Exercise 4: Biogeochemical-Ecological Lake Model

ETH Zurich Course 701-0426-00L: Modelling Aquatic Ecosystems (Schuwirth/Reichert)

08.04.2020

Goals:

- Understand the concepts and process formulations of the coupled biogeochemical-ecological lake model described in section 11.4.
- Understand the implementation of this model based on the R packages `stoichcalc` and `ecosim`.
- Understand the behaviour (time courses of the state variables and overall mass fluxes) of this model.
- Perform some simple sensitivity analyses to deepen the understanding of the behaviour of the model.

Task 1: Model formulation

Study and try to understand the model formulation given in section 11.4. Note that it may be useful to study first the "intermediately complex" model described in section 11.3.

Task 2: Model implementation

Study the implementation of the model given below and run the model based on the accompanying file `exercise_4.R`.

Task 3: Model results

Study the time courses of the state variables and the overall fluxes of phosphorus and nitrogen resulting from executing the file `exercise_4.R` and interpret the results.

Task 3: Homework: Model sensitivity

Perform a sensitivity analysis with respect to the most important kinetic parameters and interpret the results.

Questions

1. Why is it important that some stoichiometric coefficients are indicated as 0/+?
2. How is the metalimnion represented in the model?
3. Look at the process rates of mineralization in the sediment. Why are they dfferent from those in chapter 8.5?
4. Look at the mass balance for P and N. If there is a difference between input and output + accumulation, where does it come from? Hint: Have a look at the stoichiometric coeffcients for anoxic mineralization.

Solution of Task 2

Load the package `ecosim` (and install if it is not yet installed).

```
# load required packages:

if ( !require("ecosim") ) {install.packages("ecosim"); library(ecosim) }
```

```
## Loading required package: ecosim
```

```
## Loading required package: deSolve
```

```
## Loading required package: stoichcalc
```

Note that the packages `deSolve`, to numerially solve systems of ordinary differential equations, and `stoichcalc`, to calculate process stoichiometry were loaded automatically.

Define parameter values for stoichiometry, kinetics, reactor configuration and input:

```
# Define parameter values:

param <- list(alpha.O.ALG          = 0.50,      # gO/gALG
              alpha.H.ALG          = 0.07,      # gH/gALG
              alpha.N.ALG          = 0.06,      # gN/gALG
              alpha.P.ALG          = 0.005,     # gP/gALG
              alpha.O.ZOO          = 0.50,      # gO/gZOO
              alpha.H.ZOO          = 0.07,      # gH/gZOO
              alpha.N.ZOO          = 0.06,      # gN/gZOO
              alpha.P.ZOO          = 0.01,      # gP/gZOO
              alpha.O.POM          = 0.39,      # gO/gPOM
              alpha.H.POM          = 0.07,      # gH/gPOM
              alpha.N.POM          = 0.06,      # gN/gPOM
              alpha.P.POM          = 0.007,     # gP/gPOM
              Y.ZOO                = 0.2,       # gZOO/gALG
              f.e                  = 0.2,       # gPOM/gALG
              f.I                  = 0.2,       # gPOMI/(gPOMD+gPOMI)
              k.gro.ALG            = 0.8,       # 1/d
              k.gro.ZOO            = 0.4,       # m3/gDM/d
              k.resp.ALG           = 0.10,      # 1/d
              k.resp.ZOO           = 0.10,      # 1/d
              k.death.ALG          = 0.10,      # 1/d
              k.death.ZOO          = 0.05,      # 1/d
              k.nitri              = 0.1,       # gN/m3/d
              k.miner.ox.POM       = 0.02,      # 1/d
              k.miner.ox.POM.sed   = 5.0,       # gDM/m2/d
              k.miner.anox.POM.sed = 5.0,       # gDM/m2/d
              K.POM.miner.sed      = 10,        # gDM/m2
              K.HPO4               = 0.002,     # gP/m3
              K.N                  = 0.04,      # gN/m3
              p.NH4                = 5,         # -
              K.O2.ZOO             = 0.2,       # gO/m3
              K.O2.resp            = 0.5,       # gO/m3
              K.O2.nitri           = 0.4,       # gO/m3
              K.O2.miner           = 0.5,       # gO/m3
              K.NO3.miner          = 0.1,       # gN/m3
              K.NH4.nitri          = 0.5,       # gN/m3
              A                    = 5e+006,    # m2
```

```
                h.epi                 = 5,            # m
                h.hypo                = 10,           # m
                Q.in                  = 5,            # m3/s
                C.HPO4.in             = 0.04,         # gP/m3
                C.NO3.in              = 0.5,          # gN/m3
                C.O2.in               = 10,           # gO/m3
                C.ALG.ini             = 0.1,          # gDM/m3
                C.ZOO.ini             = 0.1,          # gDM/m3
                C.POMD.ini            = 0.0,          # gDM/m3
                C.POMI.ini            = 0.0,          # gDM/m3
                C.HPO4.ini            = 0.04,         # gP/m3
                C.NH4.ini             = 0.1,          # gN/m3
                C.NO3.ini             = 0.5,          # gN/m3
                C.O2.ini              = 10,           # gO/m3
                D.POMD.ini            = 0,            # gDM/m2
                D.POMI.ini            = 0,            # gDM/m2
                beta.ALG              = 0.046,        # 1/degC
                beta.ZOO              = 0.08,         # 1/degC
                beta.BAC              = 0.046,        # 1/degC
                T0                    = 20,           # degC
                K.I                   = 30,           # W/m2
                lambda.1              = 0.10,         # 1/m
                lambda.2              = 0.10,         # m2/gDM
                v.ex.O2               = 1,            # m/d
                v.sed.POM             = 1,            # m/d
                Kz.summer             = 0.02,         # m2/d
                Kz.winter             = 20,           # m2/d
                h.meta                = 5,            # m
                t.max                 = 230,          # d
                I0.min                = 25,           # W/m2
                I0.max                = 225,          # W/m2
                T.min                 = 5,            # degC
                T.max                 = 25,           # degC
                p                     = 101325)       # Pa
```

This set of parameters contains the elemental mass fractions of nitrogen, phosphorus, oxygen and hydrogen. The largest mass fraction, of carbon, is then calculated as the difference to unity:

```
# choose carbon fractions to guarantee that the fractions sum to unity:

param$alpha.C.ALG <- 1 - (param$alpha.O.ALG + param$alpha.H.ALG +
                          param$alpha.N.ALG + param$alpha.P.ALG)
param$alpha.C.ZOO <- 1 - (param$alpha.O.ZOO + param$alpha.H.ZOO +
                          param$alpha.N.ZOO + param$alpha.P.ZOO)
param$alpha.C.POM <- 1 - (param$alpha.O.POM + param$alpha.H.POM +
                          param$alpha.N.POM + param$alpha.P.POM)
```

