

Modelling Aquatic Ecosystems

Course 701-0426-00

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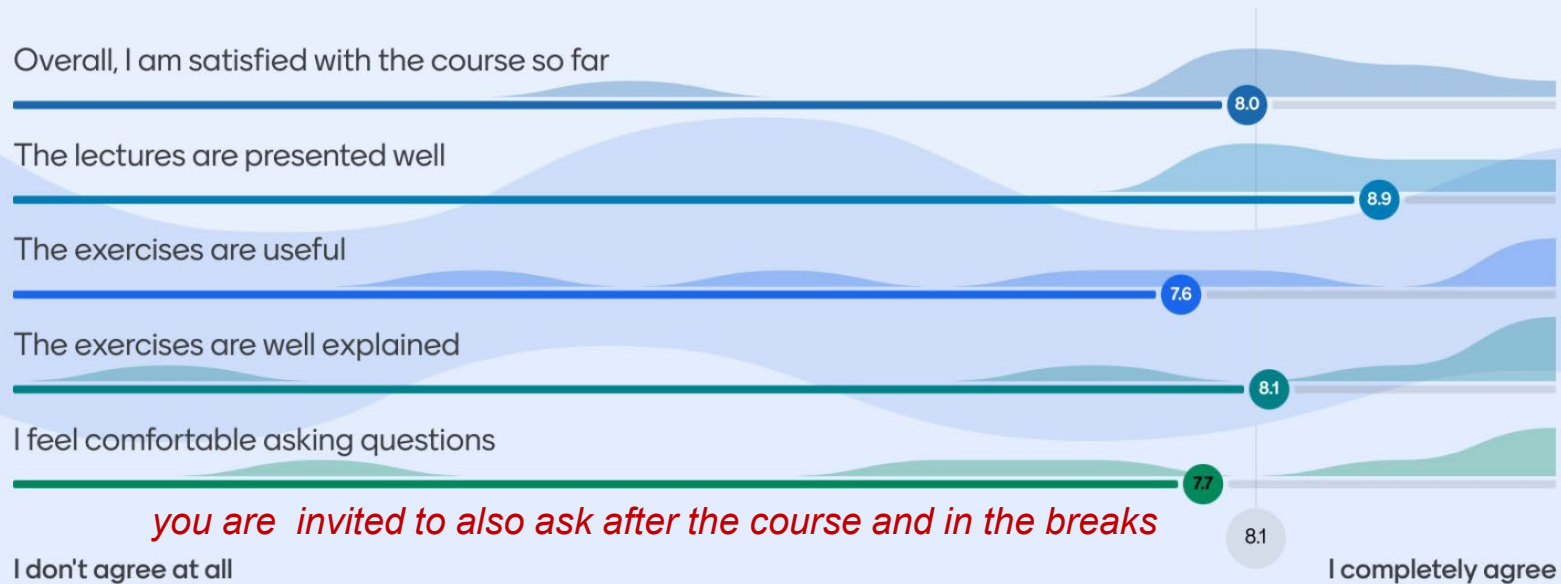
1. Introduction, principles of modelling environmental systems, mass balance in a mixed reactor, process table notation, simple lake plankton model
Exercise: R, ecosim-package, simple lake plankton model
Exercise: lake phytoplankton-zooplankton model
2. **Process stoichiometry** Exercises: analytical 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 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

Check-in about the course

Thank you for your feedback!

Course evaluation

Please rate the extent to which you were satisfied or dissatisfied about the following:



We always welcome suggestions for improvements!

Questions from last week?

Any cake recipes you want to share?

Short repetition of last week:

- Learn to calculate stoichiometric coefficients
 - from chemical substance notation (section 4.3.1)
 - using parameterized elemental mass fractions (section 4.3.2)

Today:

- general solution of stoichiometric equations: theory (section 4.3.3)
- general solution of stoichiometric equations: exercise (R-package `stoichcalc`; chapter 15)

Process table

Process i	Substances j					Rate
	s_1	s_2	s_3	\dots	s_{n_s}	
p_1	ν_{11}	ν_{12}	ν_{13}	\dots	ν_{1n_s}	ρ_1
p_2	ν_{21}	ν_{22}	ν_{23}	\dots	ν_{2n_s}	ρ_2
\vdots	\vdots	\vdots	\vdots	\ddots	\vdots	\vdots
p_{n_p}	$\nu_{n_p 1}$	$\nu_{n_p 2}$	$\nu_{n_p 3}$	\dots	$\nu_{n_p n_s}$	ρ_{n_p}

$$r_j = \sum_{i=1}^{n_p} \nu_{ij} \rho_i$$

How to derive the stoichiometric coefficients ν_{ij} ?

Idea: Conservation of mass of elements and charge constrain the stoichiometric coefficients

3 ways to derive stoichiometric coefficients:

- Chemical substance notation
- Parameterized elemental mass fractions
- General solution of stoichiometric equations

Processes i	Substances j					Rates
	s_1	s_2	s_3	\dots	s_{n_s}	
p_1	ν_{11}	ν_{12}	ν_{13}	\dots	ν_{1n_s}	ρ_1
p_2	ν_{21}	ν_{22}	ν_{23}	\dots	ν_{2n_s}	ρ_2
\vdots	\vdots	\vdots	\vdots	\ddots	\vdots	\vdots
p_{n_p}	$\nu_{n_p 1}$	$\nu_{n_p 2}$	$\nu_{n_p 3}$	\dots	$\nu_{n_p n_s}$	ρ_{n_p}
Elements k						
e_1	α_{11}	α_{12}	α_{13}	\dots	α_{1n_s}	
e_2	α_{21}	α_{22}	α_{23}	\dots	α_{2n_s}	
\vdots	\vdots	\vdots	\vdots	\ddots	\vdots	
e_{n_e}	$\alpha_{n_e 1}$	$\alpha_{n_e 2}$	$\alpha_{n_e 3}$	\dots	$\alpha_{n_e n_s}$	

ν_{ij} : stoich. coeff. = relative trans. rate of substance j in process i

α_{kj} : mass fraction of element k in substance j

$\nu_{ij}\alpha_{kj}$: rel. trans. rate by proc. i of element k contained in subst. j

