

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

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)

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

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	NO3	HPO4	HCO3	O2	H	H2O	ALG	ZOO	POM
		[mol]	[gDM]	[gDM]	[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)



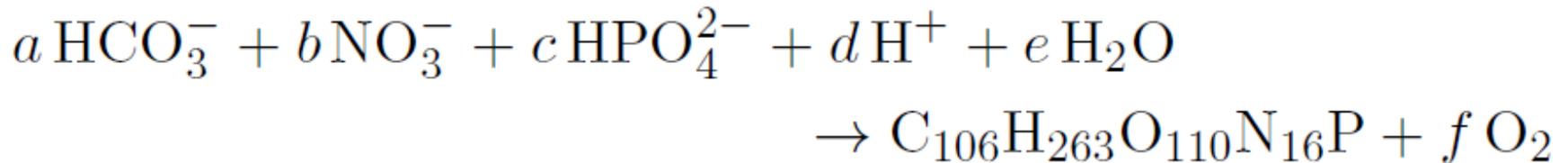
Total “molar” mass

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

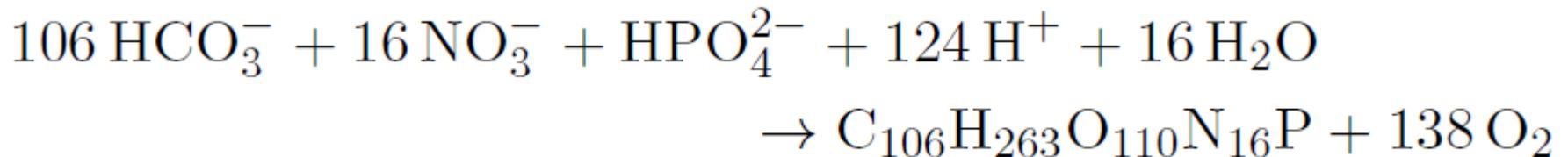
$$\begin{aligned} m &= 106 \cdot 12 \frac{\text{gC}}{\text{“mol”}} + 263 \frac{\text{gH}}{\text{“mol”}} + 110 \cdot 16 \frac{\text{gO}}{\text{“mol”}} \\ &\quad + 16 \cdot 14 \frac{\text{gN}}{\text{“mol”}} + 31 \frac{\text{gP}}{\text{“mol”}} \\ &= 3550 \frac{\text{gDM}}{\text{“mol”}} \quad . \end{aligned}$$

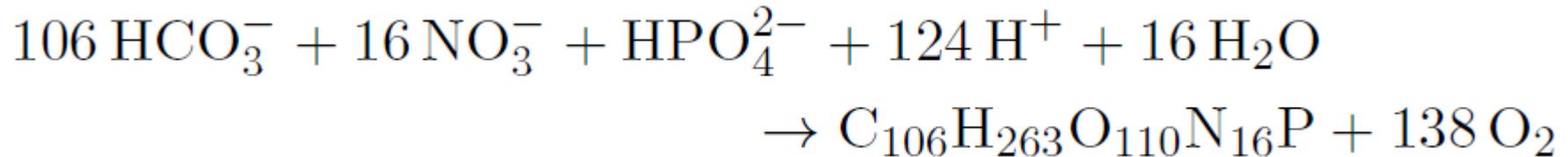
Example: Algae growth

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:

$$\begin{aligned} \nu_{\text{gro,ALG,NO3 HCO}_3^-} &= -\frac{106}{3550} \frac{\text{molHCO}_3^-}{\text{gDM}} \\ \nu_{\text{gro,ALG,NO3 NO}_3^-} &= -\frac{16}{3550} \frac{\text{molNO}_3^-}{\text{gDM}} \\ \nu_{\text{gro,ALG,NO3 HPO}_4^{2-}} &= -\frac{1}{3550} \frac{\text{molHPO}_4^{2-}}{\text{gDM}} \\ \nu_{\text{gro,ALG,NO3 H}^+} &= -\frac{124}{3550} \frac{\text{molH}^+}{\text{gDM}} \\ \nu_{\text{gro,ALG,NO3 H}_2\text{O}} &= -\frac{16}{3550} \frac{\text{molH}_2\text{O}}{\text{gDM}} \\ \nu_{\text{gro,ALG,NO3 ALG}} &= 1 \frac{\text{gDM}}{\text{gDM}} \\ \nu_{\text{gro,ALG,NO3 O}_2} &= \frac{138}{3550} \frac{\text{molO}_2}{\text{gDM}} \end{aligned}$$

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

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

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
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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

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

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

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: $f_r = 1 - Y_{ZOO} - f_e$

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

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

ν		NH4	NO3	HPO4	HCO3	O2	H	H2O	ALG	ZOO	POM
		[mol]	[gDM]	[gDM]	[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 \rightarrow can be solved

Conclusion?

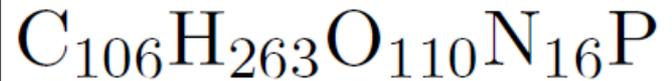
Concept is straightforward but quite some manual work!

If composition changes: redo the calculation!

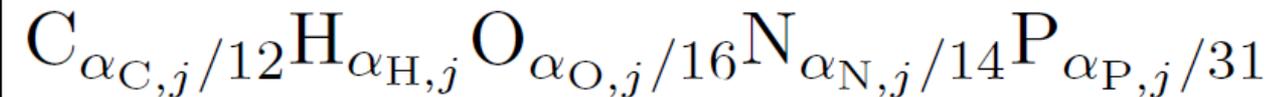
3 ways to derive stoichiometric coefficients:

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

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



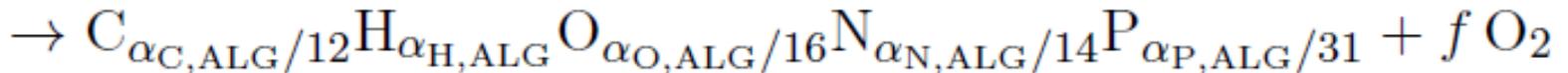
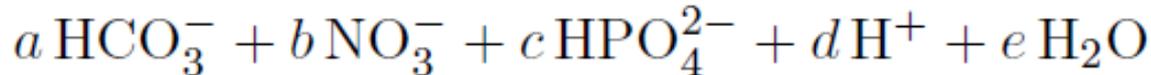
use parameterized mass fractions:



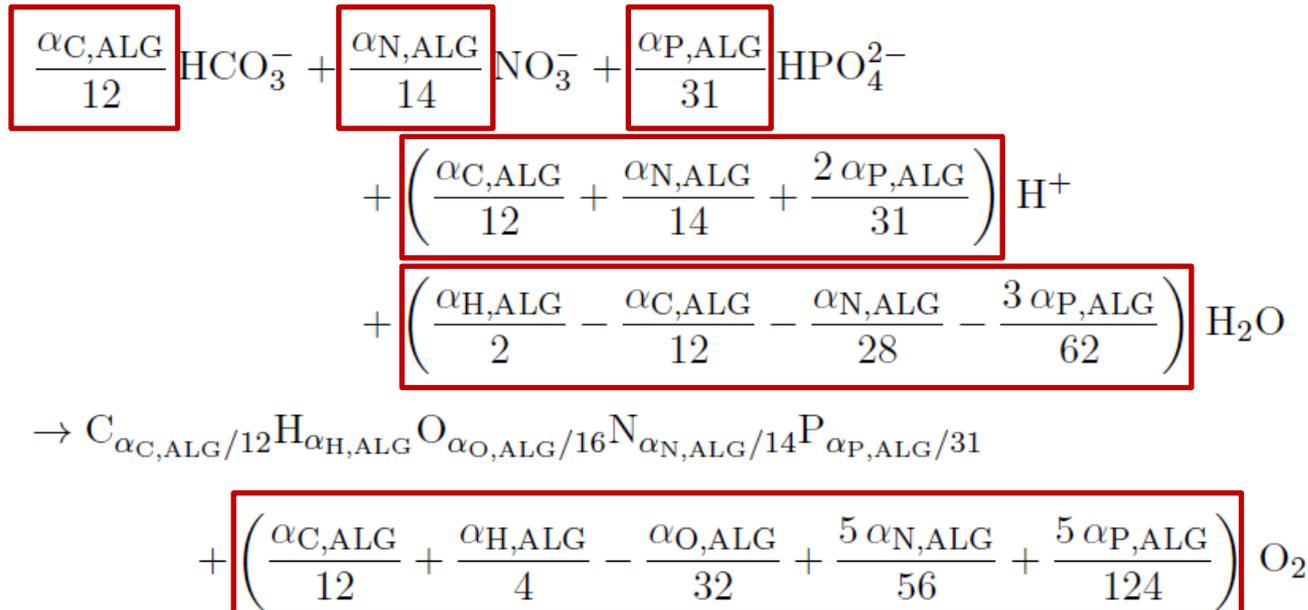
with:

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

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):



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

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

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

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

→ Swiss Army Knife of Linear Algebra



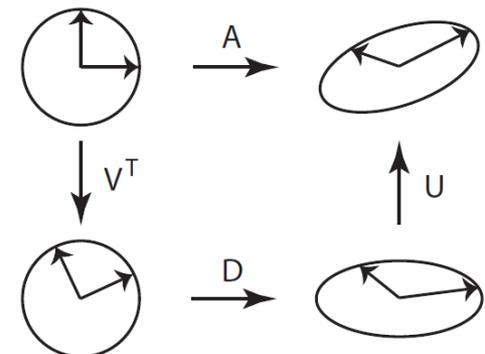
What did you find out?

The Singular Value Decomposition Theorem decomposes any $n \cdot m$ matrix A (with $n \geq m$) into three matrices:

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

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

→ The rows of U^T corresponding to elements of D that are zero build a basis of the left null space of A . They are a solution of our linear algebra problem. See R-function `svd()`



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.Z00 <-  
  calc.stoich.coef(alpha      = alpha.2,  
                  name       = "gro.Z00",  
                  subst      = c("NH4", "HPO4", "HCO3", "O2", "H",  
                                "H2O", "ALG", "Z00", "POM"),  
                  subst.norm = "Z00",  
                  nu.norm    = 1,  
                  constraints = list(c("Z00" = 1,  
                                     "ALG" = param$Y.Z00),  
                                   c("POM" = 1,  
                                     "ALG" = param$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 dependencies in compositions or constraints.**