Next we define the composition of all substances to be considered for the calculation of the stoichiometries of all processes considered in the model. Note that we have to be careful with the units. The natural unit to measure the amount of inorganic chemical compounds is moles. THis is not the case for organic compounds as they consist of a large number of different organic molecules and we just consider their mean composition. For this reason, we measure organic compounds as dry mass. As we have to consider conservation of charge as well as conservation of the elements, we need to add charge to the composition vectors:

```
# Construct composition matrix:

NH4    <- c(H      = 4*1/14,              # gH/gNH4-N
            N      = 1,                   # gN/gNH4-N
            charge = 1/14)                # chargeunits/gNH4-N
NO3    <- c(O      = 3*16/14,             # gO/gNO3-N
            N      = 1,                   # gN/gNO3-N
            charge = -1/14)               # chargeunits/gNO3-N
N2     <- c(N      = 1)                   # gN/gN2-N
HPO4   <- c(O      = 4*16/31,             # gO/gHPO4-P
            H      = 1*1/31,              # gH/gHPO4-P
            P      = 1,                   # gP/gHPO4-P
            charge = -2/31)               # chargeunits/gHPO4-P
HCO3   <- c(C      = 1,                   # gC/gHCO3-C
            O      = 3*16/12,             # gO/gHCO3-C
            H      = 1*1/12,              # gH/gHCO3-C
            charge = -1/12)               # chargeunits/gHCO3-C
O2     <- c(O      = 1)                   # gO/gO2-O
H      <- c(H      = 1,                   # gH/molH
            charge = 1)                   # chargeunits/molH
H2O    <- c(O      = 1*16,                # gO/molH2O
            H      = 2*1)                 # gH/molH2O
ALG    <- c(C      = param$alpha.C.ALG,   # gC/gALG
            O      = param$alpha.O.ALG,   # gO/gALG
            H      = param$alpha.H.ALG,   # gH/gALG
            N      = param$alpha.N.ALG,   # gN/gALG
            P      = param$alpha.P.ALG)   # gP/gALG
ZOO    <- c(C      = param$alpha.C.ZOO,   # gC/gZOO
            O      = param$alpha.O.ZOO,   # gO/gZOO
            H      = param$alpha.H.ZOO,   # gH/gZOO
            N      = param$alpha.N.ZOO,   # gN/gZOO
            P      = param$alpha.P.ZOO)   # gP/gZOO
POM    <- c(C      = param$alpha.C.POM,   # gC/gPOM
            O      = param$alpha.O.POM,   # gO/gPOM
            H      = param$alpha.H.POM,   # gH/gPOM
            N      = param$alpha.N.POM,   # gN/gPOM
            P      = param$alpha.P.POM)   # gP/gPOM
```

Once all substances are defined, we can construct a composition matrix by passing the list of substances to the function `calc.comp.matrix` of the package `stoichcalc`:

```
subst.comp <- list(C.NH4    = NH4,
                   C.NO3    = NO3,
                   C.N2     = N2,
                   C.HPO4   = HPO4,
                   C.HCO3   = HCO3,
                   C.O2     = O2,
                   C.H      = H,
                   C.H2O    = H2O,
                   C.ALG    = ALG,
                   C.ZOO    = ZOO,
                   C.POMD   = POM,
                   D.POMD   = POM,
                   C.POMI   = POM,
```

```
                  D.POMI   = POM)

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

```
## [1] "Composition matrix (6x14) successfully constructed:"
## [1] "el. const.: H,N,charge,O,P,C"
## [1] "substances: C.NH4,C.NO3,C.N2,C.HPO4,C.HCO3,C.O2,C.H,C.H2O,C.ALG,C.ZOO,C.POMD,D.POMD,C.POMI,D.POI
```

```
print(round(alpha,3))
```

```
##        C.NH4  C.NO3 C.N2 C.HPO4 C.HCO3 C.O2 C.H C.H2O C.ALG C.ZOO C.POMD
## H      0.286  0.000    0  0.032  0.083    0   1     2 0.070  0.07  0.070
## N      1.000  1.000    1  0.000  0.000    0   0     0 0.060  0.06  0.060
## charge 0.071 -0.071    0 -0.065 -0.083    0   1     0 0.000  0.00  0.000
## O      0.000  3.429    0  2.065  4.000    1   0    16 0.500  0.50  0.390
## P      0.000  0.000    0  1.000  0.000    0   0     0 0.005  0.01  0.007
## C      0.000  0.000    0  0.000  1.000    0   0     0 0.365  0.36  0.473
##        D.POMD C.POMI D.POMI
## H       0.070  0.070  0.070
## N       0.060  0.060  0.060
## charge  0.000  0.000  0.000
## O       0.390  0.390  0.390
## P       0.007  0.007  0.007
## C       0.473  0.473  0.473
```

Death converts living algae or zooplankton into dead particulate organic matter. The typical stoichiometry of this process would be -1 for algae or zooplankton and +1 for particulate organic matter. However, we run into troubles if the composition of some of these organic components are different. This could be resolved by introducing dead organic particles with all different compositions of living organisms. To avoid this increase in the number of state variables (in particular if there would be more organisms to distinguish) and as most of the dead organic particles will be mineralized later anyway, we introduced a "yield" for death so that part of the organism becomes dead particulate organic matter and the remaining part is mineralized. The idea is to keep the fraction that becomes particulate organic matter as large as possible and not to have negative stoichiometric coefficients of nutrients or oxygen. The criteria we apply here are that we do not need an uptake of nitrogen or phosphorus for dying. Oxygen will have to be checked in the resulting stoichiometry. This leads to the following expressions for the yield:

```
# choose yield of death to guarantee that no nutrients are required
# (oxygen content of POM was reduced to avoid need of oxygen):

param$Y.ALG.death <-  min(1,
                          param$alpha.N.ALG/param$alpha.N.POM,
                          param$alpha.P.ALG/param$alpha.P.POM,
                          param$alpha.C.ALG/param$alpha.C.POM)
param$Y.ZOO.death <-  min(1,
                          param$alpha.N.ZOO/param$alpha.N.POM,
                          param$alpha.P.ZOO/param$alpha.P.POM,
                          param$alpha.C.ZOO/param$alpha.C.POM)

print(param$Y.ALG.death)
```

```
## [1] 0.7142857
```

```
print(param$Y.ZOO.death)
```

```
## [1] 0.7610994
```

Having defined the composition matrix and the stoichiometric parameters, we can define the stoichiometries of the processes to be considered by the model. Each process requires the composition matrix, it has a name, a list of substances to be considered, an indication of which coefficient should be chosen to make the stoichiometry unique, the value to which this coefficient is set (typically +1 or -1), and, optionally, the coefficients of additional constraints. These coefficients have to be provided in the form $\sum_j \nu_j \gamma_j = 0$. This means that e.g. the condition $\nu_{\mathrm{ZOO}} = -Y\nu_{ALG}$ indicating that one mass unit of algae is only converted into Y (= yield) mass units of zooplanktion has to be transformed into $\nu_{\mathrm{ZOO}} + Y\nu_{ALG} = 0$ to read the coefficients (see the first constraint below for the growth of zooplankton).