Processes i	Substances j					Rates
	s_1	s_2	s_3	\dots	s_{n_s}	
p_1	ν_{11}	ν_{12}	ν_{13}	\dots	ν_{1n_s}	ρ_1
p_2	ν_{21}	ν_{22}	ν_{23}	\dots	ν_{2n_s}	ρ_2
\vdots	\vdots	\vdots	\vdots	\ddots	\vdots	\vdots
p_{n_p}	$\nu_{n_p 1}$	$\nu_{n_p 2}$	$\nu_{n_p 3}$	\dots	$\nu_{n_p n_s}$	ρ_{n_p}
Elements k						
e_1	α_{11}	α_{12}	α_{13}	\dots	α_{1n_s}	
e_2	α_{21}	α_{22}	α_{23}	\dots	α_{2n_s}	
\vdots	\vdots	\vdots	\vdots	\ddots	\vdots	
e_{n_e}	$\alpha_{n_e 1}$	$\alpha_{n_e 2}$	$\alpha_{n_e 3}$	\dots	$\alpha_{n_e n_s}$	

Mass conservation for element k in process i :

n_e constraints for each process from
"elemental" composition (incl. charge)

$$\sum_j \nu_{ij} \alpha_{kj} = 0$$

Example

ν	NH4 [mol]	NO3 [mol]	HPO4 [mol]	HCO3 [mol]	O2 [mol]	H [mol]	H2O [mol]	ALG [gDM]	ZOO [gDM]	POM [gDM]
gro.ALG.NH4	-		-	-	+	?	?	1		
gro.ALG.NO3		-	-	-	+	?	?	1		
resp.ALG	+		+	+	-	?	?	-1		
death.ALG	0/+		0/+	0/+	+	?	?	-1		+
gro.ZOO	+		+	+	-	?	?	-	1	+
resp.ZOO	+		+	+	-	?	?		-1	
death.ZOO	0/+		0/+	0/+	+	?	?		-1	+

Choice of units: We measure inorganic compounds in moles, but organic compounds and organisms as dry mass.

Moles do not make much sense for organic compounds, because even if we use chemical notation, this is not meant to represent molecules.

Extended Process Table Notation

ν		NH4 [mol]	NO3 [mol]	HPO4 [mol]	HCO3 [mol]	O2 [mol]	H [mol]	H2O [mol]	ALG [gDM]	ZOO [gDM]	POM [gDM]
gro.ALG.NH4		-		-	-	+	?	?	1		
gro.ALG.NO3			-	-	-	+	?	?	1		
resp.ALG		+		+	+	-	?	?	-1		
death.ALG		0/+		0/+	0/+	+	?	?	-1		+
gro.ZOO		+		+	+	-	?	?	-	1	+
resp.ZOO		+		+	+	-	?	?		-1	
death.ZOO		0/+		0/+	0/+	+	?	?		-1	+
α											
C	[mol]	0	0	0	1	0	0	0	0.030417	0.03	0.04025
H	[mol]	4	0	1	1	0	1	2	0.07	0.07	0.07
O	[mol]	0	3	4	3	2	0	1	0.03125	0.03125	0.025
N	[mol]	1	1	0	0	0	0	0	0.004286	0.004286	0.002857
P	[mol]	0	0	1	0	0	0	0	0.000161	0.000323	0.000226
charge	[mol]	1	-1	-2	-1	0	1	0	0	0	0

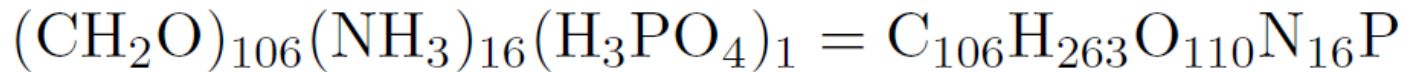
$$\sum_j \nu_{ij} \alpha_{kj} = 0$$

For growth of algae on nitrate:

6 unknown stoichiometric coefficients ν ,
6 mass balance equations (C,H,O,N,P,charge)
→ can be solved

Example: Algae growth

Typical composition of marine algae (Redfield, 1958)



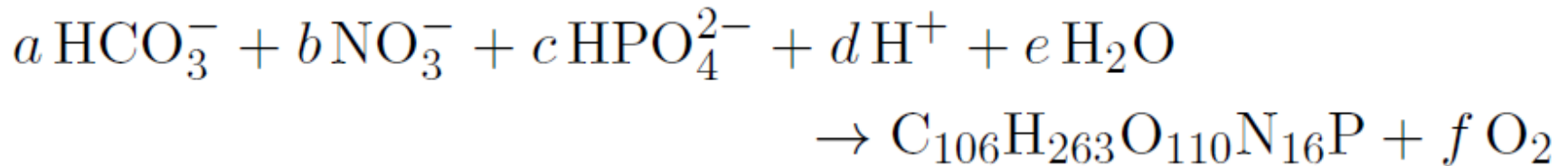
Total “molar” mass

(this is an average composition that does not represent a molecule):

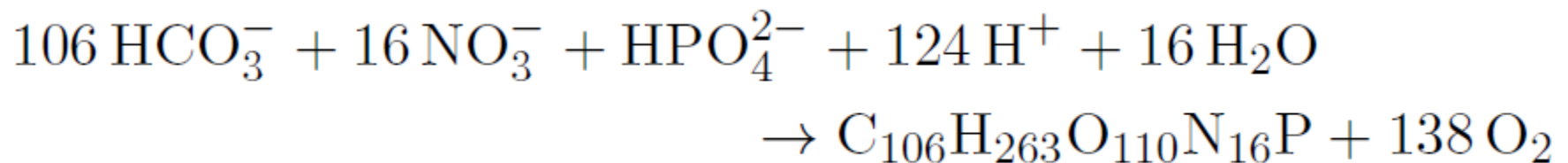
$$\begin{aligned} m &= 106 \cdot 12 \frac{\text{gC}}{\text{“mol”}} + 263 \frac{\text{gH}}{\text{“mol”}} + 110 \cdot 16 \frac{\text{gO}}{\text{“mol”}} \\ &\quad + 16 \cdot 14 \frac{\text{gN}}{\text{“mol”}} + 31 \frac{\text{gP}}{\text{“mol”}} \\ &= 3550 \frac{\text{gDM}}{\text{“mol”}} \quad . \end{aligned}$$

