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

2. Behavior of solutions, numerics, lake phytoplankton-zooplankton model  
   Exercise: lake phytoplankton-zooplankton model


4. Biological processes in lakes

5. Physical processes in lakes, mass balance in multi-box and continuous systems. Exercise: structured, biogeochemical-ecological lake model  
   Homework: build your own model by implementing model extensions

6. Physical processes in rivers, bacterial growth, river model for benthic populations. Exercise: river model for benthic populations, nutrients and oxygen

7. Stochasticity and uncertainty. Exercise: uncertainty, stochasticity

8. Overview model structures, additional processes, model extensions

9. Existing models and applications in research and practice, examples and case studies, preparation of the oral exam
Goals

• Review exercise 2 and clarify open questions

• Acquire knowledge in process stoichiometry to bridge between ecological and biogeochemical processes.

• Learn to calculate stoichiometric coefficients from chemical substance notation (chapter 4.3.1) and parameterized elemental mass fractions (chapter 4.3.2).
### Review exercise 2: Model description

#### chapter 11.2

<table>
<thead>
<tr>
<th>Process</th>
<th>Substances / Organisms</th>
<th>Rate</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>HPO4 [gP/m³]</td>
<td>ALG [gDM/m³]</td>
</tr>
<tr>
<td>Growth of algae</td>
<td>$-\alpha_{P, ALG}$</td>
<td>1</td>
</tr>
<tr>
<td>Death of algae</td>
<td></td>
<td>$-1$</td>
</tr>
<tr>
<td>Growth of zooplankton</td>
<td>$\frac{1}{Y_{ZOO}}$</td>
<td>1</td>
</tr>
<tr>
<td>Death of zooplankton</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Rate expression**

- $\rho_{gro, ALG} = k_{gro, ALG, T_0} \cdot \exp(\beta_{ALG}(T - T_0)) \cdot \frac{1}{\lambda h} \log \left( \frac{K_I + I_0}{K_I + I_0 \exp(-\lambda h)} \cdot \frac{C_{HPO_4^-}}{K_{HPO_4^-, ALG} + C_{HPO_4^-}} \cdot C_{ALG} \right)$
- $\rho_{death, ALG} = k_{death, ALG} \cdot C_{ALG}$
- $\rho_{gro, ZOO} = k_{gro, ZOO, T_0} \cdot \exp(\beta_{ZOO}(T - T_0)) \cdot C_{ALG} \cdot C_{ZOO}$
- $\rho_{death, ZOO} = k_{death, ZOO} \cdot C_{ZOO}$
1. Are the algae concentrations controlled bottom-up (by phosphate limitation) or top-down (by grazing of zooplankton)?

2. What is the reason for oscillating concentrations under constant driving forces? What happens when you introduce periodic driving forces?

3. What are the main deficits of the model compared to a real lake?

4. What is your expectation regarding the response of the model to the change in each parameter, does the result match your expectation and can you explain the observed changes?
Review exercise 2: Model results

Results for constant environmental conditions

Results for periodic environmental conditions
Review exercise 2: Sensitivity Analysis
Review exercise 2: Sensitivity Analysis
Review exercise 2: Sensitivity Analysis
Review exercise 2: Sensitivity Analysis

Graphs showing changes over time for different scenarios involving C.HPO4, C.ALG, and C.ZOO.
Review exercise 2: Sensitivity Analysis
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Review exercise 2: Sensitivity Analysis
Review exercise 2: Sensitivity Analysis
Review Exercise 2: Lessons learned?
Stoichiometry