```
# Calculate stoichiometric coefficients of selected processes:

# Growth of algae on ammonium:

nu.gro.ALG.NH4 <-
   calc.stoich.coef(alpha       = alpha,
                    name        = "gro.ALG.NH4",
                    subst       = c("C.NH4","C.HPO4","C.HCO3","C.O2",
                                    "C.H","C.H2O","C.ALG"),
                    subst.norm  = "C.ALG",
                    nu.norm     = 1)
```

```
## [1] "Number of substances:                    7"
## [1] "Number of elementary constituents:       6"
## [1] "Number of constraints:                   0"
## [1] "Number of independent processes:         1"
## [1] "Stoichiometric coefficients successfully calculated."
```

```
# Growth of algae on nitrate:

nu.gro.ALG.NO3 <-
   calc.stoich.coef(alpha       = alpha,
                    name        = "gro.ALG.NO3",
                    subst       = c("C.NO3","C.HPO4","C.HCO3","C.O2",
                                    "C.H","C.H2O","C.ALG"),
                    subst.norm  = "C.ALG",
                    nu.norm     = 1)
```

```
## [1] "Number of substances:                    7"
## [1] "Number of elementary constituents:       6"
## [1] "Number of constraints:                   0"
## [1] "Number of independent processes:         1"
## [1] "Stoichiometric coefficients successfully calculated."
```

```
# Respiration of algae:

nu.resp.ALG <-
   calc.stoich.coef(alpha       = alpha,
                    name        = "resp.ALG",
                    subst       = c("C.NH4","C.HPO4","C.HCO3","C.O2",
                                    "C.H","C.H2O","C.ALG"),
                    subst.norm  = "C.ALG",
                    nu.norm     = -1)
```

```
## [1] "Number of substances:                    7"
## [1] "Number of elementary constituents:       6"
## [1] "Number of constraints:                   0"
## [1] "Number of independent processes:         1"
```

```
## [1] "Stoichiometric coefficients successfully calculated."
```

```
# Death of algae:

nu.death.ALG <-
   calc.stoich.coef(alpha       = alpha,
                    name        = "death.ALG",
                    subst       = c("C.NH4","C.HPO4","C.HCO3","C.O2",
                                    "C.H","C.H2O","C.ALG","C.POMD","C.POMI"),
                    subst.norm  = "C.ALG",
                    nu.norm     = -1,
                    constraints = list(c("C.ALG"  = param$Y.ALG.death,
                                         "C.POMD" = 1,
                                         "C.POMI" = 1),
                                       c("C.POMD" = -param$f.I,
                                         "C.POMI" = 1-param$f.I)))
```

```
## [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."
```

```
# Growth of zooplankton:

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

```
## [1] "Number of substances:                    10"
## [1] "Number of elementary constituents:       6"
## [1] "Number of constraints:                   3"
## [1] "Number of independent processes:         1"
## [1] "Stoichiometric coefficients successfully calculated."
```

```
# Respiration of zooplankton:

nu.resp.ZOO <-
   calc.stoich.coef(alpha       = alpha,
                    name        = "resp.ZOO",
                    subst       = c("C.NH4","C.HPO4","C.HCO3","C.O2",
                                    "C.H","C.H2O","C.ZOO"),
                    subst.norm  = "C.ZOO",
                    nu.norm     = -1)
```

```
## [1] "Number of substances:                       7"
## [1] "Number of elementary constituents:          6"
## [1] "Number of constraints:                      0"
## [1] "Number of independent processes:            1"
## [1] "Stoichiometric coefficients successfully calculated."
```

```
# Death of zooplankton:

nu.death.ZOO <-
   calc.stoich.coef(alpha       = alpha,
                    name        = "death.ZOO",
                    subst       = c("C.NH4","C.HPO4","C.HCO3","C.O2",
                                    "C.H","C.H2O","C.ZOO","C.POMD","C.POMI"),
                    subst.norm  = "C.ZOO",
                    nu.norm     = -1,
                    constraints = list(c("C.ZOO"  = param$Y.ZOO.death,
                                         "C.POMD" = 1,
                                         "C.POMI" = 1),
                                       c("C.POMD" = -param$f.I,
                                         "C.POMI" = 1-param$f.I)))
```

```
## [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."
```

```
# Nitrification:

nu.nitri <-
   calc.stoich.coef(alpha       = alpha,
                    name        = "nitri",
                    subst       = c("C.NH4","C.NO3","C.O2","C.H","C.H2O"),
                    subst.norm  = "C.NH4",
                    nu.norm     = -1)
```

```
## [1] "Number of substances:                       5"
## [1] "Number of elementary constituents:          6"
## [1] "Number of constraints:                      0"
## [1] "Number of independent processes:            1"
## [1] "Stoichiometric coefficients successfully calculated."
```

```
# Oxic mineralization of suspended organic particles:

nu.miner.ox.POM <-
   calc.stoich.coef(alpha       = alpha,
                    name        = "miner.ox.POM",
                    subst       = c("C.NH4","C.HPO4","C.HCO3","C.O2",
                                    "C.H","C.H2O","C.POMD"),
                    subst.norm  = "C.POMD",
                    nu.norm     = -1)
```

```
## [1] "Number of substances:                       7"
## [1] "Number of elementary constituents:          6"
## [1] "Number of constraints:                      0"
## [1] "Number of independent processes:            1"
## [1] "Stoichiometric coefficients successfully calculated."
```

```
# Oxic mineralization of sedimented organic particles:

nu.miner.ox.POM.sed <-
   calc.stoich.coef(alpha       = alpha,
                    name        = "miner.ox.POM.sed",
                    subst       = c("C.NH4","C.HPO4","C.HCO3","C.O2",
                                    "C.H","C.H2O","D.POMD"),
                    subst.norm  = "D.POMD",
                    nu.norm     = -1)
```

```
## [1] "Number of substances:                    7"
## [1] "Number of elementary constituents:       6"
## [1] "Number of constraints:                   0"
## [1] "Number of independent processes:         1"
## [1] "Stoichiometric coefficients successfully calculated."
```

```
# Anoxic mineralization of sedimented organic particles:

nu.miner.anox.POM.sed <-
   calc.stoich.coef(alpha       = alpha,
                    name        = "miner.anox.POM.sed",
                    subst       = c("C.NH4","C.NO3","C.HPO4","C.HCO3","C.N2",
                                    "C.H","C.H2O","D.POMD"),
                    subst.norm  = "D.POMD",
                    nu.norm     = -1,
                    constraints = list(c("C.NO3" = 1,
                                         "C.N2"  = 1)))
```

```
## [1] "Number of substances:                    8"
## [1] "Number of elementary constituents:       6"
## [1] "Number of constraints:                   1"
## [1] "Number of independent processes:         1"
## [1] "Stoichiometric coefficients successfully calculated."
```

```
# Sedimentation of degradable organic particles:

nu.sed.POMD <-
   calc.stoich.coef(alpha       = alpha,
                    name        = "sed.POMD",
                    subst       = c("C.POMD","D.POMD"),
                    subst.norm  = "C.POMD",
                    nu.norm     = -1)
```

```
## [1] "Number of substances:                    2"
## [1] "Number of elementary constituents:       6"
## [1] "Number of constraints:                   0"
## [1] "Number of independent processes:         1"
## [1] "Stoichiometric coefficients successfully calculated."
```

```
# Sedimentation of inert organic particles:

nu.sed.POMI <-
   calc.stoich.coef(alpha       = alpha,
                    name        = "sed.POMI",
                    subst       = c("C.POMI","D.POMI"),
                    subst.norm  = "C.POMI",
```

```
                    nu.norm     = -1)
```

```
## [1] "Number of substances:                      2"
## [1] "Number of elementary constituents:         6"
## [1] "Number of constraints:                     0"
## [1] "Number of independent processes:           1"
## [1] "Stoichiometric coefficients successfully calculated."
```