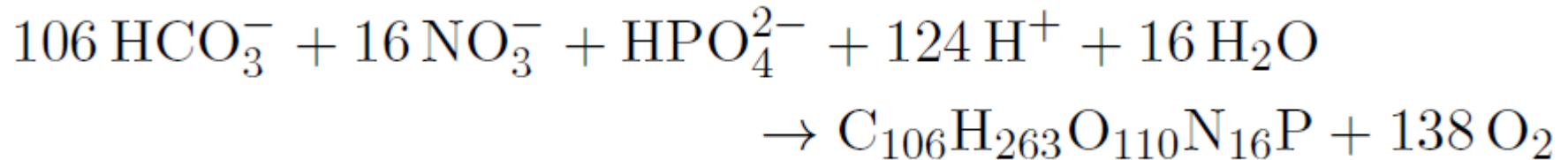
Example: Algae growth

Write down the chemical reaction equation including all substances that are needed to close the mass balance:



Solving the mass balance equations for C, H, O, N, P and charge leads to the unique solution (6 eq. for 6 unknowns):





Conversion of units:

$$\begin{aligned} \nu_{\text{gro,ALG,NO}_3 \text{ HCO}_3^-} &= -\frac{106}{3550} \frac{\text{molHCO}_3^-}{\text{gDM}} \\ \nu_{\text{gro,ALG,NO}_3 \text{ NO}_3^-} &= -\frac{16}{3550} \frac{\text{molNO}_3^-}{\text{gDM}} \\ \nu_{\text{gro,ALG,NO}_3 \text{ HPO}_4^{2-}} &= -\frac{1}{3550} \frac{\text{molHPO}_4^{2-}}{\text{gDM}} \\ \nu_{\text{gro,ALG,NO}_3 \text{ H}^+} &= -\frac{124}{3550} \frac{\text{molH}^+}{\text{gDM}} \\ \nu_{\text{gro,ALG,NO}_3 \text{ H}_2\text{O}} &= -\frac{16}{3550} \frac{\text{molH}_2\text{O}}{\text{gDM}} \\ \nu_{\text{gro,ALG,NO}_3 \text{ ALG}} &= 1 \frac{\text{gDM}}{\text{gDM}} \\ \nu_{\text{gro,ALG,NO}_3 \text{ O}_2} &= \frac{138}{3550} \frac{\text{molO}_2}{\text{gDM}} \end{aligned}$$

Chemical Substance Notation

ν		NH4	NO3	HPO4	HCO3	O2	H	H2O	ALG	ZOO	POM
		[mol]	[mol]	[mol]	[mol]	[mol]	[mol]	[mol]	[gDM]	[gDM]	[gDM]
gro.ALG.NH4		-		-	-	+	?	?	1		
gro.ALG.NO3			-0.00429	-0.00016	-0.030417	0.03785	-0.0350	-0.00220	1		
resp.ALG		+		+	+	-	?	?	-1		
death.ALG		0/+		0/+	0/+	+	?	?	-1		+
gro.ZOO		+		+	+	-	?	?	-	1	+
resp.ZOO		+		+	+	-	?	?		-1	
death.ZOO		0/+		0/+	0/+	+	?	?		-1	+
α											
C	[mol]	0	0	0	1	0	0	0	0.030417	0.03	0.04025
H	[mol]	4	0	1	1	0	1	2	0.07	0.07	0.07
O	[mol]	0	3	4	3	2	0	1	0.03125	0.03125	0.025
N	[mol]	1	1	0	0	0	0	0	0.004286	0.004286	0.002857
P	[mol]	0	0	1	0	0	0	0	0.000161	0.000323	0.000226
charge	[mol]	1	-1	-2	-1	0	1	0	0	0	0

$$\sum_j \nu_{ij} \alpha_{kj} = 0$$

Chemical Substance Notation

ν		NH4 [mol]	NO3 [mol]	HPO4 [mol]	HCO3 [mol]	O2 [mol]	H [mol]	H2O [mol]	ALG [gDM]	ZOO [gDM]	POM [gDM]
gro.ALG.NH4		-		-	-	+	?	?	1		
gro.ALG.NO3			-	-	-	+	?	?	1		
resp.ALG		+		+	+	-	?	?	-1		
death.ALG		0/+		0/+	0/+	+	?	?	-1		+
gro.ZOO		+		+	+	-	?	?	-	1	+
resp.ZOO		+		+	+	-	?	?		-1	
death.ZOO		0/+		0/+	0/+	+	?	?		-1	+
α											
C	[mol]	0	0	0	1	0	0	0	0.030417	0.03	0.04025
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P	[mol]	0	0	1	0	0	0	0	0.000161	0.000323	0.000226
charge	[mol]	1	-1	-2	-1	0	1	0	0	0	0

$$\sum_j \nu_{ij} \alpha_{kj} = 0$$

For growth of zooplankton:

8 unknown stoichiometric coefficients ν ,
6 mass balance equations (C,H,O,N,P,charge)
→ the system of equations is underdetermined

Zooplankton Growth:

8 unknown stoichiometric coefficients

6 mass balance equations

2 additional constraints required:

Fraction of zooplankton biomass produced per algal biomass consumed (yield): Y_{ZOO}

Fraction of dead particles produced (excretion + sloppy feeding) per algal biomass consumed: f_e

The fraction of algal biomass respired is then: $f_r = 1 - Y_{ZOO} - f_e$

$$1 \text{ ALG} = Y_{ZOO} \text{ Zoo} + f_e \text{ POM} + (1 - Y_{ZOO} - f_e) * (\text{"nutrients"})$$

$$1 \text{ Zoo} - 1/Y_{ZOO} \text{ ALG} + f_e/Y_{ZOO} \text{ POM} + (1 - Y_{ZOO} - f_e) (\text{"nutrients"}) = 0$$

