion prevents spreading of the tracer into the epilimnion:



Transport and Mixing in Lakes

Sedimentation

Imagine you are a particle floating around in a lake.

What do you think are important properties that influence if you are sedimented or you stay in suspension?

Sedimentation

chapter 6.2

Estimate of the sedimentation velocity:

$$v_{\mathrm{sed}} = f_{\mathrm{st}} \frac{g}{18} \frac{\rho_{\mathrm{p}} - \rho_{\mathrm{w}}}{\mu} d_{\mathrm{p}}^2$$

g: gravitational acceleration (LT^{-2}).
ρ_{p}: density of the particle (ML^{-3}).
ρ_{w}: density of water (ML^{-3}).
μ: dynamic viscosity of water ($\mathrm{ML}^{-1}\mathrm{T}^{-1}$).
d_{p}: particle diameter (L).
f_{st}: shape factor (1.0 for spheres).

Typical sedimentation velocities of algae, organic particles, clay and silt particles are in the following range:

$$\begin{aligned} v_{\mathrm{sed,ALG}} &\approx 0.0 - 0.3\ \mathrm{m/d} \\ v_{\mathrm{sed,POM}} &\approx 0.2 - 2.5\ \mathrm{m/d} \\ v_{\mathrm{sed,clay}} &\approx 0.3 - 1.0\ \mathrm{m/d} \\ v_{\mathrm{sed,silt}} &\approx 3.0 - 30\ \mathrm{m/d} \end{aligned}$$

These estimates allow us to get an estimate of the sedimentation flux in the lake:

$$J_{\mathrm{sed,POM}} = A_{\mathrm{sed}}\, v_{\mathrm{sed,POM}}\, C_{\mathrm{POM}}$$

Gas Exchange

chapter 6.3

Equilibrium concentration according to Henry's law:

$$C_{\mathrm{w,eq}}(C_{\mathrm{a}}) = \frac{C_{\mathrm{a}}}{H}$$

$C_{\mathrm{w,eq}}(C_{\mathrm{a}})$	equilibrium concentration in water depending on T and p
C_{a}	concentration in the air
H	Henry's law constant, O_2 in water at 25°C, 1 atm: 0.032

If gas is produced or consumed:

Gas exchange flux between the atmosphere and the water

$$J_{\mathrm{gasex}} = A\, v_{\mathrm{ex}} \left(C_{\mathrm{w,eq}}(C_{\mathrm{a}}) - C_{\mathrm{w}} \right)$$

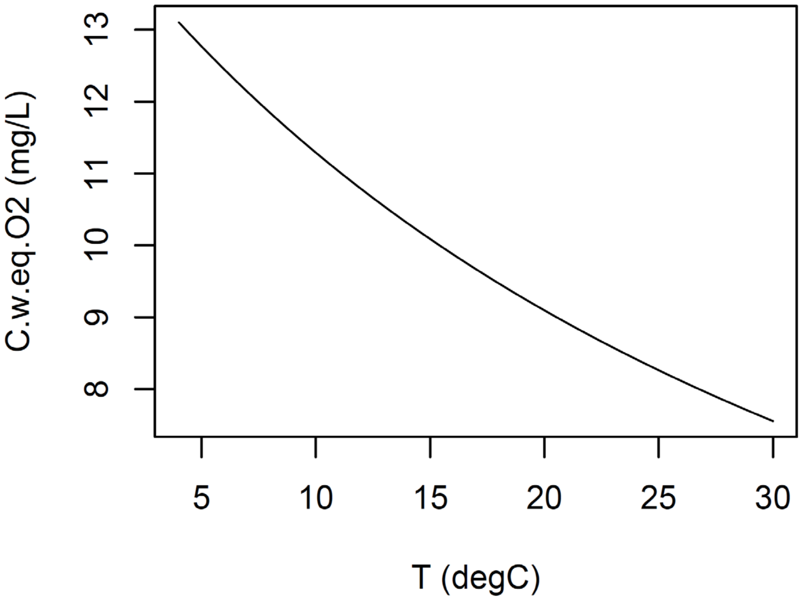
[M/T] [L^2] [L/T] [M/L^3]