Finally, we bind the stoichiometries together for the full stoichiometric matrix:

```
# Construct stoichiometric matrix:

nu <- rbind(nu.gro.ALG.NH4,
            nu.gro.ALG.NO3,
            nu.resp.ALG,
            nu.death.ALG,
            nu.gro.ZOO,
            nu.resp.ZOO,
            nu.death.ZOO,
            nu.nitri,
            nu.miner.ox.POM,
            nu.miner.ox.POM.sed,
            nu.miner.anox.POM.sed,
            nu.sed.POMD,
            nu.sed.POMI)
print(round(nu,3))
```

```
##                    C.NH4  C.NO3  C.N2 C.HPO4 C.HCO3   C.O2    C.H  C.H2O
## gro.ALG.NH4       -0.060  0.000 0.000 -0.005 -0.365  0.937 -0.026  0.002
## gro.ALG.NO3        0.000 -0.060 0.000 -0.005 -0.365  1.211 -0.035 -0.002
## resp.ALG           0.060  0.000 0.000  0.005  0.365 -0.937  0.026 -0.002
## death.ALG          0.017  0.000 0.000  0.000  0.027  0.018  0.001  0.006
## gro.ZOO            0.180  0.000 0.000  0.008  0.992 -2.417  0.070  0.003
## resp.ZOO           0.060  0.000 0.000  0.010  0.360 -0.930  0.026 -0.002
## death.ZOO          0.014  0.000 0.000  0.005  0.000  0.088 -0.001  0.007
## nitri             -1.000  1.000 0.000  0.000  0.000 -4.571  0.143  0.071
## miner.ox.POM       0.060  0.000 0.000  0.007  0.473 -1.338  0.036 -0.011
## miner.ox.POM.sed   0.060  0.000 0.000  0.007  0.473 -1.338  0.036 -0.011
## miner.anox.POM.sed 0.060 -0.468 0.468  0.007  0.473  0.000  0.002  0.006
## sed.POMD           0.000  0.000 0.000  0.000  0.000  0.000  0.000  0.000
## sed.POMI           0.000  0.000 0.000  0.000  0.000  0.000  0.000  0.000
##                   C.ALG C.ZOO C.POMD D.POMD C.POMI D.POMI
## gro.ALG.NH4           1     0  0.000      0  0.000      0
## gro.ALG.NO3           1     0  0.000      0  0.000      0
## resp.ALG             -1     0  0.000      0  0.000      0
## death.ALG            -1     0  0.571      0  0.143      0
## gro.ZOO              -5     1  0.800      0  0.200      0
## resp.ZOO              0    -1  0.000      0  0.000      0
## death.ZOO             0    -1  0.609      0  0.152      0
## nitri                 0     0  0.000      0  0.000      0
## miner.ox.POM          0     0 -1.000      0  0.000      0
## miner.ox.POM.sed      0     0  0.000     -1  0.000      0
## miner.anox.POM.sed    0     0  0.000     -1  0.000      0
## sed.POMD              0     0 -1.000      1  0.000      0
## sed.POMI              0     0  0.000      0 -1.000      1
```

This stoichiometric matrix should be checked in particular for the signs of the stoichiometric coefficients. As we chose the yields for death accordingly above, death of neither algae or zooplankton consumes phosphate or ammonium. However, we also have to check that it does not consume oxygen, which is not so easy to avoid. If it would consume oxygen, we would have to switch to the approach of using multiple fractions of dead organic matter (we do not have this problem if the compostion of dead organic matter is the same as that of the dying organism).

We can now proceed with the definition of transformation processes. This is analogous as we did it in the exercises 1 and 2 with the exception that we can use the stoichiometries as calculated above with `stoichcalc`. As we pass the numerical values of the stoichiometric coefficients that were evaluated above using the model parameters, we will not be able to do sensitivity analyses of the model with regard to parameters that affect the stoichiomtry by just redoing simulations with modified parameter values (we can still do so for the parameters that characterize kinetics, input, etc.). If we are interested in sensitivity regarding stoichiometric parameters, we have to re-evaluate stoichiometry with modified parameter values, pass the modified stoichiometry to the processes in the model and then redo the simulations.

```
# Definition of transformation processes:

# Growth of algae on ammonium:

gro.ALG.NH4 <-
   new(Class  = "process",
       name   = "gro.ALG.NH4",
       rate   = expression(k.gro.ALG
                           *exp(beta.ALG*(T-T0))
                           *log((K.I+I0)/
                               (K.I+I0*exp(-(lambda.1+lambda.2*C.ALG)*h.epi)))
                               /((lambda.1+lambda.2*C.ALG)*h.epi)
                           *min(C.HPO4/(K.HPO4+C.HPO4),
                               (C.NH4+C.NO3)/(K.N+C.NH4+C.NO3))
                           *(p.NH4*C.NH4/(p.NH4*C.NH4+C.NO3))
                           *C.ALG),
       stoich = as.list(nu["gro.ALG.NH4",]))

# Growth of algae on nitrate:

gro.ALG.NO3 <-
   new(Class  = "process",
       name   = "gro.ALG.NO3",
       rate   = expression(k.gro.ALG
                          *exp(beta.ALG*(T-T0))
                          *log((K.I+I0)/
                               (K.I+I0*exp(-(lambda.1+lambda.2*C.ALG)*h.epi)))
                               /((lambda.1+lambda.2*C.ALG)*h.epi)
                          *min(C.HPO4/(K.HPO4+C.HPO4),
                               (C.NH4+C.NO3)/(K.N+C.NH4+C.NO3))
                          *(C.NO3/(p.NH4*C.NH4+C.NO3))
                          *C.ALG),
       stoich = as.list(nu["gro.ALG.NO3",]))

# Respiration of algae:

resp.ALG <-
   new(Class  = "process",
       name   = "resp.ALG",
```