Chemical Substance Notation

ν		NH4 [mol]	NO3 [mol]	HPO4 [mol]	HCO3 [mol]	O2 [mol]	H [mol]	H2O [mol]	ALG [gDM]	ZOO [gDM]	POM [gDM]
gro.ALG.NH4		-		-	-	+	?	?	1		
gro.ALG.NO3											
resp.ALG		+		+	+	-	?	?	-1		
death.ALG		0/+		0/+	0/+	+	?	?	-1		+
gro.ZOO		+		+	+	-	?	?	-1/Y.ZOO	1	fe/Y.ZOO
resp.ZOO		+		+	+	-	?	?		-1	
death.ZOO		0/+		0/+	0/+	+	?	?		-1	+
α											
C	[mol]	0	0	0	1	0	0	0	0.030417	0.03	0.04025
H	[mol]	4	0	1	1	0	1	2	0.07	0.07	0.07
O	[mol]	0	3	4	3	2	0	1	0.03125	0.03125	0.025
N	[mol]	1	1	0	0	0	0	0	0.004286	0.004286	0.002857
P	[mol]	0	0	1	0	0	0	0	0.000161	0.000323	0.000226
charge	[mol]	1	-1	-2	-1	0	1	0	0	0	0

$$\sum_j \nu_{ij} \alpha_{kj} = 0$$

For growth of zooplankton:
8 unknown stoichiometric coefficients ν ,
6 mass balance equations (C,H,O,N,P,charge)
+ 2 additional constraints → can be solved

Conclusion?

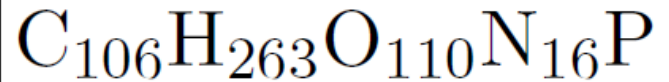
Concept is straightforward but quite some manual work!

If composition changes: redo the calculation!

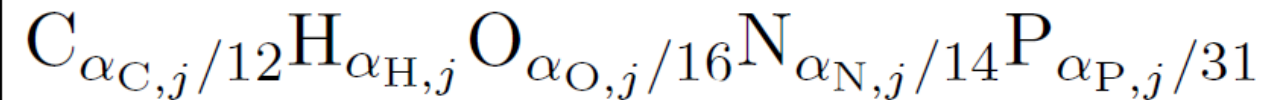
3 ways to derive stoichiometric coefficients:

- Chemical substance notation
- **Parameterized elemental mass fractions**
- General solution of stoichiometric equations

Instead of assuming a fixed chemical composition (e.g. Redfield:)



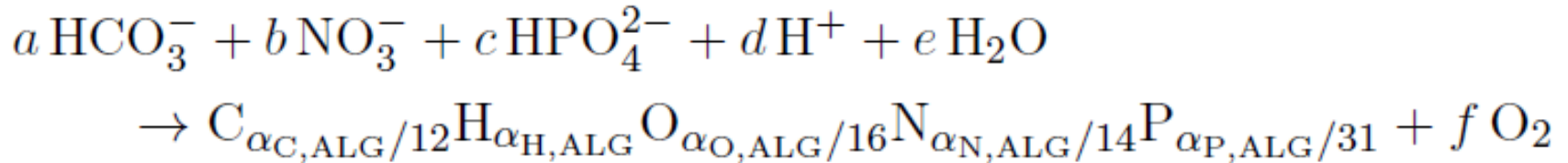
use parameterized mass fractions:



with:

$$\alpha_{\text{C},j} + \alpha_{\text{H},j} + \alpha_{\text{O},j} + \alpha_{\text{N},j} + \alpha_{\text{P},j} = 1$$

Algae growth



Solving the mass balance equations for C, H, O, N and P and charge leads to the unique solution (6 eq. for 6 unknowns):

$$\begin{aligned} & \frac{\alpha_{\text{C,ALG}}}{12} \text{HCO}_3^- + \frac{\alpha_{\text{N,ALG}}}{14} \text{NO}_3^- + \frac{\alpha_{\text{P,ALG}}}{31} \text{HPO}_4^{2-} \\ & + \left(\frac{\alpha_{\text{C,ALG}}}{12} + \frac{\alpha_{\text{N,ALG}}}{14} + \frac{2 \alpha_{\text{P,ALG}}}{31} \right) \text{H}^+ \\ & + \left(\frac{\alpha_{\text{H,ALG}}}{2} - \frac{\alpha_{\text{C,ALG}}}{12} - \frac{\alpha_{\text{N,ALG}}}{28} - \frac{3 \alpha_{\text{P,ALG}}}{62} \right) \text{H}_2\text{O} \\ & \rightarrow \text{C}_{\alpha_{\text{C,ALG}}/12} \text{H}_{\alpha_{\text{H,ALG}}} \text{O}_{\alpha_{\text{O,ALG}}/16} \text{N}_{\alpha_{\text{N,ALG}}/14} \text{P}_{\alpha_{\text{P,ALG}}/31} \\ & + \left(\frac{\alpha_{\text{C,ALG}}}{12} + \frac{\alpha_{\text{H,ALG}}}{4} - \frac{\alpha_{\text{O,ALG}}}{32} + \frac{5 \alpha_{\text{N,ALG}}}{56} + \frac{5 \alpha_{\text{P,ALG}}}{124} \right) \text{O}_2 \end{aligned}$$

Once we decided about the α parameters, we can calculate the ν

$$\alpha_{\text{C,ALG}}^{\text{Redfield}} = \frac{106 \cdot 12}{3550} \frac{\text{gC}}{\text{gDM}} \approx 0.36 \frac{\text{gC}}{\text{gDM}}$$

$$\alpha_{\text{H,ALG}}^{\text{Redfield}} = \frac{263}{3550} \frac{\text{gH}}{\text{gDM}} \approx 0.07 \frac{\text{gH}}{\text{gDM}}$$

$$\alpha_{\text{O,ALG}}^{\text{Redfield}} = \frac{110 \cdot 16}{3550} \frac{\text{gO}}{\text{gDM}} \approx 0.50 \frac{\text{gO}}{\text{gDM}}$$

$$\alpha_{\text{N,ALG}}^{\text{Redfield}} = \frac{16 \cdot 14}{3550} \frac{\text{gN}}{\text{gDM}} \approx 0.06 \frac{\text{gN}}{\text{gDM}}$$

$$\alpha_{\text{P,ALG}}^{\text{Redfield}} = \frac{1 \cdot 31}{3550} \frac{\text{gP}}{\text{gDM}} \approx 0.01 \frac{\text{gP}}{\text{gDM}}$$

Conclusions?