<table>
<thead>
<tr>
<th>Process $i$</th>
<th>Substances $j$</th>
<th>Rate</th>
</tr>
</thead>
<tbody>
<tr>
<td>$p_1$</td>
<td>$s_1$</td>
<td>$\nu_{11}$ $\nu_{12}$ $\nu_{13}$ $\cdots$ $\nu_{1n_s}$</td>
</tr>
<tr>
<td>$p_2$</td>
<td>$s_2$</td>
<td>$\nu_{21}$ $\nu_{22}$ $\nu_{23}$ $\cdots$ $\nu_{2n_s}$</td>
</tr>
<tr>
<td>$\vdots$</td>
<td>$s_3$</td>
<td>$\vdots$ $\vdots$ $\vdots$ $\cdots$ $\vdots$</td>
</tr>
<tr>
<td>$p_{n_P}$</td>
<td>$s_{n_s}$</td>
<td>$\nu_{n_p1}$ $\nu_{n_p2}$ $\nu_{n_p3}$ $\cdots$ $\nu_{n_Pn_s}$</td>
</tr>
</tbody>
</table>

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

How to derive the stoichiometric coefficients $\nu_{ij}$?
Stoichiometry: Ingredients for 1 cake?

Best recipe: https://tinyurl.com/Schoggikuchen
Stoichiometry

https://openclipart.org/detail/263810/chemist
3 ways to derive stoichiometric coefficients:

- Chemical substance notation
- Parameterized elemental mass fractions
- General solution
## Chemical Substance Notation

<table>
<thead>
<tr>
<th>Process</th>
<th>( \text{NH}_4^+ \text{ mol} )</th>
<th>( \text{NO}_3^- \text{ mol} )</th>
<th>( \text{HPO}_{2}^- \text{ mol} )</th>
<th>( \text{O}_2 \text{ mol} )</th>
<th>( \text{ALG} \text{ gDM} )</th>
<th>( \text{ZOO} \text{ gDM} )</th>
<th>( \text{POM} \text{ gDM} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Growth of ALG,NH4</td>
<td>?</td>
<td>?</td>
<td>?</td>
<td>?</td>
<td>1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Growth of ALG,NO3</td>
<td>?</td>
<td>?</td>
<td>?</td>
<td>?</td>
<td>1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Death of ALG</td>
<td>-1</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>Death of ZOO</td>
<td>-1</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>1</td>
<td></td>
</tr>
</tbody>
</table>

Additional substances for calculation of the stoichiometric coefficients: \( \text{HCO}_3^- \), \( \text{H}^+ \), \( \text{H}_2\text{O} \)
Chemical Substance Notation

1. Example: Growth of algae

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:

\[
m = 106 \cdot 12 \text{ gC mol}^{-1} + 263 \text{ gH mol}^{-1} + 110 \cdot 16 \text{ gO mol}^{-1} \\
+ 16 \cdot 14 \text{ gN mol}^{-1} + 31 \text{ gP mol}^{-1} \\
= 3550 \text{ gDM mol}^{-1}
\]
1. Example: Growth of algae with nitrate:

\[ a \text{HCO}_3^- + b \text{NO}_3^- + c \text{HPO}_4^{2-} + d \text{H}^+ + e \text{H}_2\text{O} \rightarrow \text{C}_{106}\text{H}_{263}\text{O}_{110}\text{N}_{16}\text{P} + f \text{O}_2 \]

6 unknowns \((a, b, c, d, e, f)\)

equations for the conservation of "mass": ?
1. Example: Growth of algae with nitrate:

\[
a \text{HCO}_3^- + b \text{NO}_3^- + c \text{HPO}_4^{2-} + d \text{H}^+ + e \text{H}_2\text{O} \\
\rightarrow \text{C}_{106}\text{H}_{263}\text{O}_{110}\text{N}_{16}\text{P} + f \text{O}_2
\]

\[
106 \text{HCO}_3^- + 16 \text{NO}_3^- + \text{HPO}_4^{2-} + 124 \text{H}^+ + 16 \text{H}_2\text{O} \\
\rightarrow \text{C}_{106}\text{H}_{263}\text{O}_{110}\text{N}_{16}\text{P} + 138 \text{O}_2
\]
Stoichiometric coefficients for growth of algae:

\[
\begin{align*}
\nu_{\text{gro,ALG,NO}_3 \text{ HCO}_3^-} &= -\frac{106}{3550} \frac{\text{molHCO}_3^-}{\text{gDM}} \\
\nu_{\text{gro,ALG,NO}_3 \text{ NO}_3^-} &= -\frac{16}{3550} \frac{\text{molNO}_3^-}{\text{gDM}} \\
\nu_{\text{gro,ALG,NO}_3 \text{ HPO}_4^{2-}} &= -\frac{1}{3550} \frac{\text{molHPO}_4^{2-}}{\text{gDM}} \\
\nu_{\text{gro,ALG,NO}_3 \text{ H}^+} &= -\frac{124}{3550} \frac{\text{molH}^+}{\text{gDM}} \\
\nu_{\text{gro,ALG,NO}_3 \text{ H}_2\text{O}} &= -\frac{16}{3550} \frac{\text{molH}_2\text{O}}{\text{gDM}} \\
\nu_{\text{gro,ALG,NO}_3 \text{ ALG}} &= 1 \frac{\text{gDM}}{\text{gDM}} \\
\nu_{\text{gro,ALG,NO}_3 \text{ O}_2} &= \frac{138}{3550} \frac{\text{molO}_2}{\text{gDM}}
\end{align*}
\]
Do exercise L3 Task 1
Similarly for algal growth with ammonium:

\[ 106 \text{HCO}_3^- + 16 \text{NH}_4^+ + \text{HPO}_4^{2-} + 92 \text{H}^+ \rightarrow C_{106}\text{H}_{263}\text{O}_{110}\text{N}_{16}\text{P} + 106 \text{O}_2 \]

Respiration:

\[ C_{106}\text{H}_{263}\text{O}_{110}\text{N}_{16}\text{P} + 106 \text{O}_2 \rightarrow 106 \text{HCO}_3^- + 16 \text{NH}_4^+ + \text{HPO}_4^{2-} + 92 \text{H}^+ \]

Death:

\[ C_{106}\text{H}_{263}\text{O}_{110}\text{N}_{16}\text{P} \rightarrow C_{106}\text{H}_{263}\text{O}_{110}\text{N}_{16}\text{P} \]
### Chemical Substance Notation

<table>
<thead>
<tr>
<th>Process</th>
<th>( \text{NH}_4^+ )</th>
<th>( \text{NO}_3^- )</th>
<th>( \text{HPO}_4^{2-} )</th>
<th>( \text{O}_2 )</th>
<th>ALG</th>
<th>ZOO</th>
<th>POM</th>
</tr>
</thead>
<tbody>
<tr>
<td>Growth of ALG,NO(_3)</td>
<td>?</td>
<td>?</td>
<td>?</td>
<td>?</td>
<td>1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Death of ALG</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>-1</td>
<td></td>
<td>1</td>
</tr>
<tr>
<td>Death of ZOO</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>-1</td>
<td></td>
<td>1</td>
</tr>
</tbody>
</table>

→ how many unknowns?

Additional substances for calculation of the stoichiometric coefficients: \( \text{HCO}_3^- \), \( \text{H}^+ \), \( \text{H}_2\text{O} \)
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: $f_r = 1 - Y_{ZOO} - f_e$
## Chemical Substance Notation

<table>
<thead>
<tr>
<th>Process</th>
<th>NH(_4^+) mol</th>
<th>NO(_3^-) mol</th>
<th>HPO(_4^{2-}) mol</th>
<th>O(_2) mol</th>
<th>ALG gDM</th>
<th>ZOO gDM</th>
<th>POM gDM</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gro. ALG,NH4</td>
<td>16/3550</td>
<td>1/3550</td>
<td>106</td>
<td>1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Gro. ALG,NO3</td>
<td>16/3550</td>
<td>1/3550</td>
<td>138</td>
<td>1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Resp. ALG</td>
<td>16/3550</td>
<td>1/3550</td>
<td>106</td>
<td>-1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Death ALG</td>
<td>-1</td>
<td></td>
<td></td>
<td>1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Growth ZOO</td>
<td>(\frac{f_r}{Y_{ZOO}}) 16/3550</td>
<td>(\frac{f_r}{Y_{ZOO}}) 1/3550</td>
<td>(\frac{f_r}{Y_{ZOO}}) 106/3550</td>
<td>(\frac{1}{Y_{ZOO}}) 1</td>
<td>(\frac{f_e}{Y_{ZOO}})</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Resp. ZOO</td>
<td>16/3550</td>
<td>1/3550</td>
<td>106</td>
<td>-1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Death ZOO</td>
<td>-1</td>
<td></td>
<td></td>
<td>1</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Chemical Substance Notation:

Quite some handwork!