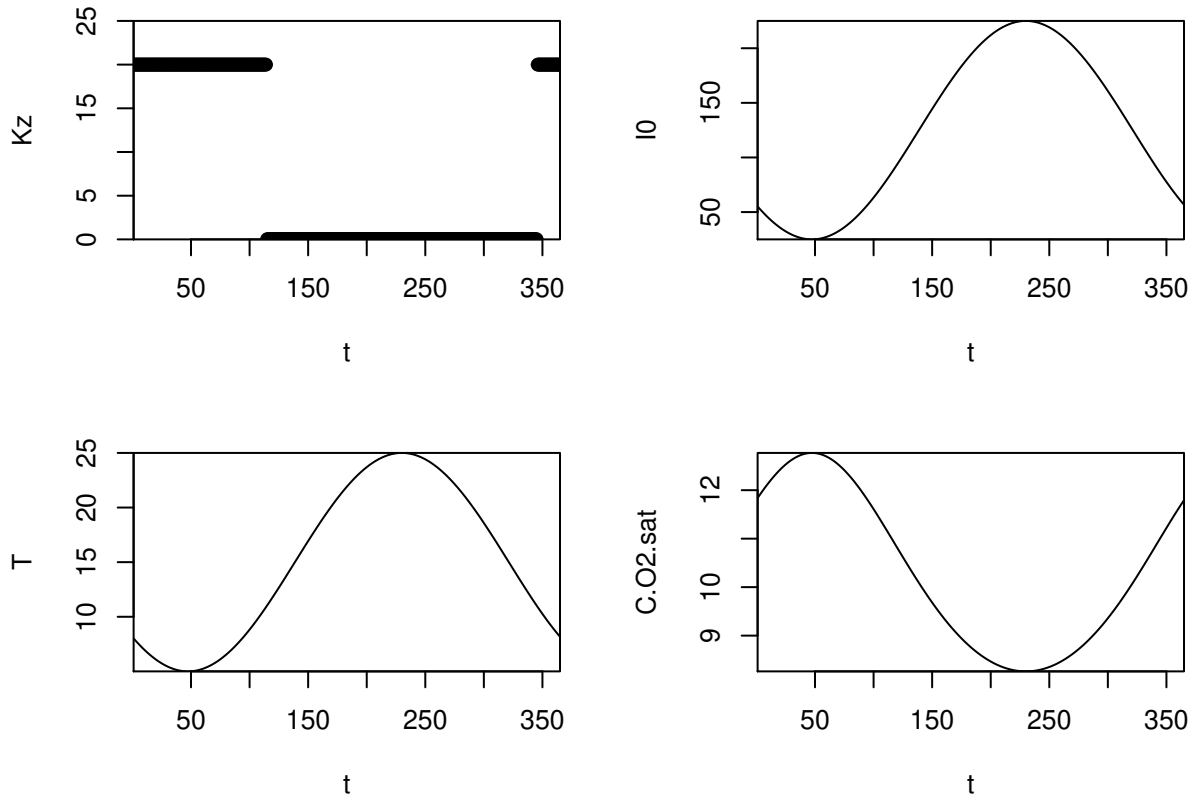
```
       rate   = expression(k.resp.ALG*exp(beta.ALG*(T-T0))*(C.O2/(K.O2.resp+C.O2))*C.ALG),
       stoich = as.list(nu["resp.ALG",]))

# Death of algae:

death.ALG <-
   new(Class = "process",
       name   = "death.ALG",
       rate   = expression(k.death.ALG*C.ALG),
       stoich = as.list(nu["death.ALG",]))

# Growth of zooplankton:

gro.ZOO <-
   new(Class  = "process",
       name   = "gro.ZOO",
       rate   = expression(k.gro.ZOO*exp(beta.ZOO*(T-T0))
                           *(C.O2/(K.O2.ZOO+C.O2))
                           *C.ALG
                           *C.ZOO),
       stoich = as.list(nu["gro.ZOO",]))

# Respiration of zooplankton:

resp.ZOO <-
   new(Class  = "process",
       name   = "resp.ZOO",
       rate   = expression(k.resp.ZOO*exp(beta.ZOO*(T-T0))*(C.O2/(K.O2.resp+C.O2))*C.ZOO),
       stoich = as.list(nu["resp.ZOO",]))

# Death of zooplankton:

death.ZOO <-
   new(Class = "process",
       name   = "death.ZOO",
       rate   = expression(k.death.ZOO*C.ZOO),
       stoich = as.list(nu["death.ZOO",]))

# Nitrification:

nitri <-
   new(Class = "process",
       name   = "nitri",
       rate   = expression(k.nitri
                           *exp(beta.BAC*(T-T0))
                           *min(C.NH4/(K.NH4.nitri+C.NH4),C.O2/(K.O2.nitri+C.O2))),
       stoich = as.list(nu["nitri",]))

# Oxic mineralization of suspended organic particles:

miner.ox.POM <-
   new(Class  = "process",
       name   = "miner.ox.POM",
```

```
       rate   = expression(k.miner.ox.POM
                           *exp(beta.BAC*(T-T0))
                           *C.O2/(K.O2.miner+C.O2)
                           *C.POMD),
       stoich = as.list(nu["miner.ox.POM",]))

# Oxic mineralization of sedimented organic particles:

miner.ox.POM.sed <-
   new(Class  = "process",
       name   = "miner.ox.POM.sed",
       rate   = expression(k.miner.ox.POM.sed
                           *exp(beta.BAC*(T-T0))
                           *C.O2/(K.O2.miner+C.O2)
                           *D.POMD/(K.POM.miner.sed+D.POMD)),
       stoich = as.list(nu["miner.ox.POM.sed",]),
       pervol = F)

# Anoxic mineralization of sedimented organic particles:

miner.anox.POM.sed <-
   new(Class  = "process",
       name   = "miner.anox.POM.sed",
       rate   = expression(k.miner.anox.POM.sed
                           *exp(beta.BAC*(T-T0))
                           *C.NO3/(K.NO3.miner+C.NO3)
                           *(D.POMD/(K.POM.miner.sed+D.POMD))^2),
       stoich = as.list(nu["miner.anox.POM.sed",]),
       pervol = F)

# Sedimentation of degradable organic particles:

sed.POMD <-
   new(Class  = "process",
       name   = "sed.POMD",
       rate   = expression(v.sed.POM/h.hypo*C.POMD),
       stoich = as.list(nu["sed.POMD",]))

# Sedimentation of inert organic particles:

sed.POMI <-
   new(Class  = "process",
       name   = "sed.POMI",
       rate   = expression(v.sed.POM/h.hypo*C.POMI),
       stoich = as.list(nu["sed.POMI",]))
```

