Exercise 3

Modelling Aquatic Ecosystems FS24

20.3.2024

Introduction of the ‘`stoichcalc`’ package

- An R package that implements the general solution to calculate stoichiometric coefficients of substances and organisms for different processes.

- The package contains three functions:

– ‘`calc.comp.matrix`’ constructs the **substance composition matrix**

– ‘`calc.stoich.coef`’ calculates the **stoichiometric coefficients**

– ‘`calc.stoich.basis`’ calculates the basis of the **stoichiometry space** (used by the function calc.stoich.coef, not directly in the exercises)

- Using ‘`?stoichcalc`’ in R for more details.

'calc.comp.matrix'

```r
HPO4    <- c(P        = 1)                 # gP/gHPO4-P
ALG     <- c(P        = 0.01)              # gP/gALG

subst.comp <- list(HPO4    = HPO4,
                   ALG     = ALG)

alpha.1 <- calc.comp.matrix(subst.comp)

print(alpha.1)
```

```r
HPO4    <- c(P        = 1)                 # gP/gHPO4-P
NH4     <- c(N        = 1)                 # gN/gNH4-N
ALG     <- c(P        = 0.01,              # gP/gALG
             N        = 0.06)              # gN/gALG

subst.comp <- list(HPO4    = HPO4,
                   NH4     = NH4,
                   ALG     = ALG)

alpha.1 <- calc.comp.matrix(subst.comp)

print(alpha.1)
```

Vectors for each substance/organism providing the elemental composition

Named list with the elementary composition of each substance/organism

```
[1] "Composition matrix (1x2) successfully constructed:"
[1] "el. const.: P"
[1] "substances: HPO4,ALG"
  HPO4   ALG
P    1  0.01
```

```
[1] "Composition matrix (2x3) successfully constructed:"
[1] "el. const.: P,N"
[1] "substances: HPO4,NH4,ALG"
  HPO4 NH4  ALG
P    1   0 0.01
N    0   1 0.06
```

Elementary constituents

Substances & organisms

Composition matrix
with elementary constituents as rows
and substances/organisms as columns

‘calc.stoich.coef’

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

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

nu.1 <- rbind(nu.gro.ALG,
              nu.resp.ALG)

print(nu.1)
```

- For each process we need to calculate the stoichiometric coefficients separately (growth of algae, respiration of algae ……)
- ‘alpha’ is the composition matrix
- ‘subst.norm’ is the substance you choose to normalize the stoichiometric coefficients, ‘nu.norm’ is the value you choose to normalize.

```
[1] "Number of substances:                  2"      → HPO4, ALG
[1] "Number of elementary constituents:     1"      → P
[1] "Number of constraints:                 0"      → No additional constraint
[1] "Number of independent processes:       1"      → Growth of algae
[1] "Stoichiometric coefficients successfully calculated."
[1] "Number of substances:                  2"      → HPO4, ALG
[1] "Number of elementary constituents:     1"      → P
[1] "Number of constraints:                 0"      → No constraint
[1] "Number of independent processes:       1"      → Respiration of algae
[1] "Stoichiometric coefficients successfully calculated."
            HPO4  ALG
growth.ALG -0.01    1
resp.ALG    0.01   -1
```

→ Stoichiometric coefficient matrix nu

Try to do Task 1 in Exercise 3!

Stoichiometry of a complex process model

- Parameterized mass fractions (Algae as an example)

Sum of mass fractions [g element per g algae]
for all elements in a substance/organism should be 1

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

```
param <- list(a.O.ALG     = 0.50,          # gO/gALG
              a.H.ALG     = 0.07,          # gH/gALG
              a.N.ALG     = 0.06,          # gN/gALG
              a.P.ALG     = 0.005,         # gP/gALG
param$a.C.ALG = 1-(param$a.O.ALG+param$a.H.ALG+param$a.N.ALG+param$a.P.ALG)
```

In order to guarantee
that the fractions sum to 1

This tells you how many mole of each element
per gram of algae.

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

```
ALG    <- c(C      = param$a.C.ALG/12,   # molC/gALG
            O      = param$a.O.ALG/16,   # molO/gALG
            H      = param$a.H.ALG,      # molH/gALG
            N      = param$a.N.ALG/14,   # molN/gALG
            P      = param$a.P.ALG/31)   # molP/gALG
```

Elemental mass fractions of organisms are
known according to different compositions. Here
we use the Redfield composition for algae.

Stoichiometry of a complex process model

- Constraints γ have to be formulated to fulfill $\boxed{\boldsymbol{\nu}_i \cdot (\boldsymbol{\gamma}_{(i)})^{\mathrm{T}} = \mathbf{0}}$

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

```
param$Y.ALG.death = min(1,param$a.N.ALG/param$a.N.POM,param$a.P.ALG/param$a.P.POM)
param$Y.ZOO.death = min(1,param$a.N.ZOO/param$a.N.POM,param$a.P.ZOO/param$a.P.POM)
```

$\boldsymbol{Y.death} \leq \mathbf{1}$, otherwise it means dead particulate organic matter (POM) takes up nutrients from algae or zooplankton. Here we choose it as close to 1 as possible and as small as necessary to avoid negative coefficients for the nutrients.

Constraints provide the relation between two substances/org. We choose one organism to be 1, then the other can be quantified by parameters.

```
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)))
```

```
[1] "Number of substances:                        9"
[1] "Number of elementary constituents:           6"
[1] "Number of constraints:                       2"
[1] "Number of independent processes:             1"
[1] "Stoichiometric coefficients successfully calculated."
          NH4 NO3 HPO4  HCO3     O2    H   H2O ALG ZOO POM
gro.ZOO 0.011   0    0 0.042 -0.031 0.03 0.011  -5   1   2
```

No. Substances & Organisms = elementary constituents +
No. Constraints +
1 normalized substance/organism

In this example, **9 substances** = **6 elements** (C,N,P,O,H,charge) + **2** (constraints) + **1** (normalized zooplankton)

Try to do Task 2 in Exercise 3!

Homework

- Task 3: Homework: Extend the process stoichiometry to sulfur
- Think about theory questions in Exercise 3.

Don’t hesitate to ask if you have any questions!

Have a great day!