If composition changes: redo the calculation!

-> instead of fixed composition use parameters for elemental mass fractions
3 ways to derive stoichiometric coefficients:

- Chemical substance notation
- Parameterized elemental mass fractions
- General solution
### Extended Process Table Notation

<table>
<thead>
<tr>
<th>Processes $i$</th>
<th>Substances $j$</th>
<th>Rates</th>
</tr>
</thead>
<tbody>
<tr>
<td>$p_1$</td>
<td>$s_1$</td>
<td>$\nu_{11}$</td>
</tr>
<tr>
<td>$p_2$</td>
<td>$s_2$</td>
<td>$\nu_{21}$</td>
</tr>
<tr>
<td>$\vdots$</td>
<td>$s_3$</td>
<td>$\vdots$</td>
</tr>
<tr>
<td>$p_{n_P}$</td>
<td>$s_{n_s}$</td>
<td>$\nu_{n_P1}$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Elements $k$</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>$e_1$</td>
<td>$\alpha_{11}$</td>
</tr>
<tr>
<td>$e_2$</td>
<td>$\alpha_{21}$</td>
</tr>
<tr>
<td>$\vdots$</td>
<td>$\vdots$</td>
</tr>
<tr>
<td>$e_{n_e}$</td>
<td>$\alpha_{n_e1}$</td>
</tr>
</tbody>
</table>

$\nu_{ij}$: stoich. coeff. = relative transf. rate of substance $j$ in proc. $i$

$\alpha_{kj}$: mass fraction of element $k$ on substance $j$

$\nu_{ij}\alpha_{kj}$: relative transf. rate of element $k$ contained in subst. $j$
## Extended Process Table Notation

<table>
<thead>
<tr>
<th>Processes $i$</th>
<th>Substances $j$</th>
<th>Rates</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$s_1$</td>
<td>$s_2$</td>
</tr>
<tr>
<td>$p_1$</td>
<td>$\nu_{11}$</td>
<td>$\nu_{12}$</td>
</tr>
<tr>
<td>$p_2$</td>
<td>$\nu_{21}$</td>
<td>$\nu_{22}$</td>
</tr>
<tr>
<td>$\vdots$</td>
<td>$\vdots$</td>
<td>$\vdots$</td>
</tr>
<tr>
<td>$p_{n_P}$</td>
<td>$\nu_{n_P1}$</td>
<td>$\nu_{n_P2}$</td>
</tr>
</tbody>
</table>

### Elements $k$

| $e_1$ | $\alpha_{11}$ | $\alpha_{12}$ | $\alpha_{13}$ | $\cdots$ | $\alpha_{1n_s}$ |
|-------|----------------|----------------|----------------|-------|
| $e_2$ | $\alpha_{21}$ | $\alpha_{22}$ | $\alpha_{23}$ | $\cdots$ | $\alpha_{2n_s}$ |
| $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\ddots$ | $\vdots$ |
| $e_{n_e}$ | $\alpha_{n_e1}$ | $\alpha_{n_e2}$ | $\alpha_{n_e3}$ | $\cdots$ | $\alpha_{n_en_s}$ |

Mass conservation for element $k$ in process $i$: \[ \sum_{j} \nu_{ij} \alpha_{kj} = 0 \]
### Parameterized Mass Fractions

