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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

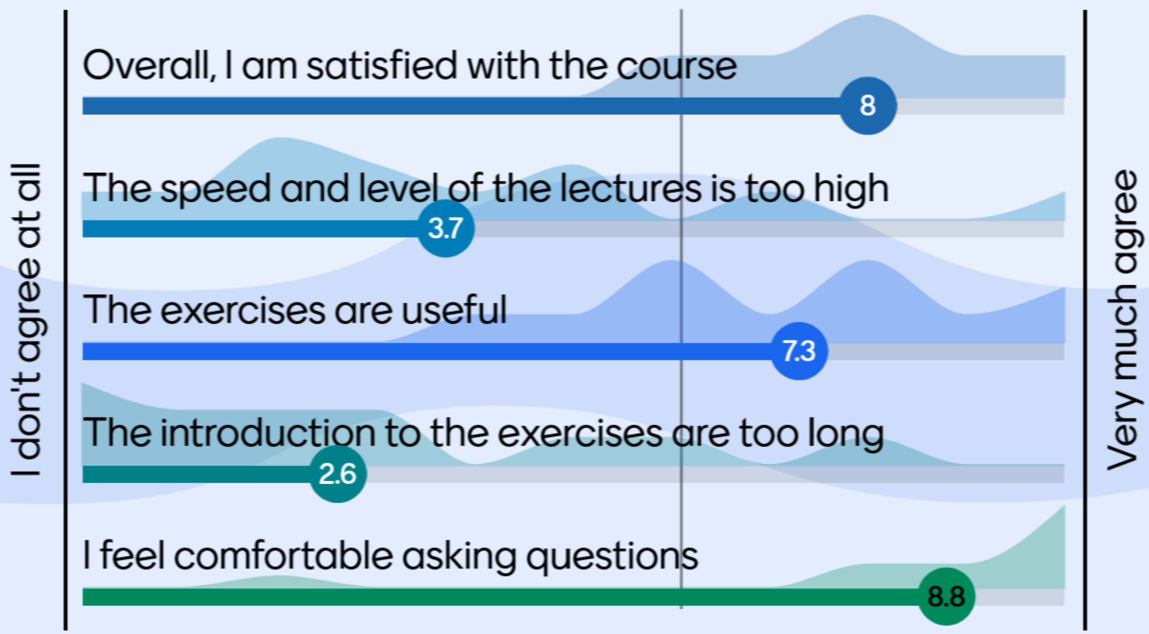
Structure of the Course

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

Check-in about the course

COURSE EVALUATION

How much do I agree about the following so far:



please interrupt at any time

feel free to ask after the course

What could be improved?

3 responses

12

- Maybe recording the lectures and exercices sessions would be help us understand better as we could rewatch if something was not understood
- Maybe going through examples together more often would help to understand the processes
- .

Questions from last week?

Goals

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)

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Process table

Process i	Substances j					Rate
	s_1	s_2	s_3	$\cdots$	$\mathsf{s}_{n_\mathrm{s}}$	
p_1	ν_{11}	ν_{12}	ν_{13}	$\cdots$	ν_{1n_s}	ρ_1
p_2	ν_{21}	ν_{22}	ν_{23}	$\cdots$	ν_{2n_s}	ρ_2
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$
$\mathsf{p}_{n_\mathrm{p}}$	$\nu_{n_\mathrm{p}1}$	$\nu_{n_\mathrm{p}2}$	$\nu_{n_\mathrm{p}3}$	$\cdots$	$\nu_{n_\mathrm{p}n_\mathrm{s}}$	ρ_{n_p}

$$r_j = \sum_{i=1}^{n_\mathrm{p}} \nu_{ij}\ \rho_i$$

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

Extended Process Table Notation

Processes i	Substances j					Rates
	s_1	s_2	s_3	$\cdots$	s_{n_s}	
p_1	ν_{11}	ν_{12}	ν_{13}	$\cdots$	ν_{1n_s}	ρ_1
p_2	ν_{21}	ν_{22}	ν_{23}	$\cdots$	ν_{2n_s}	ρ_2
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$
p_{n_p}	ν_{n_p1}	ν_{n_p2}	ν_{n_p3}	$\cdots$	$\nu_{n_pn_s}$	ρ_{n_p}
Elements k						
e_1	α_{11}	α_{12}	α_{13}	$\cdots$	α_{1n_s}	
e_2	α_{21}	α_{22}	α_{23}	$\cdots$	α_{2n_s}	
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	
e_{n_e}	α_{n_e1}	α_{n_e2}	α_{n_e3}	$\cdots$	$\alpha_{n_en_s}$	