Gas Exchange

chapter 6.3

Equilibrium concentration of O_2 in water depending on T and air pressure p:

$$C_{\mathrm{w,eq,O_2}}(T,p) = \exp\big(7.7117 - 1.31403\log(T/1^{\circ}\mathrm{C} + 45.93)\big) \cdot 1\,\mathrm{gO/m^3} \cdot \frac{p}{1013.25\,\mathrm{hPa}}$$



heat stress can also be due to lack of oxygen

Two Box Lake Model

chapter 11.4

Important substance fluxes not related to directed water transport:

Exchange of oxygen at the lake surface between atmosphere and epilimnion:

$$J_{\mathrm{gasex}} = A\, v_{\mathrm{ex}} \left(C_{\mathrm{w,eq}}(C_{\mathrm{a}}) - C_{\mathrm{w}} \right)$$

Exchange between epilimnion and hypolimnion through turbulent diffusion (all dissolved and suspended substances or organisms):

$$\mathbf{J}^{\mathrm{epi\,hypo}} = A_{\mathrm{meta}} \frac{K_{\mathrm{z,meta}}}{h_{\mathrm{meta}}} \left(\mathbf{C}^{\mathrm{epi}} - \mathbf{C}^{\mathrm{hypo}} \right)$$

Sedimentation flux of dead organic particles from epilimnion to hypolimnion:

$$J_{\mathrm{POM}}^{\mathrm{epi\,hypo}} = A_{\mathrm{meta}}\, v_{\mathrm{sed,POM}}\, C_{\mathrm{POM}}$$

Note: For technical reasons (sediment layer part of box), we describe sedimentation from the hypolimnion to the sediment formally as a transformation process

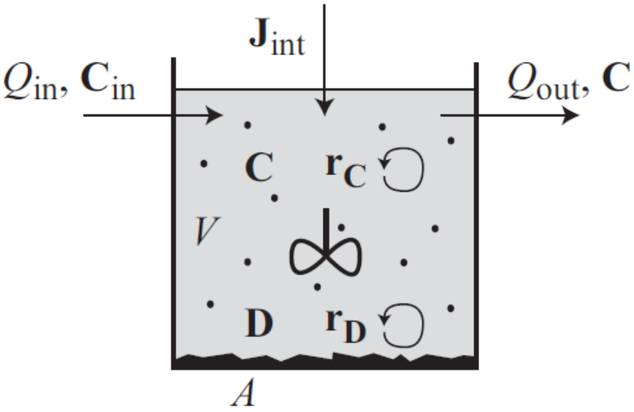
Transport and Mixing in Lakes

Comment on Dissolved/Suspended and Attached Substances

In our mixed reactors, we distinguish substances that are dissolved or suspended in the water and transported with water flow and substances that are attached/ sedimented/sessile on surfaces.

Substances in the water column are characterized by concentrations, C, (mass per volume), substances on surfaces by surface densities, D, (mass per area).

For processes involving substances of both types (e.g. mineralization of sedimented particles consuming dissolved oxygen from the water column), we have to consider this “geometric” difference.



We have to calculate total transformation rates $A\,r_D$, $V\,r_C$ to calculate fluxes between different types of substances.

This leads to conversion factors of A/V or V/A if converting per area into per volume rates or vice versa

`ecosim` does this automatically for us!