- Even more tedious to solve the equations manually.
 - Changes in composition are now easy to handle, just change the numerical values of the parameters!
 - However, when adding elements, all calculations have to be revised.
- Try to find a general solution of stoichiometric equations

3 ways to derive stoichiometric coefficients:

- Chemical substance notation
- Parameterized elemental mass fractions
- General solution of stoichiometric equations

Processes i	Substances j					Rates
	s_1	s_2	s_3	\dots	s_{n_s}	
p_1	ν_{11}	ν_{12}	ν_{13}	\dots	ν_{1n_s}	ρ_1
p_2	ν_{21}	ν_{22}	ν_{23}	\dots	ν_{2n_s}	ρ_2
\vdots	\vdots	\vdots	\vdots	\ddots	\vdots	\vdots
p_{n_p}	$\nu_{n_p 1}$	$\nu_{n_p 2}$	$\nu_{n_p 3}$	\dots	$\nu_{n_p n_s}$	ρ_{n_p}
Elements k						
e_1	α_{11}	α_{12}	α_{13}	\dots	α_{1n_s}	
e_2	α_{21}	α_{22}	α_{23}	\dots	α_{2n_s}	
\vdots	\vdots	\vdots	\vdots	\ddots	\vdots	
e_{n_e}	$\alpha_{n_e 1}$	$\alpha_{n_e 2}$	$\alpha_{n_e 3}$	\dots	$\alpha_{n_e n_s}$	

Mass conservation for element k in process i :

n_e constraints for each process from
the "elemental" composition

$$\sum_j \nu_{ij} \alpha_{kj} = 0$$

Mass conservation for element k in process i :
$$\sum_{j=1}^{n_s} \nu_{ij} \alpha_{kj} = 0$$

in matrix notation: $\boldsymbol{\nu}_i \cdot (\boldsymbol{\alpha}_{(i)})^T = \mathbf{0}$

Constraints:
$$\sum_{j=1}^{n_s} \nu_{ij} \gamma_{(i),kj} = 0$$

$\boldsymbol{\alpha}_{(i)}$: composition matrix with only the columns of substances involved in process i

in matrix notation: $\boldsymbol{\nu}_i \cdot (\boldsymbol{\gamma}_{(i)})^T = \mathbf{0}$

Combined conditions:
$$\boldsymbol{\nu}_i \cdot \begin{pmatrix} \boldsymbol{\alpha}_{(i)} \\ \boldsymbol{\gamma}_{(i)} \end{pmatrix}^T = \mathbf{0}$$

→ Solving stoichiometric equations is a problem of linear algebra:
Finding the “left null-space” of a matrix

→ Swiss Army Knife of Linear Algebra



What did you find out?


What is the "Swiss Army Knife of Linear Algebra"? Please explain it in simple words

people.inf.ethz
[PDF] SVD -- the Swiss Army Knife of Linear...

cmps-people.ok.ubc
[PDF] Projection Methods: Swiss Army Knives for...

PB peterbloem
The Singular Value Decomposition [...]

+6 sources

 Answer

The "Swiss Army Knife of Linear Algebra" is the Singular Value Decomposition (SVD) ¹ ³ ⁴ . This term is used to describe SVD because of its versatility and wide range of applications in mathematics, data science, and machine learning ³ ⁴ .

SVD is a powerful mathematical technique that decomposes any matrix into three simpler matrices ⁶ . This decomposition allows us to analyze and manipulate complex data more easily, much like how a Swiss Army knife provides various tools for different tasks ⁴ .

Here's why SVD is considered so versatile:

1. It can be used for dimensionality reduction, which is crucial in data analysis and machine learning ³ .
2. It helps in solving various problems like semantic search, prediction, pattern extraction, clustering, and topic modeling ⁴ .
3. SVD is fundamental to many important operations in linear algebra, including linear regression, principal component analysis (PCA), and matrix approximation ³ ⁶ .
4. It's useful in a wide range of fields, from image processing to natural language processing ⁴ ⁶ .

In simple terms, SVD is like a multi-tool that can help solve many different types of mathematical and data-related problems, making it an essential technique for anyone working with large datasets or complex mathematical structures ⁴ ⁶ .

What is the "Swiss Army Knife of Linear Algebra"? Please explain **how it works** in simple words

en.wikipedia
Singular value
decomposition - Wikipedia

builtin
Singular Value
Decomposition (SVD)...

gregorygundersen
Singular Value
Decomposition as Simply...

+4 sources

Answer

The "Swiss Army Knife of Linear Algebra" is the Singular Value Decomposition (SVD). It's called this because of its versatility and wide range of applications in mathematics, data science, and machine learning ¹ ² .

SVD works by decomposing any matrix into three simpler matrices:

1. A left singular matrix (U)
2. A diagonal matrix of singular values (Σ)
3. A right singular matrix (V^T)

In simple terms, SVD breaks down a complex matrix into three parts that are easier to work with ¹ ² .

Here's how SVD works in simple words:

1. Rotation: The matrix V^T rotates the original data.
2. Scaling: The diagonal matrix Σ scales the rotated data.
3. Another rotation: The matrix U performs a final rotation.

This process can be thought of as transforming data through a series of simple steps: rotate, stretch or shrink, and rotate again ¹ .

The power of SVD lies in its ability to reveal important structures and patterns in the data. The singular values in the diagonal matrix Σ represent the importance of different features or components in the data. Larger singular values correspond to more significant patterns ¹ ² .



Anonymous

What is the "Swiss Army Knife of Linear Algebra"? Please explain it in simple words.



ChatGPT

The "Swiss Army Knife of Linear Algebra" often refers to the Singular Value Decomposition (SVD). Just like a Swiss Army knife, which is valued for its versatility and utility in various situations, SVD is highly versatile and useful in the field of linear algebra and beyond.