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

Extended Process Table Notation

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Processes i	Substances j					Rates
	s_1	s_2	s_3	$\cdots$	$\mathsf{s}_{n_\mathrm{s}}$	
p_1	ν_{11}	ν_{12}	ν_{13}	$\cdots$	ν_{1n_s}	ρ_1
p_2	ν_{21}	ν_{22}	ν_{23}	$\cdots$	ν_{2n_s}	ρ_2
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$
$\mathsf{p}_{n_\mathrm{p}}$	$\nu_{n_\mathrm{p}1}$	$\nu_{n_\mathrm{p}2}$	$\nu_{n_\mathrm{p}3}$	$\cdots$	$\nu_{n_\mathrm{p}n_\mathrm{s}}$	ρ_{n_p}
Elements k						
e_1	α_{11}	α_{12}	α_{13}	$\cdots$	α_{1n_s}	
e_2	α_{21}	α_{22}	α_{23}	$\cdots$	α_{2n_s}	
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	
$\mathsf{e}_{n_\mathrm{e}}$	$\alpha_{n_\mathrm{e}1}$	$\alpha_{n_\mathrm{e}2}$	$\alpha_{n_\mathrm{e}3}$	$\cdots$	$\alpha_{n_\mathrm{e}n_\mathrm{s}}$	

Mass conservation for element k in process i:

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

n_e constraints for each process

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 growth on nitrate:
6 unknown stoichiometric coefficients ν,
6 mass balance equations (C,H,O,N,P,charge)
$\rightarrow$ can be solved

Chemical Substance Notation

Example: Algae growth

Typical composition of marine algae (Redfield, 1958)

$$(CH_2O)_{106}(NH_3)_{16}(H_3PO_4)_1 = C_{106}H_{263}O_{110}N_{16}P$$

Total “molar” mass
(this is an average composition that does not represent a molecule):

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

Chemical Substance Notation

Example: Algae growth

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

$$a\,\mathrm{HCO_3^-} + b\,\mathrm{NO_3^-} + c\,\mathrm{HPO_4^{2-}} + d\,\mathrm{H^+} + e\,\mathrm{H_2O} \rightarrow \mathrm{C_{106}H_{263}O_{110}N_{16}P} + f\,\mathrm{O_2}$$

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

$$106\,\mathrm{HCO_3^-} + 16\,\mathrm{NO_3^-} + \mathrm{HPO_4^{2-}} + 124\,\mathrm{H^+} + 16\,\mathrm{H_2O} \rightarrow \mathrm{C_{106}H_{263}O_{110}N_{16}P} + 138\,\mathrm{O_2}$$

Chemical Substance Notation

$$106\,HCO_3^- + 16\,NO_3^- + HPO_4^{2-} + 124\,H^+ + 16\,H_2O \rightarrow C_{106}H_{263}O_{110}N_{16}P + 138\,O_2$$

Conversion of units:

$$\nu_{\mathrm{gro,ALG,NO3}\ \mathrm{HCO_3^-}} = -\frac{106}{3550}\,\frac{\mathrm{molHCO_3^-}}{\mathrm{gDM}}$$

$$\nu_{\mathrm{gro,ALG,NO3}\ \mathrm{NO_3^-}} = -\frac{16}{3550}\,\frac{\mathrm{molNO_3^-}}{\mathrm{gDM}}$$

$$\nu_{\mathrm{gro,ALG,NO3}\ \mathrm{HPO_4^{2-}}} = -\frac{1}{3550}\,\frac{\mathrm{molHPO_4^{2-}}}{\mathrm{gDM}}$$

$$\nu_{\mathrm{gro,ALG,NO3}\ \mathrm{H+}} = -\frac{124}{3550}\,\frac{\mathrm{molH^+}}{\mathrm{gDM}}$$

$$\nu_{\mathrm{gro,ALG,NO3}\ \mathrm{H_2O}} = -\frac{16}{3550}\,\frac{\mathrm{molH_2O}}{\mathrm{gDM}}$$

$$\nu_{\mathrm{gro,ALG,NO3}\ \mathrm{ALG}} = 1\,\frac{\mathrm{gDM}}{\mathrm{gDM}}$$

$$\nu_{\mathrm{gro,ALG,NO3}\ \mathrm{O_2}} = \frac{138}{3550}\,\frac{\mathrm{molO_2}}{\mathrm{gDM}}$$

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		-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
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)
→ the system of equations is underdetermined

Chemical Substance Notation

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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: $f_{\mathrm{r}} = 1 - Y_{\mathrm{ZOO}} - f_{\mathrm{e}}$

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

1 Zoo $-1/Y_{Zoo}$ ALG + f_e/Y_{Zoo} POM + $(1 - Y_{Zoo} - f_e)$ ("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

Chemical Substance Notation

Conclusion?