We now define the seasonally varying light intensity and temperature and, as a consequence of temperature variation, the seasonally varying saturation concentration of dissolved oxygen. In addition, we define the turbulent diffusion coefficient, K_z, that quantifies mixing between the hypolimnion (deep water) and the epiliminion (upper part of the water column). To describe, mixing during the winter and stratification in the summer, we use a large value in winter and a small value in summer.

```
# Definition of environmental conditions:
```

```
cond.epi  <- list(I0       = expression( 0.5*(I0.min+I0.max)
                                        +0.5*(I0.max-I0.min)
                                            *cos(2*pi/365.25*(t-t.max))),
                  T        = expression( 0.5*(T.min+T.max)
                                        +0.5*(T.max-T.min)
                                            *cos(2*pi/365.25*(t-t.max))),
                  C.O2.sat = expression(exp(7.7117-1.31403*log(T+45.93))
                                        *p/101325))

cond.hypo <- list(I0 = 0,
                  T  = 5)

cond.gen  <- list(Kz=expression( 0.5*(Kz.summer+Kz.winter)
                                -0.5*(Kz.winter-Kz.summer)
                                    *sign(cos(2*pi/365.25*(t-t.max))+0.4)))

# Plot the environmental conditions

t <-  1:365

Kz <- numeric(0)
I0 <- numeric(0)
T <- numeric(0)
C.O2.sat <- numeric(0)

for(i in 1:length(t))
{
   Kz[i]       <- eval(cond.gen$Kz, envir=c(param, t=t[i]))
   I0[i]       <- eval(cond.epi$I0, envir=c(param, t=t[i]))
   T[i]        <- eval(cond.epi$T, envir=c(param, t=t[i]))
   C.O2.sat[i] <- eval(cond.epi$C.O2.sat, envir=c(param, T=T[i]))
}

#Plots
par.def <- par(no.readonly=TRUE)  # store current plotting parameter
par(mfrow=c(2,2),xaxs="i",yaxs="i",mar=c(4.5,4.5,2,1.5)+0.1) # modify plot parameters
plot(t, Kz , ylim=c(0,25))
plot(t, I0, type="l")
plot(t, T, type="l")
plot(t, C.O2.sat, type="l")
```




```
par(par.def)  # restore previous plotting parameters
```

We now define the two boxes that allow us to describe mixed and stratified conditions of the lake. Inflow and outflow are into and out of the upper box, called epilimnion. In the lower box, called hypolimnion, there is no primary production due to the absence of light. Also the sediment is assumed to be only relevant in the hypoliminion which is typical for deep lakes with steep banks.

```
# Definition of reactors:

# Epilimnion:

epilimnion <-
   new(Class            = "reactor",
       name             = "Epi",
       volume.ini       = expression(A*h.epi),
       conc.pervol.ini  = list(C.HPO4 = expression(C.HPO4.ini),  # gP/m3
                               C.NH4  = expression(C.NH4.ini),   # gN/m3
                               C.NO3  = expression(C.NO3.ini),   # gN/m3
                               C.O2   = expression(C.O2.ini),    # gO/m3
                               C.ALG  = expression(C.ALG.ini),   # gDM/m3
                               C.ZOO  = expression(C.ZOO.ini),   # gDM/m3
                               C.POMD = expression(C.POMD.ini),  # gDM/m3
                               C.POMI = expression(C.POMI.ini)), # gDM/m3
       input            = list(C.O2   = expression(v.ex.O2*A
                                                   *(C.O2.sat-C.O2))), # gas ex.
       inflow           = expression(Q.in*86400),                # m3/d
       inflow.conc      = list(C.HPO4 = expression(C.HPO4.in),
```

```
                              C.NH4  = 0,
                              C.NO3  = expression(C.NO3.in),
                              C.O2   = expression(C.O2.in),
                              C.ALG  = 0,
                              C.ZOO  = 0,
                              C.POMD = 0,
                              C.POMI = 0),
       outflow          = expression(Q.in*86400),
       cond             = cond.epi,
       processes        = list(gro.ALG.NH4,gro.ALG.NO3,resp.ALG,death.ALG,
                              gro.ZOO,resp.ZOO,death.ZOO,
                              nitri,miner.ox.POM))

# Hypolimnion:

hypolimnion <-
   new(Class            = "reactor",
       name             = "Hypo",
       volume.ini       = expression(A*h.hypo),
       area             = expression(A),
       conc.pervol.ini  = list(C.HPO4 = expression(C.HPO4.ini),  # gP/m3
                              C.NH4  = expression(C.NH4.ini),   # gN/m3
                              C.NO3  = expression(C.NO3.ini),   # gN/m3
                              C.O2   = expression(C.O2.ini),    # gO/m3
                              C.ALG  = expression(C.ALG.ini),   # gDM/m3
                              C.ZOO  = expression(C.ZOO.ini),   # gDM/m3
                              C.POMD = expression(C.POMD.ini),  # gDM/m3
                              C.POMI = expression(C.POMI.ini)), # gDM/m3
       conc.perarea.ini = list(D.POMD = expression(D.POMD.ini),  # gDM/m2
                              D.POMI = expression(D.POMI.ini)), # gDM/m2
       cond             = cond.hypo,
       processes        = list(resp.ALG,death.ALG,
                              gro.ZOO,resp.ZOO,death.ZOO,
                              nitri,
                              miner.ox.POM,miner.ox.POM.sed,miner.anox.POM.sed,
                              sed.POMD,sed.POMI))
```

The final element needed ist the metalimnion that separates the epilimnion from the hypolimnion. We neglect its volume (this means we expand the epilimnion and the metalimnion) and specify directed flow of dead organic particles through sedimentation from the epilimnion to the metalimnion and diffusive exchange of all substances with the turbulent diffusion coefficient K_z that was defined above to be large in winter and small in summer.

```
# Definition of links:

# Exchange between epilimnion and hypolimnion:

metalimnion <-
   new(Class      = "link",
       name       = "Metalimnion",
       from       = "Epi",
       to         = "Hypo",
       qadv.spec  = list(C.POMD = expression(v.sed.POM*A),
                         C.POMI = expression(v.sed.POM*A)),
```

```
       qdiff.gen  = expression(A/h.meta*Kz))
```

The definition of the model is concluded with the system definition that contains the reactors, links, environmental conditions, parameters and output time points for simulations:

```
#Definition of the lake system:

system.11.4 <- new(Class    = "system",
                   name     = "Lake",
                   reactors = list(epilimnion,hypolimnion),
                   links    = list(metalimnion),
                   cond     = cond.gen,
                   param    = param,
                   t.out    = seq(0,730,by=1)) #number of days 365, 730, 1095 ,1460
```

Now, we start simulations. The default option is to use an implicit integration scheme that is stable also for large time steps; as an alternative, we could apply an explicit Runge-Kutta scheme that is faster for each time step but needs more of them:

```
# Perform simulation:

ptm <- proc.time()
res.11.4 <- calcres(system.11.4)
print(proc.time()-ptm)
```

