Eawag: Swiss Federal Institute of Aquatic Science and Technology

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Modelling Aquatic Ecosystems Course 701-0426-00

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- ETH zürich eawag aquatic research 80000
- 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





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 (chapter 6.1.1)
- introduction to the biogeochemical ecological lake model (11.4)

Assignments of topics for own model

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There will be an **oral exam in the second week** after the semester (7./10./11. June 24). 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: 09.05.24

Deadline for submission of R-files, results and interpretation: 24.05.24

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.





(topic of today and next exercise)

Motivation

Assess management scenarios to reduce eutrophication of a lake

<u>Assignment</u>

- Start from model 11.4
- Add a deep water extraction (outflow from hypolimnion)
- Investigate the following scenarios separately:
- 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



inflow



Topic 2: insecticide contamination and coexistence of two zooplankton groups



- introduce two zooplankton groups differing in ۰
 - half-saturation constant for food limitation
 - sensitivity towards insecticide •

۰

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





Clarification of terms

- 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 bygravitational 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 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)

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General Principles and One Box Model



 \mathbf{m}

tegral form:

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

$$\mathbf{d}\mathbf{m}$$

differential form:

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

special case: one box $Q_{in}, C_{in} \xrightarrow{J_{int}} Q_{out}, C$

 $\cdot \mathbf{C} \mathbf{r}_{\mathbf{C}}$

A

$$= \begin{pmatrix} V \\ VC_{1} \\ VC_{2} \\ \vdots \\ VC_{n_{v}} \\ AD_{1} \\ AD_{2} \\ \vdots \\ AD_{n_{a}} \end{pmatrix}, \mathbf{J} = \begin{pmatrix} Q_{\text{in}} - Q_{\text{out}} \\ Q_{\text{in}}C_{\text{in},1} - Q_{\text{out}}C_{1} + J_{\text{int},1} \\ Q_{\text{in}}C_{\text{in},2} - Q_{\text{out}}C_{2} + J_{\text{int},2} \\ \vdots \\ Q_{\text{in}}C_{\text{in},n_{v}} - Q_{\text{out}}C_{n_{v}} + J_{\text{int},n_{v}} \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \mathbf{R} = \begin{pmatrix} 0 \\ Vr_{C_{1}} \\ Vr_{C_{2}} \\ \vdots \\ Vr_{C_{n_{v}}} \\ Ar_{D_{1}} \\ Ar_{D_{2}} \\ \vdots \\ Ar_{D_{n_{a}}} \end{pmatrix}$$

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General Principles and One Box Model



Multi-Reactor System



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Multi-Reactor System



Multi-Reactor System

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



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Multi-Reactor System

directed mass flows

Transport proportional to the concentration of the originating reactor:

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

flow direction logical: notation to choose concentration from originating reactor

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

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

sedimentation: proportionality coefficient [L³/T] equal to cross-sectional area A times sedimentation velocity v_{sed}

Multi-Reactor System

diffusive mass flows

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

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

 q^{diff} : proportionality coefficient [L³/T] equal to the cross-sectional area *A* times the diffusion coefficient *D* divided by the thickness of the diffusive layer L_{diff}

-







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chapter 3.4

Continuous System in Three Dimensions

m J

integral form: $\mathbf{m}(t_{\text{end}}) = \mathbf{m}(t_{\text{ini}}) + \int_{0}^{t_{\text{end}}} \mathbf{J}(t) \, \mathrm{d}t + \int_{0}^{t_{\text{end}}} \mathbf{R}(t) \, \mathrm{d}t$

differential form:

 $t_{\rm ini}$

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

total mass = volume integral of mass density

> net total flux = surface integral of flux density

net transformation rate = $\mathbf{R}(t) = \int \mathbf{r}(\vec{x}, t) \, \mathrm{d}V \qquad \text{volume integral of trans-}$ formation rate per volume



 $\mathbf{m}(t) = \int_{U} \boldsymbol{\rho}(\vec{x}, t) \, \mathrm{d}V$ $\mathbf{J}(t) = -\int \vec{\mathbf{j}}(\vec{x},t) \cdot \mathrm{d}\vec{A}$





Continuous System in Three Dimensions

3D - Advection-Diffusion-Reaction equation



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Density of Water

chapter 6.1.1

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



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



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.