Concept is straightforward but quite some manual work!

If composition changes: redo the calculation!

Stoichiometry

3 ways to derive stoichiometric coefficients:

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

Parameterized Mass Fractions

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

$$C_{106}H_{263}O_{110}N_{16}P$$

use parameterized mass fractions:

$$C_{\alpha_{C,j}/12}H_{\alpha_{H,j}}O_{\alpha_{O,j}/16}N_{\alpha_{N,j}/14}P_{\alpha_{P,j}/31}$$

with:

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

Parameterized Mass Fractions

Algae growth

$$a\,\mathrm{HCO_3^-} + b\,\mathrm{NO_3^-} + c\,\mathrm{HPO_4^{2-}} + d\,\mathrm{H^+} + e\,\mathrm{H_2O}$$
$$\rightarrow \mathrm{C}_{\alpha_{\mathrm{C,ALG}}/12}\mathrm{H}_{\alpha_{\mathrm{H,ALG}}}\mathrm{O}_{\alpha_{\mathrm{O,ALG}}/16}\mathrm{N}_{\alpha_{\mathrm{N,ALG}}/14}\mathrm{P}_{\alpha_{\mathrm{P,ALG}}/31} + f\,\mathrm{O_2}$$

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

$$\boxed{\frac{\alpha_{\mathrm{C,ALG}}}{12}}\mathrm{HCO_3^-} + \boxed{\frac{\alpha_{\mathrm{N,ALG}}}{14}}\mathrm{NO_3^-} + \boxed{\frac{\alpha_{\mathrm{P,ALG}}}{31}}\mathrm{HPO_4^{2-}}$$
$$+ \boxed{\left(\frac{\alpha_{\mathrm{C,ALG}}}{12} + \frac{\alpha_{\mathrm{N,ALG}}}{14} + \frac{2\,\alpha_{\mathrm{P,ALG}}}{31}\right)}\mathrm{H^+}$$
$$+ \boxed{\left(\frac{\alpha_{\mathrm{H,ALG}}}{2} - \frac{\alpha_{\mathrm{C,ALG}}}{12} - \frac{\alpha_{\mathrm{N,ALG}}}{28} - \frac{3\,\alpha_{\mathrm{P,ALG}}}{62}\right)}\mathrm{H_2O}$$
$$\rightarrow \mathrm{C}_{\alpha_{\mathrm{C,ALG}}/12}\mathrm{H}_{\alpha_{\mathrm{H,ALG}}}\mathrm{O}_{\alpha_{\mathrm{O,ALG}}/16}\mathrm{N}_{\alpha_{\mathrm{N,ALG}}/14}\mathrm{P}_{\alpha_{\mathrm{P,ALG}}/31}$$
$$+ \boxed{\left(\frac{\alpha_{\mathrm{C,ALG}}}{12} + \frac{\alpha_{\mathrm{H,ALG}}}{4} - \frac{\alpha_{\mathrm{O,ALG}}}{32} + \frac{5\,\alpha_{\mathrm{N,ALG}}}{56} + \frac{5\,\alpha_{\mathrm{P,ALG}}}{124}\right)}\mathrm{O_2}$$

Parameterized Mass Fractions

Once we decided about the α parameters, we can calulate the v

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

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

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

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

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

Parameterized Mass Fractions

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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

Extended Process Table Notation

Processes i	Substances j					Rates
	s_1	s_2	s_3	$\cdots$	$\mathsf{s}_{n_\mathrm{s}}$	
p_1	ν_{11}	ν_{12}	ν_{13}	$\cdots$	ν_{1n_s}	ρ_1
p_2	ν_{21}	ν_{22}	ν_{23}	$\cdots$	ν_{2n_s}	ρ_2
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$
$\mathsf{p}_{n_\mathrm{p}}$	$\nu_{n_\mathrm{p}1}$	$\nu_{n_\mathrm{p}2}$	$\nu_{n_\mathrm{p}3}$	$\cdots$	$\nu_{n_\mathrm{p}n_\mathrm{s}}$	ρ_{n_p}
Elements k						
e_1	α_{11}	α_{12}	α_{13}	$\cdots$	α_{1n_s}	
e_2	α_{21}	α_{22}	α_{23}	$\cdots$	α_{2n_s}	
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	
$\mathsf{e}_{n_\mathrm{e}}$	$\alpha_{n_\mathrm{e}1}$	$\alpha_{n_\mathrm{e}2}$	$\alpha_{n_\mathrm{e}3}$	$\cdots$	$\alpha_{n_\mathrm{e}n_\mathrm{s}}$	