SVD is a method that breaks down a matrix into three simpler matrices. Imagine you have a complex puzzle (the original matrix); SVD allows you to separate it into three easier puzzles (the matrices U , Σ , and V^*), where:

- U is a matrix containing what are called the left singular vectors,
- Σ (Sigma) is a diagonal matrix with singular values (these values can be thought of as the importance or weight of each corresponding singular vector),
- V^* (the conjugate transpose of V) contains the right singular vectors.

This decomposition helps in understanding the structure and properties of the original matrix. It's like having a tool that can adapt to perform a wide range of tasks:

Data compression, Noise reduction, **Solving linear equations**, Principal component analysis...

Full Answers (always to be treated with a grain of salt)

What is the "Swiss Army Knife of Linear Algebra"?

Please explain it in simple words:

<https://chat.openai.com/share/b2035ee9-382c-43d2-9591-9dab098d9de0>

Please explain step by step, how the singular value decomposition works.

Explain it on three levels: first for a 5 year old, then for a college students and finally for experts with all mathematical details.

<https://chat.openai.com/share/a69e6f50-b5cb-4ae6-98a1-ea7b8a8ebabc>

I have the process table of a chemical reaction. How can I translate this to the corresponding ODE system? Please give me a small example.

<https://chat.openai.com/share/f3466e31-772b-4aa4-83a9-3e8a6f46f80f>

(note that it doesn't refer to the process table concept as we use it here)

Thanks to Andreas Scheidegger!



Solving homogeneous linear equations

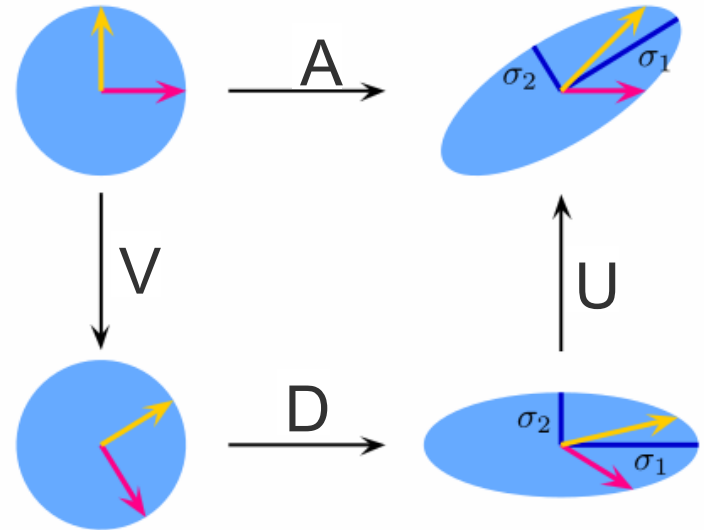
A set of homogeneous linear equations can be written as $\mathbf{Ax} = \mathbf{0}$ for a matrix \mathbf{A} and vector \mathbf{x} .

A typical situation is that \mathbf{A} is known and a non-zero \mathbf{x} is to be determined which satisfies the equation.

Such an \mathbf{x} belongs to \mathbf{A} 's null space and is sometimes called a (right) null vector of \mathbf{A} .

The vector \mathbf{x} can be characterized as a right-singular vector corresponding to a singular value of \mathbf{A} that is zero.

If \mathbf{A} is a square matrix and has no vanishing singular value, the equation has no non-zero \mathbf{x} as a solution. If there are several vanishing singular values, any linear combination of the corresponding right-singular vectors is a valid solution. Analogously to the definition of a (right) null vector, a non-zero \mathbf{x} satisfying $\mathbf{x}^* \mathbf{A} = \mathbf{0}$, with \mathbf{x}^* denoting the conjugate transpose of \mathbf{x} , is called a left null vector of \mathbf{A} .



$$\mathbf{A} = \mathbf{U} \mathbf{D} \mathbf{V}^T$$

We can profit from implementations of the Singular Value Decomposition Theorem (Swiss army knife of linear algebra)

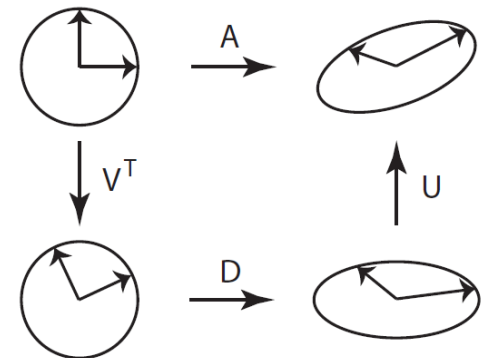


each $n \times m$ matrix \mathbf{A} with $n \geq m$ can be decomposed

$$\mathbf{A} = \mathbf{U} \cdot \mathbf{D} \cdot \mathbf{V}^T$$

- \mathbf{U} is an $n \times m$ matrix with orthonormal columns: $\mathbf{U}^T \cdot \mathbf{U} = \mathbf{I}$.
- \mathbf{D} is an $m \times m$ diagonal matrix with non-negative elements in its diagonal. These values in the diagonal of \mathbf{D} are called singular values of the matrix \mathbf{A} .
- \mathbf{V} is an $m \times m$ matrix with orthonormal columns: $\mathbf{V}^T \cdot \mathbf{V} = \mathbf{I}$.

→ The rows of \mathbf{U}^T corresponding to elements of \mathbf{D} that are zero build a basis of the left null space of \mathbf{A} . This solves our linear algebra problem.



Recipe for deriving the stoichiometry:

At the model level:

- 1) Choose the elements to be considered in the model.
- 2) Choose the substances to be considered in the model.
- 3) Add substances needed for elemental mass balances (e.g. H_2O , H^+) .
- 4) Choose elemental mass fractions and construct the composition matrix.