<table>
<thead>
<tr>
<th>Process</th>
<th>$\text{NH}_4^+$ mol</th>
<th>$\text{NO}_3^-$ mol</th>
<th>$\text{HPO}_4^{2-}$ mol</th>
<th>$\text{O}_2$ mol</th>
<th>ALG gDM</th>
<th>ZOO gDM</th>
<th>POM gDM</th>
</tr>
</thead>
<tbody>
<tr>
<td>Growth of ALG, NH4</td>
<td>$?$</td>
<td>$?$</td>
<td>$?$</td>
<td>$?$</td>
<td>1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Growth of ALG, NO3</td>
<td>$?$</td>
<td>$?$</td>
<td>$?$</td>
<td>$?$</td>
<td>1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Death of ALG</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>-1</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>Death of ZOO</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>-1</td>
<td>1</td>
<td></td>
</tr>
</tbody>
</table>

Additional substances for calculation of the stoichiometric coefficients: $\text{HCO}_3^-$, $\text{H}^+$, $\text{H}_2\text{O}$

Mass balance equations for C, H, O, N, P and charge
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:

\[ C_{\alpha_{C},j} H_{\alpha_{H},j} O_{\alpha_{O},j} N_{\alpha_{N},j} P_{\alpha_{P},j} /31 \]

with:

\[ \alpha_{C,j} + \alpha_{H,j} + \alpha_{O,j} + \alpha_{N,j} + \alpha_{P,j} = 1 \]
Parameterized Mass Fractions

Redfield composition:

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

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

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

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

\[
\alpha_{\text{Redfield}, P, \text{ALG}} = \frac{1 \cdot 31}{3550} \frac{\text{gP}}{\text{gDM}} \approx 0.01 \frac{\text{gP}}{\text{gDM}}
\]
Parameterized Mass Fractions

\[ a \text{HCO}_3^- + b \text{NO}_3^- + c \text{HPO}_4^{2-} + d \text{H}^+ + e \text{H}_2\text{O} \rightarrow C_{106}\text{H}_{263}\text{O}_{110}\text{N}_{16}\text{P} + f \text{O}_2 \]

Setting up equation for algal growth with unknown coefficients:

\[ a \text{HCO}_3^- + b \text{NO}_3^- + c \text{HPO}_4^{2-} + d \text{H}^+ + e \text{H}_2\text{O} \rightarrow C_{\alpha_{\text{C,ALG}/12}}\text{H}_{\alpha_{\text{H,ALG}}}\text{O}_{\alpha_{\text{O,ALG}/16}}\text{N}_{\alpha_{\text{N,ALG}/14}}\text{P}_{\alpha_{\text{P,ALG}/31}} + f \text{O}_2 \]

Conservation of C: \[ a = \frac{\alpha_{\text{C,ALG}}}{12} \]
Conservation of N: \[ b = \frac{\alpha_{\text{N,ALG}}}{14} \]
Conservation of P: \[ c = \frac{\alpha_{\text{P,ALG}}}{31} \]
Parameterized Mass Fractions

\[
\frac{\alpha_{C,ALG}}{12} \cdot \text{HCO}_3^- + \frac{\alpha_{N,ALG}}{14} \cdot \text{NO}_3^- + \frac{\alpha_{P,ALG}}{31} \cdot \text{HPO}_4^{2-} + d \cdot \text{H}^+ + e \cdot \text{H}_2\text{O} \\
\rightarrow C_{\alpha_{C,ALG}/12} \cdot \text{H}_{\alpha_{H,ALG}} \cdot \text{O}_{\alpha_{O,ALG}/16} \cdot \text{N}_{\alpha_{N,ALG}/14} \cdot \text{P}_{\alpha_{P,ALG}/31} + f \cdot \text{O}_2
\]

Conservation of H, O and charge:

**H:** \[ \frac{\alpha_{C,ALG}}{12} \cdot 1 + \frac{\alpha_{P,ALG}}{31} \cdot 1 + d \cdot 1 + e \cdot 2 = 1 \cdot \alpha_{H,ALG} \]