Biogeochemical-Ecological Lake Model

chapter 11.4

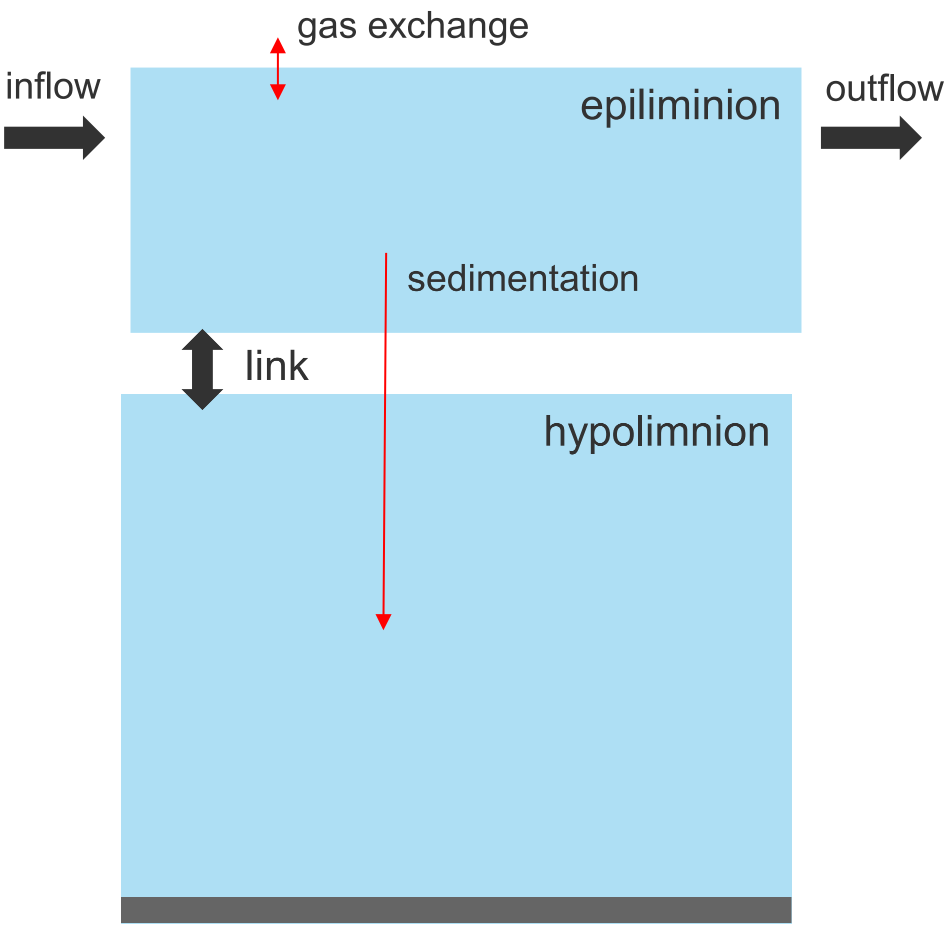
State variables:

ALG, ZOO,

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

POM: degradable/inert,

suspended/sedimented



Biogeochemical-Ecological Lake Model

Processes and stoichiometry of the biogeochemical-ecological lake model

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		$(1-f_I)Y_{\mathrm{ALG,death}}$	$f_I Y_{\mathrm{ALG,death}}$		
Growth of zooplankton	$+$	$+$		$-$	$\frac{-1}{Y_{\mathrm{ZOO}}}$	1	$\frac{(1-f_I)f_e}{Y_{\mathrm{ZOO}}}$	$\frac{f_I f_e}{Y_{\mathrm{ZOO}}}$		
Respiration of zoopl.	$+$	$+$		$-$		-1				
Death of zooplankton	$0/+$	$0/+$		$0/+$		-1	$(1-f_I)Y_{\mathrm{ZOO,death}}$	$f_I Y_{\mathrm{ZOO,death}}$		
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