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

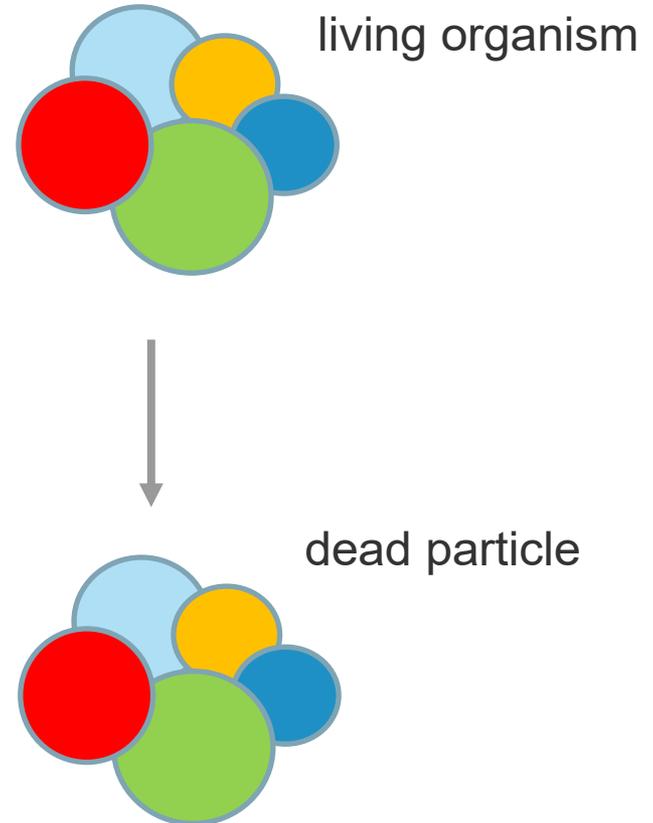
Extended Process Table Notation

ν		NH4	NO3	HPO4	HCO3	O2	H	H2O	ALG	ZOO	POM	
		[mol]	[gDM]	[gDM]	[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	