**O:** \[ \frac{\alpha_{C,ALG}}{12} \cdot 3 + \frac{\alpha_{N,ALG}}{14} \cdot 3 + \frac{\alpha_{P,ALG}}{31} \cdot 4 + e \cdot 1 = 1 \cdot \frac{\alpha_{O,ALG}}{16} + f \cdot 2 \]

**charge:** \[ \frac{\alpha_{C,ALG}}{12} \cdot (-1) + \frac{\alpha_{N,ALG}}{14} \cdot (-1) + \frac{\alpha_{P,ALG}}{31} \cdot (-2) + d \cdot (+1) = 0 \]
Parameterized Mass Fractions

\[ d = \frac{\alpha_{C, ALG}}{12} + \frac{\alpha_{N, ALG}}{14} + \frac{2 \, \alpha_{P, ALG}}{31} \]

\[ e = \frac{\alpha_{H, ALG}}{2} - \frac{\alpha_{C, ALG}}{12} - \frac{\alpha_{N, ALG}}{28} - \frac{3 \, \alpha_{P, ALG}}{62} \]

\[ f = \frac{\alpha_{C, ALG}}{12} + \frac{\alpha_{H, ALG}}{4} - \frac{\alpha_{O, ALG}}{32} + \frac{5 \, \alpha_{N, ALG}}{56} + \frac{5 \, \alpha_{P, ALG}}{124} \]
Parameterized Mass Fractions

Growth of algae:

\[
\frac{\alpha_{C,\text{ALG}}}{12} \text{HCO}_3^- + \frac{\alpha_{N,\text{ALG}}}{14} \text{NO}_3^- + \frac{\alpha_{P,\text{ALG}}}{31} \text{HPO}_4^{2-} \\
+ \left( \frac{\alpha_{C,\text{ALG}}}{12} + \frac{\alpha_{N,\text{ALG}}}{14} + \frac{2 \alpha_{P,\text{ALG}}}{31} \right) \text{H}^+ \\
+ \left( \frac{\alpha_{H,\text{ALG}}}{2} - \frac{\alpha_{C,\text{ALG}}}{12} - \frac{\alpha_{N,\text{ALG}}}{28} - \frac{3 \alpha_{P,\text{ALG}}}{62} \right) \text{H}_2\text{O} \\
\rightarrow C_{\alpha_{C,\text{ALG}}/12}\text{H}_{\alpha_{H,\text{ALG}}}\text{O}_{\alpha_{O,\text{ALG}}/16}\text{N}_{\alpha_{N,\text{ALG}}/14}\text{P}_{\alpha_{P,\text{ALG}}/31} \\
+ \left( \frac{\alpha_{C,\text{ALG}}}{12} + \frac{\alpha_{H,\text{ALG}}}{4} - \frac{\alpha_{O,\text{ALG}}}{32} + \frac{5 \alpha_{N,\text{ALG}}}{56} + \frac{5 \alpha_{P,\text{ALG}}}{124} \right) \text{O}_2
\]
Parameterized Mass Fractions

Do exercise L3 Task 2
Parameterized Mass Fractions:

Changes in composition are now easy to handle, just change the numerical values of the parameters.

What about adding additional elements?

The equations must be revised.

This is a laborious process.

Is there a general solution to this process?
→ Swiss Army Knife of Linear Algebra
Homework

1. Find out what the Swiss Army Knife of Linear Algebra is (hint: SVD)

2. Read chapter 4.3.3

3. Read chapter 14

4. Think about your open questions
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

2. Behavior of solutions, numerics, lake phytoplankton-zooplankton model
   Exercise: lake phytoplankton-zooplankton model


4. Biological processes in lakes

5. Physical processes in lakes, mass balance in multi-box and continuous systems. Exercise: structured, biogeochemical-ecological lake model
   Homework: build your own model by implementing model extensions

6. Physical processes in rivers, bacterial growth, river model for benthic populations. Exercise: river model for benthic populations, nutrients and oxygen

7. Stochasticity and uncertainty. Exercise: uncertainty, stochasticity

8. Overview model structures, additional processes, model extensions

9. Existing models and applications in research and practice, examples and case studies, preparation of the oral exam