Mass conservation for element k in process i:

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

n_e constraints for each process from the elemental composition

General Solution

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

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

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

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

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

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

→ 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?

... from ChatGPT 4.0

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...

... from ChatGPT 4.0

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

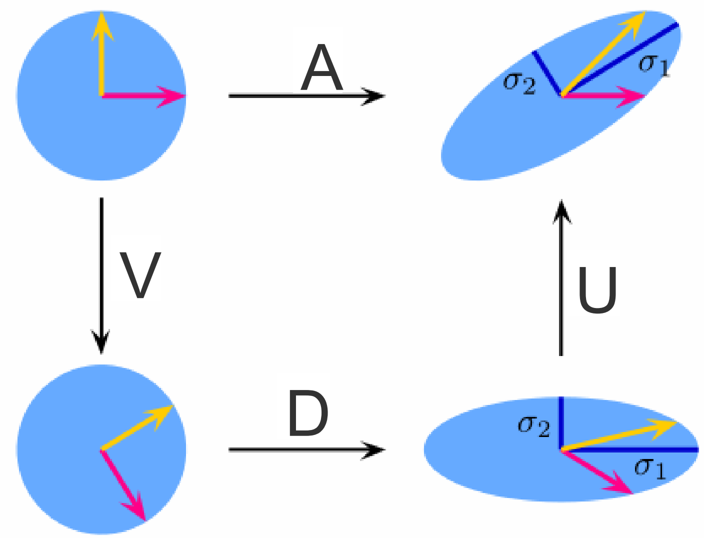
I have the process table of a chemical reaction. How can I translate this to the corresponding ODE system? Please give me a small example.
https://chat.openai.com/share/f3466e31-772b-4aa4-83a9-3e8a6f46f80f
(note that it doesn't refer to the process table concept as we use it here)

Thanks to Andreas Scheidegger!

... from Wikipedia

Solving homogeneous linear equations

A set of homogeneous linear equations can be written as **Ax** = **0** for a matrix **A** and vector **x**. A typical situation is that **A** is known and a non-zero **x** is to be determined which satisfies the equation. Such an **x** belongs to **A**'s null space and is sometimes called a (right) null vector of **A**. The vector **x** can be characterized as a right-singular vector corresponding to a singular value of **A** that is zero.



$A = U\,D\,V^T$

If **A** is a square matrix and has no vanishing singular value, the equation has no non-zero **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 **x** satisfying **x*****A** = **0**, with **x*** denoting the conjugate transpose of **x**, is called a left null vector of **A**.

General Solution

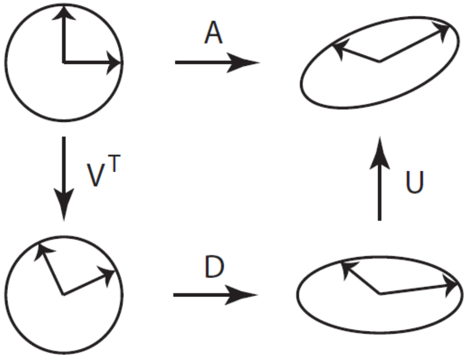
We can profit from implementations of the Singular Value Decomposition Theorem (Swiss army knife of linear algebra)

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

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

- $\mathbf{U}$ is an $n \times m$ matrix with orthonormal columns: $\mathbf{U}^{\mathrm{T}} \cdot \mathbf{U} = \mathbf{I}$.
- $\mathbf{D}$ 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: $\mathbf{V}^{\mathrm{T}} \cdot \mathbf{V} = \mathbf{I}$.

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



General Solution

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)

General Solution

The R package "`stoichcalc`" provides us with a function

`calc.stoich.coef`

that accepts

- a composition matrix ,
- coefficients of constraints,
- a list of substances to be considered, and
- a selection of a normalized coefficient and its value,

to provide a vector of stoichiometric coefficients.

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.