At the process level (for each process):

- 1) Choose the substances involved in the process and known constraints.
- 2) Determine the dimension of the left null space of the joint composition and constraint matrix.
- 3) 1: make the stoichiometry unique by normalizing one of the coefficients.
0: check whether all relevant substances were included. → Step 1)
>1: check for too many substances or missing constraints. → Step 1)

The R package “stoichcalc” provides us with a function `calc.stoich.coef` that accepts for each process

- a composition matrix `alpha`,
- a vector of substances to be considered,
- a selection of a normalized coefficient and its value,
- if required a list with coefficients of additional constraints,

and returns a vector of stoichiometric coefficients.

```
nu.gro.ALG <-  
  calc.stoich.coef(alpha      = alpha.1,  
                    name      = "growth.ALG",  
                    subst     = c("HPO4", "ALG"),  
                    subst.norm = "ALG",  
                    nu.norm    = 1)
```

```
nu.gro.ZOO <-  
  calc.stoich.coef(alpha      = alpha.2,  
                    name      = "gro.ZOO",  
                    subst     = c("NH4", "HPO4", "HCO3", "O2", "H",  
                                   "H2O", "ALG", "ZOO", "POM"),  
                    subst.norm = "ZOO",  
                    nu.norm    = 1,  
                    constraints = list(c("ZOO" = 1,  
                                          "ALG" = param$Y.ZOO),  
                                       c("POM" = 1,  
                                          "ALG" = param$f.e)))
```

As a first step, the null space is analyzed and an error message is issued if it is empty or of a higher dimension than one.

Simplified approach for estimating the need for constraints

- 1) Count the number of unknown stoichiometric coefficients (excluding the one that is normalized)
- 2) Count the number of mass balance constraints (number of elements considered for the composition; typically 5 in our examples, but see the exercises today) and add one for the charge balance constraint.
- 3) The difference of 1) minus 2) gives the number of required constraints, **if there are no linear dependences in compositions or constraints.**

The `stoichcalc` function `calc.stoich.coeff` considers these linear dependences and provides the correct answer unless there are numerical difficulties.

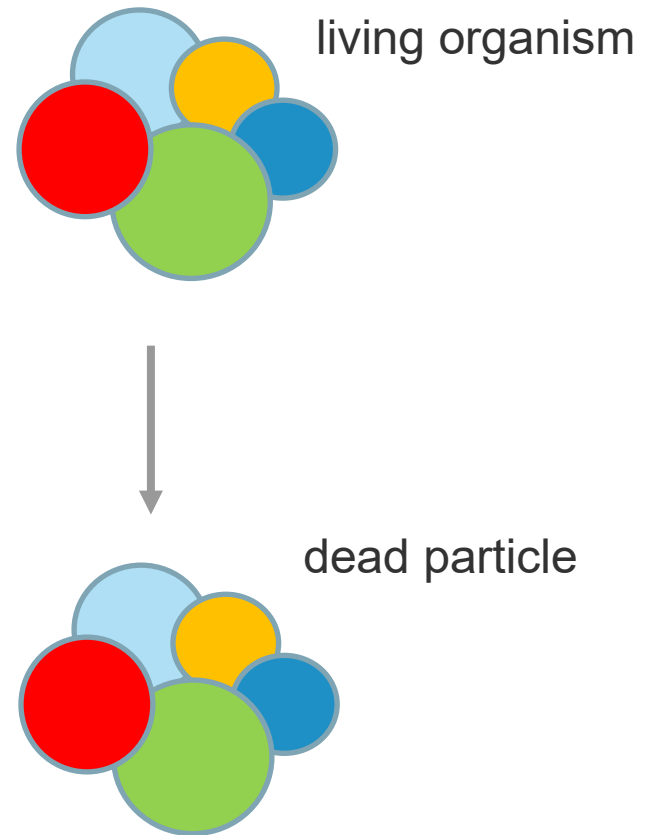
Extended Process Table Notation

ν		NH4 [mol]	NO3 [mol]	HPO4 [mol]	HCO3 [mol]	O2 [mol]	H [mol]	H2O [mol]	ALG [gDM]	ZOO [gDM]	POM [gDM]	
gro.ALG.NH4		-		-	-	+	?	?	1			6 unknowns
gro.ALG.NO3			-	-	-	+	?	?	1			6 unknowns
resp.ALG		+		+	+	-	?	?	-1			6 unknowns
death.ALG		0/+		0/+	0/+	+	?	?	-1		+	7 unknowns
gro.ZOO		+		+	+	-	?	?	-	1	+	8 unknowns
resp.ZOO		+		+	+	-	?	?		-1		6 unknowns
death.ZOO		0/+		0/+	0/+	+	?	?		-1	+	7 unknowns
α												
C	[mol]	0	0	0	1	0	0	0	0.030417	0.03	0.04025	
H	[mol]	4	0	1	1	0	1	2	0.07	0.07	0.07	
O	[mol]	0	3	4	3	2	0	1	0.03125	0.03125	0.025	
N	[mol]	1	1	0	0	0	0	0	0.004286	0.004286	0.002857	
P	[mol]	0	0	1	0	0	0	0	0.000161	0.000323	0.000226	
charge	[mol]	1	-1	-2	-1	0	1	0	0	0	0	

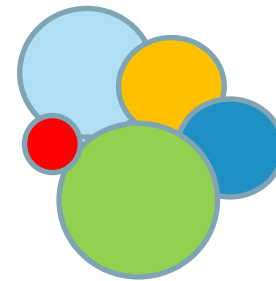
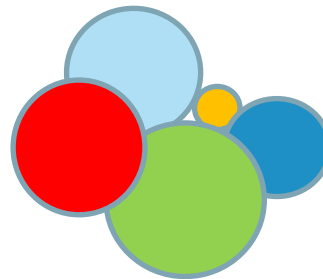
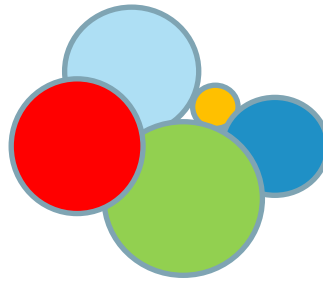
$$\sum_j \nu_{ij} \alpha_{kj} = 0$$

Death would have a trivial stoichiometry, if the dead organic matter has the same composition than the dying organisms. Then we would just turn one unit of living organisms into one unit of dead organic matter.

If we have many groups of organisms with different compositions, we would need a large number of types of dead organic matter.