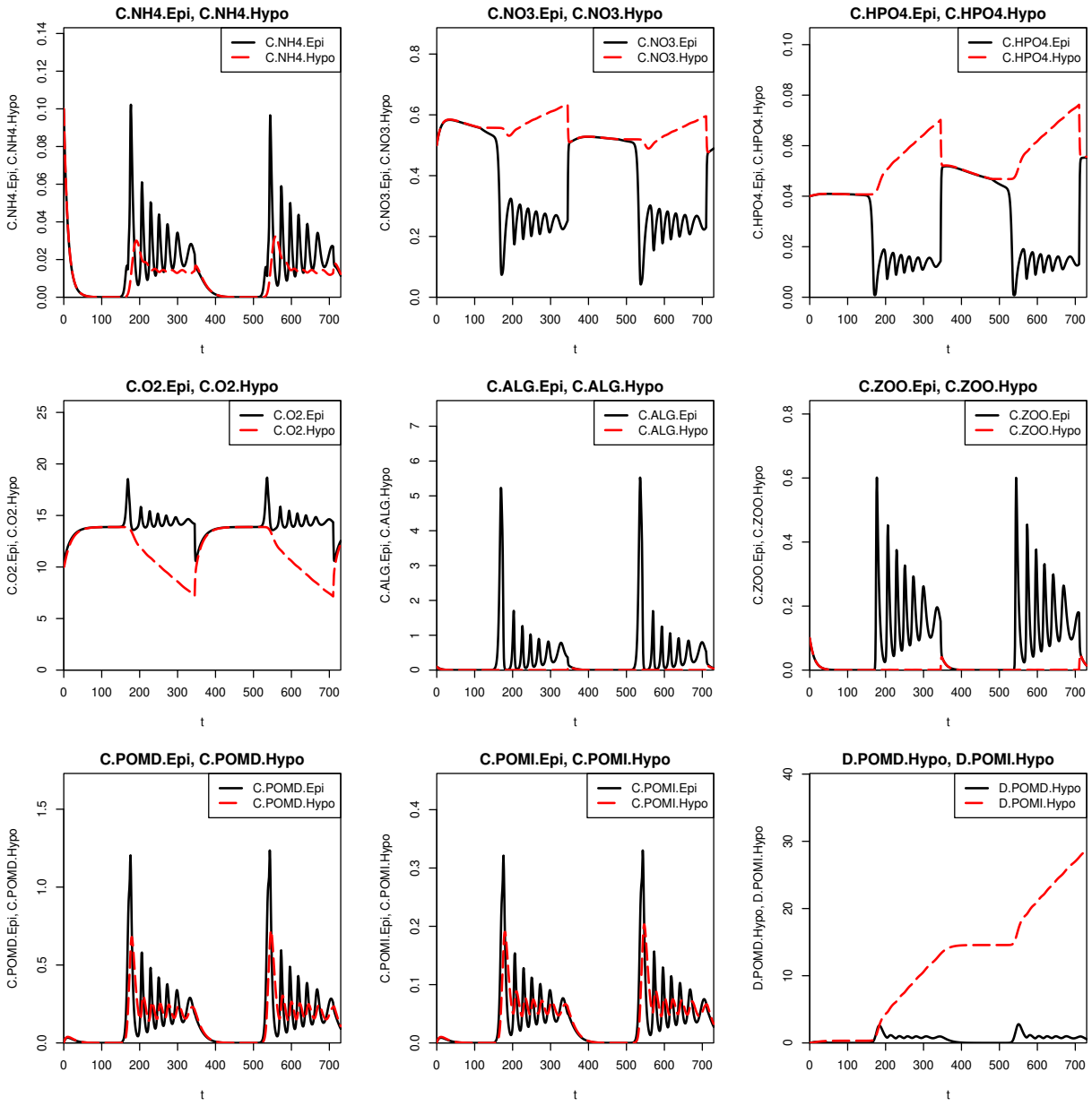
```
##    user  system elapsed
##   13.77    0.00   13.76
```

```
ptm <- proc.time()
res.11.4.rk4 <- calcres(system.11.4,method="rk4")
print(proc.time()-ptm)
```

```
##    user  system elapsed
##    8.09    0.00    8.10
```

We then plot the results to the screen and write them also with different options to files. Please note that you have to adjust the size of the pdf files with the `width` and `height` arguments to have reasonable sizes of the legend and the descriptions of the axes. You may also want to plot multiple lines into a single plot by specifying the argument `colnames` of the function `plotres` (you may type `?plotres` to get a description of the arguments of this function).

```
# Plot results:

plotres(res      = res.11.4,
        colnames =list(c("C.NH4.Epi","C.NH4.Hypo"),
                       c("C.NO3.Epi","C.NO3.Hypo"),
                       c("C.HPO4.Epi","C.HPO4.Hypo"),
                       c("C.O2.Epi","C.O2.Hypo"),
                       c("C.ALG.Epi","C.ALG.Hypo"),
                       c("C.ZOO.Epi","C.ZOO.Hypo"),
                       c("C.POMD.Epi","C.POMD.Hypo"),
                       c("C.POMI.Epi","C.POMI.Hypo"),
                       c("D.POMD.Hypo","D.POMI.Hypo")))
```




```
plotres(res      = res.11.4,
        colnames = list(c("C.NH4.Epi","C.NH4.Hypo"),
                        c("C.NO3.Epi","C.NO3.Hypo"),
                        c("C.HPO4.Epi","C.HPO4.Hypo"),
                        c("C.O2.Epi","C.O2.Hypo"),
                        c("C.ALG.Epi","C.ALG.Hypo"),
                        c("C.ZOO.Epi","C.ZOO.Hypo"),
                        c("C.POMD.Epi","C.POMD.Hypo"),
                        c("C.POMI.Epi","C.POMI.Hypo"),
                        c("D.POMD.Hypo","D.POMI.Hypo")),
        file     = "exercise_4_results.pdf",
        width    = 8,
        height   = 8)
```

```
## pdf
##   2
```

```
# compare numerical solutions:
plotres(res      = list(lsoda=res.11.4,rk4=res.11.4.rk4),
        colnames = list(c("C.NH4.Epi","C.NH4.Hypo"),
                        c("C.NO3.Epi","C.NO3.Hypo"),
                        c("C.HPO4.Epi","C.HPO4.Hypo"),
                        c("C.O2.Epi","C.O2.Hypo"),
                        c("C.ALG.Epi","C.ALG.Hypo"),
                        c("C.ZOO.Epi","C.ZOO.Hypo"),
                        c("C.POMD.Epi","C.POMD.Hypo"),
                        c("C.POMI.Epi","C.POMI.Hypo"),
                        c("D.POMD.Hypo","D.POMI.Hypo")),
        file     = "exercise_4_results_rk4.pdf",
        width    = 8,
        height   = 8)
```

```
## pdf
##   2
```