General Solution

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	

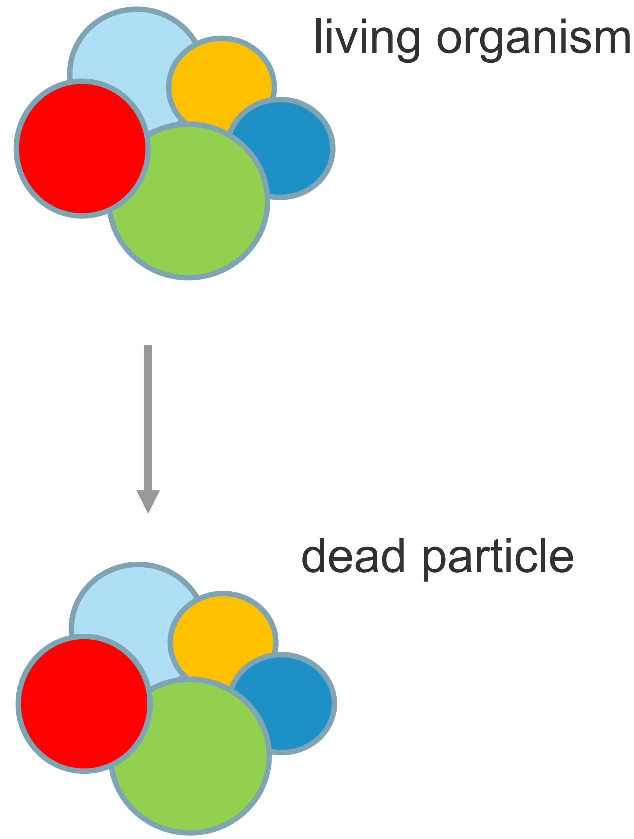
$$\sum_j \nu_{ij}\alpha_{kj} = 0$$

Death

Death

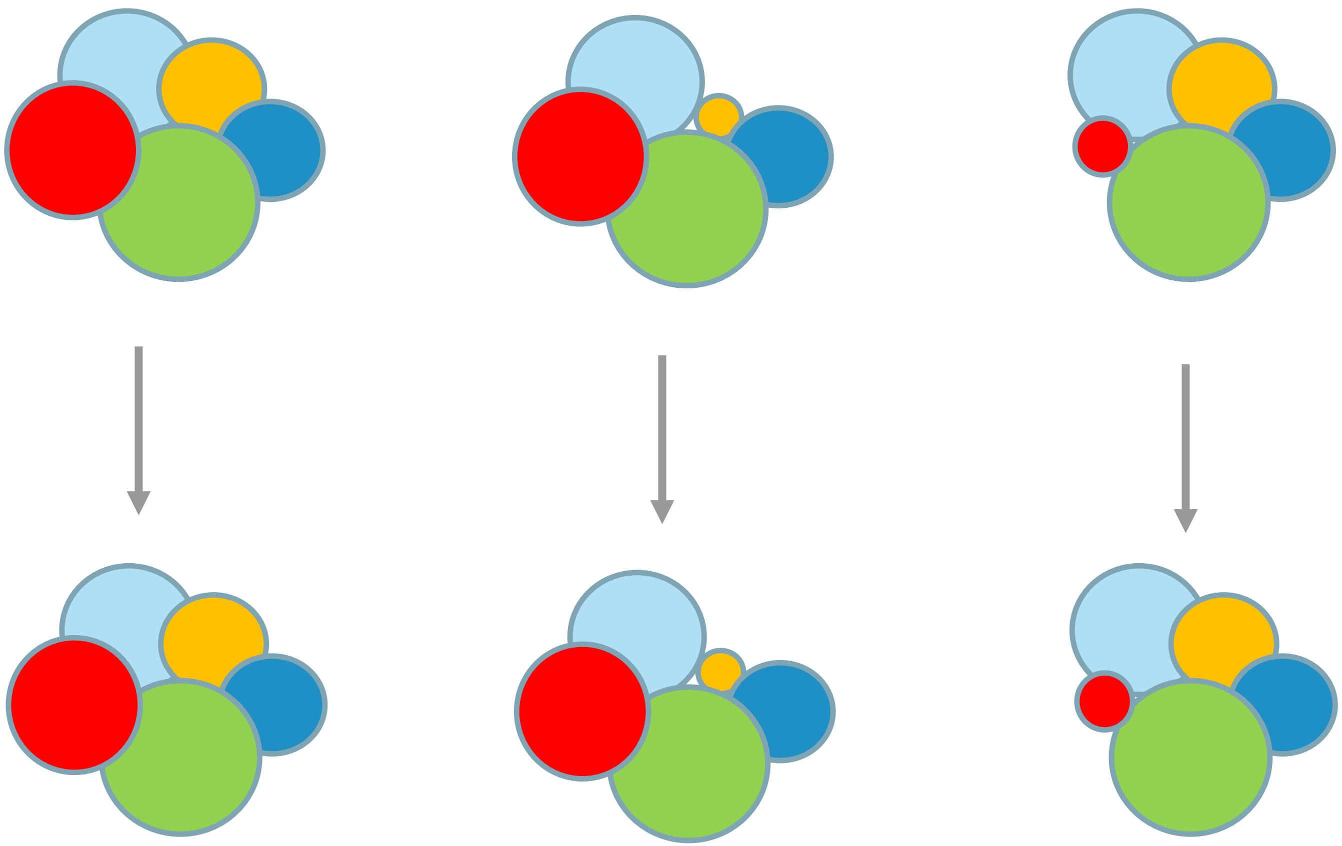
Death would have a trivial stoichiometry, if the dead organic matter has the same composition than the dying organisms. Then we would just turn one unit of living organisms into one unit of dead organic matter.