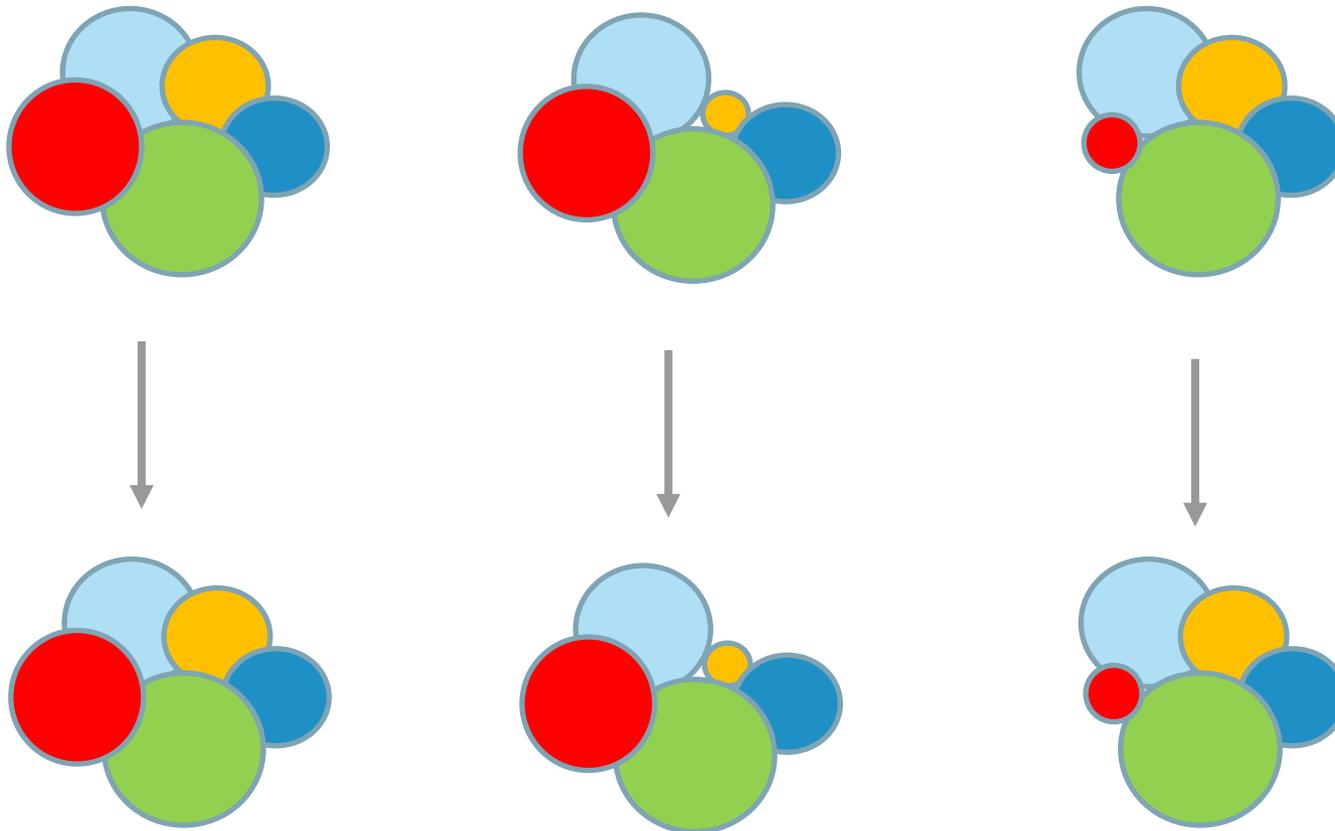
$$\sum_j \nu_{ij} \alpha_{kj} = 0$$

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



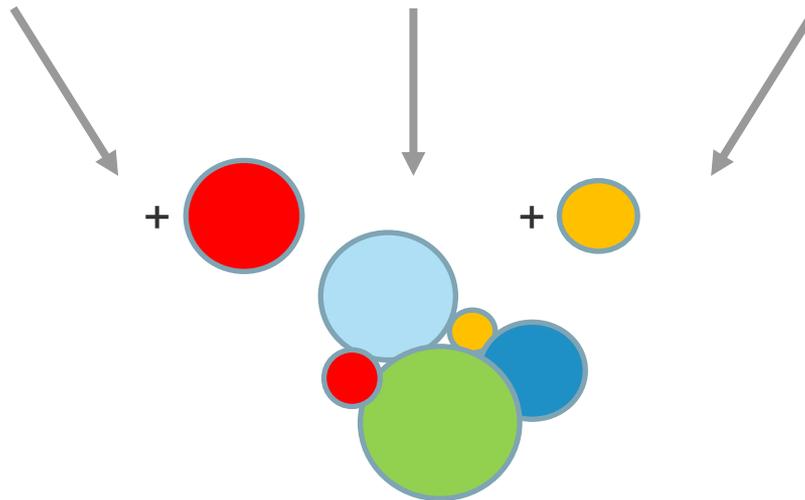
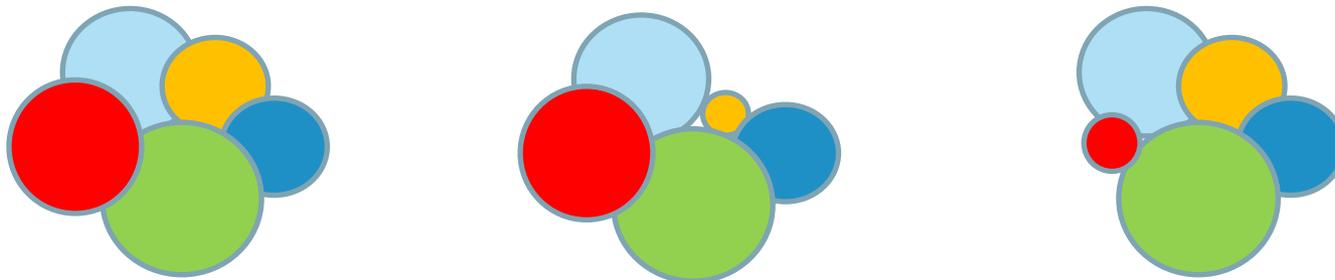
simple
stoichiometry
but many types
of POM needed

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



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										
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	-0.03	0.04025	0

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

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Exercise: R, ecosim-package, simple lake plankton model
Exercise: lake phytoplankton-zooplankton model
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3. Biological processes in lakes
4. Physical processes in lakes, mass balance in multi-box and continuous systems
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Assignments: build your own model by implementing model extensions
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Exercise: river model for benthic populations, nutrients and oxygen
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Exercise: uncertainty, stochasticity
7. Existing models and applications in research and practice, examples and case studies, preparation of the oral exam, feedback

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- think about open questions regarding stoichiometric calculations
- read chapter 8 about biological processes