Living organisms with different composition



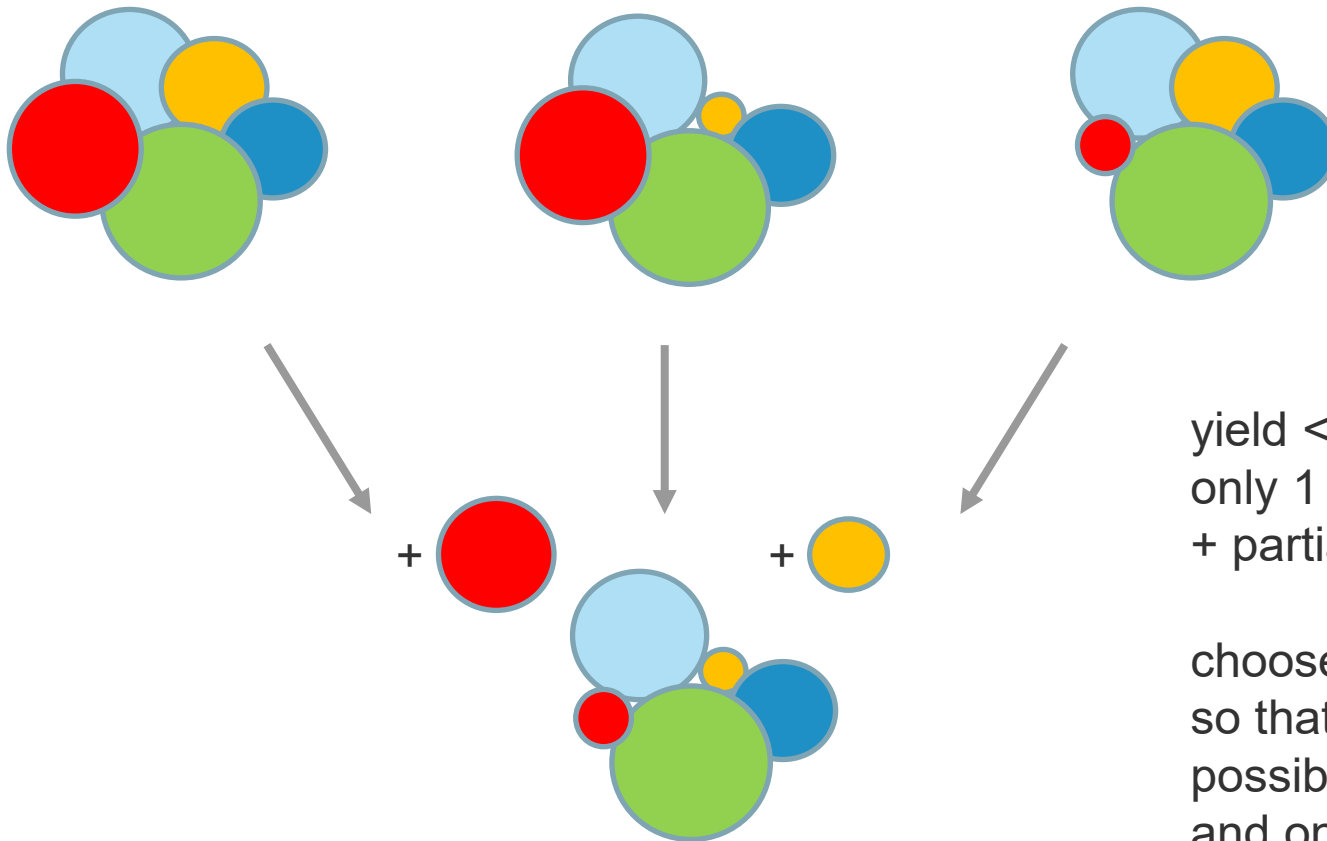
simple
stoichiometry
but many types
of POM needed

Dead particulate organic matter

Alternatively, we can formulate the model with one type of dead organic particles and mineralize part of the dying organism to keep the mass balances. This can be accepted as dead organic particles will be mineralized anyways.

Technically, we introduce a “yield” for death and adjust it so that neither nutrients nor oxygen are required for dying.

Living organisms with different composition



yield < 100%
only 1 type of POM
+ partial mineralization

choose the yield
so that as much as
possible goes to POM
and only the remainder
is respired

Dead particulate organic matter + nutrients

Check mass balance

ν	NH4	NO3	HPO4	HCO3	O2	H	H2O	ALG	ZOO	POM
	[mol]	[mol]	[mol]	[mol]	[mol]	[mol]	[mol]	[gDM]	[gDM]	[gDM]
gro.ALG.NH4	-0.00429	0	-0.00016	-0.030417	0.02928	-0.0265	0.00209	1	0	0
gro.ALG.NO3	0	-0.00429	-0.00016	-0.030417	0.03785	-0.0350	-0.00220	1	0	0
resp.ALG	0.004286	0	0.000161	0.030417	-0.02928	0.0265	-0.00209	-1	0	0
death.ALG	0.002245	0	0	0.001667	0.00171	-0.0006	0.00497	-1	0	0.714
gro.ZOO	0.011429	0	3.23E-05	0.041583	-0.03055	0.0302	0.01123	-5	1	2
resp.ZOO	0.004286	0	0.000323	0.03	-0.02906	0.0264	-0.00191	0	-1	0
death.ZOO	0.001429	0	9.68E-05	-0.01025	0.01433	-0.0115	0.00796	0	-1	1
α										
C [mol]	0	0	0	1	0	0	0	0.030417	0.03	0.04025
H [mol]	4	0	1	1	0	1	2	0.07	0.07	0.07
O [mol]	0	3	4	3	2	0	1	0.03125	0.03125	0.025
N [mol]	1	1	0	0	0	0	0	0.004286	0.004286	0.002857
P [mol]	0	0	1	0	0	0	0	0.000161	0.000323	0.000226
charge [mol]	1	-1	-2	-1	0	1	0	0	0	0

example conservation of

											sum
C - death.ZOO:	0	0	0	-0.01025	0	0	0	0	-0.03	0.04025	0

$$\sum_j \nu_{ij} \alpha_{kj} = 0$$

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 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