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



Death

Living organisms with different composition



simple stoichiometry but many types of POM needed

Dead particulate organic matter

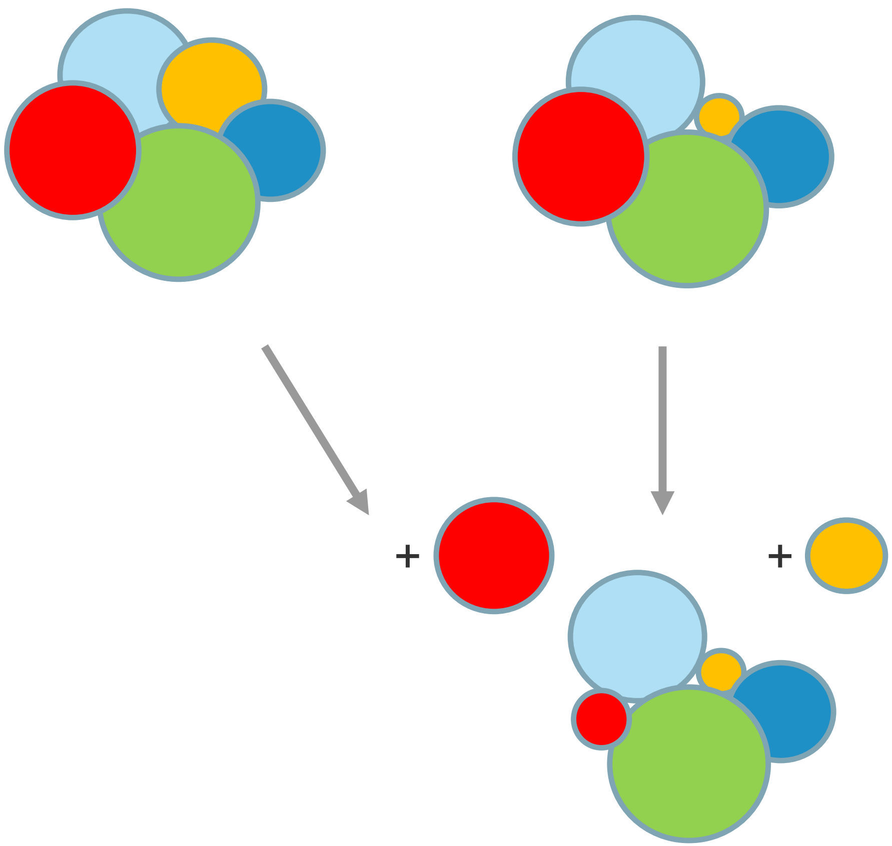
Death

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.

Death

Living organisms with different composition



Dead particulate organic matter + nutrients

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

Check mass balance

ν	NH4 [mol]	NO3 [mol]	HPO4 [mol]	HCO3 [mol]	O2 [mol]	H [mol]	H2O [mol]	ALG [gDM]	ZOO [gDM]	POM [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		NH4	NO3	HPO4	HCO3	O2	H	H2O	ALG	ZOO	POM
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	NH4	NO3	HPO4	HCO3	O2	H	H2O	ALG	ZOO	POM	**sum**
C - death.ZOO:	0	0	0	-0.01025	0	0	0	0	-0.03	0.04025	0

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

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