Stratification of Lakes

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





Plunging of Inflows

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



Transport and Mixing in Lakes

Plunging of Inflows

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



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Plunging of Inflows

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



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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:

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

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Horizontal 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:

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

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:

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

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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.

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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:

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

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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:

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

Typical ranges for the coefficient of horizontal turbulent diffusion are:

$$\begin{split} K_{z,\mathrm{epi}} &\approx 100 \ \mathrm{m}^2/\mathrm{d} \\ K_{z,\mathrm{meta}} &\approx 0.01 - 0.1 \ \mathrm{m}^2/\mathrm{d} \\ K_{z,\mathrm{hypo}} &\approx 0.1 - 10 \ \mathrm{m}^2/\mathrm{d} \end{split}$$

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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:



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Transport and Mixing in Lakes

Sedimentation

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chapter 6.2

Estimate of the sedimentation velocity:

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

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

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

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

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

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

Gas Exchange

chapter 6.3

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Equilibrium concentration according to Henry's law:

 $C_{
m w,eq}(C_{
m a}) = rac{C_{
m a}}{H}$ $C_{
m w,eq}(C_{
m a})$ equilibrium concentration in water depending on T and p $C_{
m a}$ 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 transfer flux between the atmosphere and the water

$$J_{\text{gasex}} = A v_{\text{ex}} \left(C_{\text{w,eq}}(C_{\text{a}}) - C_{\text{w}} \right)$$
$$[\text{M/T}] \quad [\text{L}^2] \quad [\text{L/T}] \quad [\text{M/L}^3]$$

Gas Exchange

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

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



chapter 6.3

Two Box Lake Model

Important substance fluxes not related to directed water transport:

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

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

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

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

Sedimentation flux of dead organic particles from epilimnion to hypolimnion:

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

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



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 subst.

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!

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chapter 11.4



Biogeochemical-Ecological Lake Model

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Processes and stoichiometry of the biogeochemical-ecological lake model

Process	Substances / Organisms										
	HPO_4^{2-}	NH_4^+	NO_3^-	O_2	ALG	ZOO	POMD	POMI	SPOMD	SPOMI	
	gP	gN	gN	gO	gDM	gDM	gDM	gDM	gDM	gDM	
Growth of algae NO_3^-	_		_	+	1						
Growth of algae NH_4^+	_	_		+	1						
Respiration of algae	+	+		_	-1						
Death of algae	0/+	0/+		0/+	-1		$(1-f_{\rm I})Y_{ m ALG,death}$	$f_{ m I}Y_{ m ALG,death}$			
Growth of zooplankton	+	+		_	$\frac{-1}{Y_{\rm ZOO}}$	1	$rac{(1-f_{ m I})f_{ m e}}{Y_{ m ZOO}}$	$\frac{f_{\rm I}f_{\rm e}}{Y_{\rm ZOO}}$			
Respiration of zoopl.	+	+		_		-1					
Death of zooplankton	0/+	0/+		0/+		$^{-1}$	$(1-f_{\rm I})Y_{ m ZOO,death}$	$f_{\rm I}Y_{\rm ZOO,death}$			
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	



chapter 5.4

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

explicit Euler scheme



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



implicit Euler scheme $\rightarrow y_j$ $\frac{\mathrm{d}\mathbf{y}}{\mathrm{d}t} \rightarrow \frac{\mathbf{y}_j - \mathbf{y}_{j-1}}{\Delta t}$ $\mathbf{y}_{j+1} = \mathbf{y}_j + \Delta t \, \mathbf{g}(\mathbf{y}_{j+1}, t_{j+1})$ $\overleftarrow{\Lambda t}$

 \rightarrow explicit schemes are faster for a single step, implicit schemes can take larger steps. 44

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 always get the description of R packages by entering the address <u>https://cran.r-project.org/package=deSolve</u>

or

https://cran.r-project.org/package=ecosim

You find there the links to the reference manuals (you can also google for that)

Function ode in desolve with a long list of numerical integrators available:

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

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

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- 5. Overview model structures, stability analysis, bistability, tipping points, applications in research including evolution
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- 7. Stochasticity and uncertainty. Exercise: uncertainty, stochasticity
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- Read the sections 11.3 and 11.4
- think about your questions (also regarding your model assignments)