Numerical Solution of ODE Models

chapter 5.4

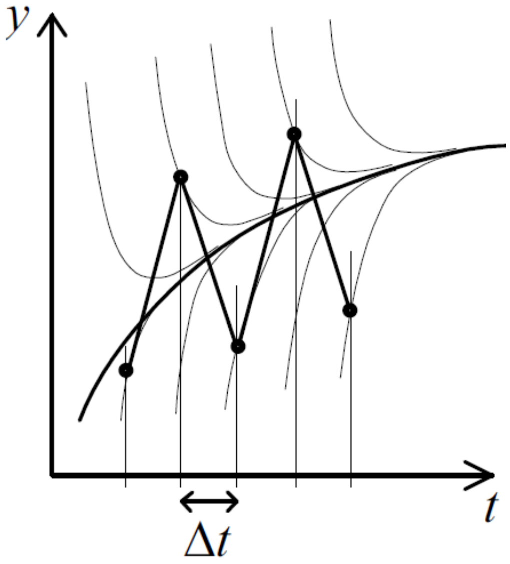
$$\frac{d\mathbf{y}}{dt} = \mathbf{g}(\mathbf{y}, t) \qquad t_j = t_0 + j \cdot \Delta t \qquad \mathbf{y}_j = \mathbf{y}(t_j)$$

explicit Euler scheme

$$\mathbf{y} \rightarrow \mathbf{y}_j$$

$$\frac{d\mathbf{y}}{dt} \rightarrow \frac{\mathbf{y}_{j+1} - \mathbf{y}_j}{\Delta t}$$

$$\mathbf{y}_{j+1} = \mathbf{y}_j + \Delta t\, \mathbf{g}(\mathbf{y}_j, t_j)$$

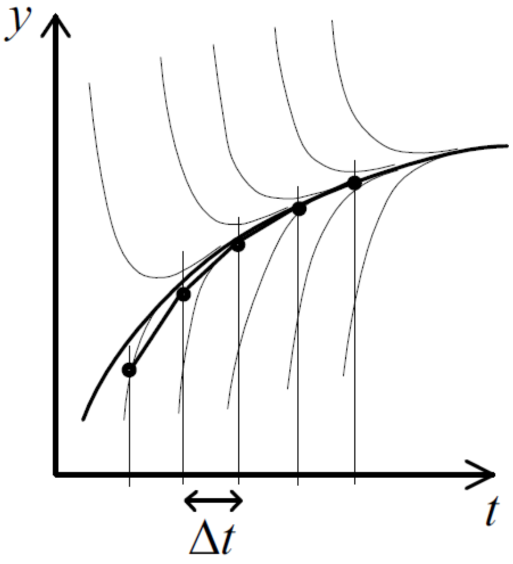


implicit Euler scheme

$$\mathbf{y} \rightarrow \mathbf{y}_j$$

$$\frac{d\mathbf{y}}{dt} \rightarrow \frac{\mathbf{y}_j - \mathbf{y}_{j-1}}{\Delta t}$$

$$\mathbf{y}_{j+1} = \mathbf{y}_j + \Delta t\, \mathbf{g}(\mathbf{y}_{j+1}, t_{j+1})$$



→ explicit schemes are faster for a single step, implicit schemes can take larger steps.

Numerical Solution of ODE Models

Numerical implementation in `ecosim`

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 get the description of R packages by entering the address
https://cran.r-project.org/package=deSolve or https://cran.r-project.org/package=ecosim
You find there the links to the reference manuals (or search them in the www).

Function `ode` in `deSolve` with 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"), ...)
```

Function `calcres` in `ecosim` allows you to choose the method and passes further arguments to `ode` (…):

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

Assignments

There will be an **oral exam in the two weeks** after the semester
8.-12. June 25 (1.-5 June if needed).
It is your responsibility to register/deregister in time.

During the semester you will develop and implement your own model (in teams of two people), interpret simulation results and perform a sensitivity analysis. We will assign topics today.

Deadline for initial code submission: **07.05.26**

Deadline for submission of R-files, results and interpretation: **22.05.26**

This is mandatory for being admitted to the exam!
In the oral exam we will start with questions about your model before moving on to other topics.

Please use the time in the exercises to ask questions and get help!
Don’t do it last minute.

Structure of the Course - next week

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

Preparation for next week:

- Read the sections 11.3 and 11.4 about the didactical models
- think about your questions (also regarding your model assignments)