Overall mass balance of phosphorus over the whole simulation period:

```
# Phosphorus mass balance:

nr.days  <- (as.numeric(rownames(res.11.4)[nrow(res.11.4)])-as.numeric(rownames(res.11.4)[1]))
nr.steps <- (nrow(res.11.4)-1)

F.in.P  <- c(HPO4    = param$Q.in*param$C.HPO4.in*nr.days*86400/1e6)
F.out.P <- c(HPO4    = sum(param$Q.in*res.11.4[,"C.HPO4.Epi"])*nr.days/nr.steps*86400/1e6,
             ALG     = sum(param$Q.in*res.11.4[,"C.ALG.Epi"]*param$alpha.P.ALG)*
                         nr.days/nr.steps*86400/1e6,
             ZOO     = sum(param$Q.in*res.11.4[,"C.ZOO.Epi"]*param$alpha.P.ZOO)*
                         nr.days/nr.steps*86400/1e6,
             POMD    = sum(param$Q.in*res.11.4[,"C.POMD.Epi"]*param$alpha.P.POM)*
                         nr.days/nr.steps*86400/1e6,
             POMI    = sum(param$Q.in*res.11.4[,"C.POMI.Epi"]*param$alpha.P.POM)*
                         nr.days/nr.steps*86400/1e6)
Acc.P   <- c(HPO4    = param$A/1e6*
                       ((param$h.epi*res.11.4[nrow(res.11.4),"C.HPO4.Epi"]+
                           param$h.hypo*res.11.4[nrow(res.11.4),"C.HPO4.Hypo"])-
                        (param$h.epi*res.11.4[1,"C.HPO4.Epi"]+
                           param$h.hypo*res.11.4[1,"C.HPO4.Hypo"])),
             ALG     = param$A/1e6*param$alpha.P.ALG*
                       ((param$h.epi*res.11.4[nrow(res.11.4),"C.ALG.Epi"]+
                           param$h.hypo*res.11.4[nrow(res.11.4),"C.ALG.Hypo"])-
                        (param$h.epi*res.11.4[1,"C.ALG.Epi"]+
                           param$h.hypo*res.11.4[1,"C.ALG.Hypo"])),
             ZOO     = param$A/1e6*param$alpha.P.ZOO*
                       ((param$h.epi*res.11.4[nrow(res.11.4),"C.ZOO.Epi"]+
                           param$h.hypo*res.11.4[nrow(res.11.4),"C.ZOO.Hypo"])-
                        (param$h.epi*res.11.4[1,"C.ZOO.Epi"]+
                           param$h.hypo*res.11.4[1,"C.ZOO.Hypo"])),
             POMD    = param$A/1e6*param$alpha.P.POM*
                       ((param$h.epi*res.11.4[nrow(res.11.4),"C.POMD.Epi"]+
                           param$h.hypo*res.11.4[nrow(res.11.4),"C.POMD.Hypo"])-
```

```
                          (param$h.epi*res.11.4[1,"C.POMD.Epi"]+
                             param$h.hypo*res.11.4[1,"C.POMD.Hypo"])),
              POMI    = param$A/1e6*param$alpha.P.POM*
                        ((param$h.epi*res.11.4[nrow(res.11.4),"C.POMI.Epi"]+
                             param$h.hypo*res.11.4[nrow(res.11.4),"C.POMI.Hypo"])-
                          (param$h.epi*res.11.4[1,"C.POMI.Epi"]+
                             param$h.hypo*res.11.4[1,"C.POMI.Hypo"])),
              POMDsed = param$A/1e6*param$alpha.P.POM*
                          (res.11.4[nrow(res.11.4),"D.POMD.Hypo"]-res.11.4[1,"D.POMD.Hypo"]),
              POMIsed = param$A/1e6*param$alpha.P.POM*
                          (res.11.4[nrow(res.11.4),"D.POMI.Hypo"]-res.11.4[1,"D.POMI.Hypo"]))

print("Input (tP)")
print(signif(F.in.P,3))
print("Output (tP)")
print(signif(F.out.P,3))
print(signif(sum(F.out.P),3))
print("Accumulation (tP)")
print(signif(Acc.P,3))
print(signif(sum(Acc.P),3))

print("Input - Output - Accumulation:")
print(sum(F.in.P)-sum(F.out.P)-sum(Acc.P))
```

```
## [1] "Input (tP)"
## HPO4
## 12.6
## [1] "Output (tP)"
##   HPO4    ALG    ZOO   POMD   POMI
## 9.2600 0.5350 0.2640 0.3240 0.0891
## [1] 10.5
## [1] "Accumulation (tP)"
##    HPO4     ALG     ZOO    POMD    POMI POMDsed POMIsed
##  1.1600 -0.0196 -0.0644  0.0532  0.0162  0.0197  1.0000
## [1] 2.17
## [1] "Input - Output - Accumulation:"
## [1] -0.02190064
```

Overall mass balance of nitrogen over the whole simulation period:

```
# Nitrogen mass balance:

nr.days <- (as.numeric(rownames(res.11.4)[nrow(res.11.4)])-as.numeric(rownames(res.11.4)[1]))
nr.steps <- (nrow(res.11.4)-1)

F.in.N  <- c(NO3     = param$Q.in*param$C.NO3.in*nr.days*86400/1e6)
F.out.N <- c(NO3     = sum(param$Q.in*res.11.4[,"C.NO3.Epi"])*nr.days/nr.steps*86400/1e6,
             NH4     = sum(param$Q.in*res.11.4[,"C.NH4.Epi"])*nr.days/nr.steps*86400/1e6,
             ALG     = sum(param$Q.in*res.11.4[,"C.ALG.Epi"]*param$alpha.N.ALG)*
                         nr.days/nr.steps*86400/1e6,
             ZOO     = sum(param$Q.in*res.11.4[,"C.ZOO.Epi"]*param$alpha.N.ZOO)*
                         nr.days/nr.steps*86400/1e6,
             POMD    = sum(param$Q.in*res.11.4[,"C.POMD.Epi"]*param$alpha.N.POM)*
                         nr.days/nr.steps*86400/1e6,
             POMI    = sum(param$Q.in*res.11.4[,"C.POMI.Epi"]*param$alpha.N.POM)*
```

```
                          nr.days/nr.steps*86400/1e6)
Acc.N   <- c(NO3     = param$A/1e6*
                       ((param$h.epi*res.11.4[nrow(res.11.4),"C.NO3.Epi"]+
                           param$h.hypo*res.11.4[nrow(res.11.4),"C.NO3.Hypo"])-
                        (param$h.epi*res.11.4[1,"C.NO3.Epi"]+
                           param$h.hypo*res.11.4[1,"C.NO3.Hypo"])),
             NH4     = param$A/1e6*
                       ((param$h.epi*res.11.4[nrow(res.11.4),"C.NH4.Epi"]+
                           param$h.hypo*res.11.4[nrow(res.11.4),"C.NH4.Hypo"])-
                        (param$h.epi*res.11.4[1,"C.NH4.Epi"]+
                           param$h.hypo*res.11.4[1,"C.NH4.Hypo"])),
             ALG     = param$A/1e6*param$alpha.N.ALG*
                       ((param$h.epi*res.11.4[nrow(res.11.4),"C.ALG.Epi"]+
                           param$h.hypo*res.11.4[nrow(res.11.4),"C.ALG.Hypo"])-
                        (param$h.epi*res.11.4[1,"C.ALG.Epi"]+
                           param$h.hypo*res.11.4[1,"C.ALG.Hypo"])),
             ZOO     = param$A/1e6*param$alpha.N.ZOO*
                       ((param$h.epi*res.11.4[nrow(res.11.4),"C.ZOO.Epi"]+
                           param$h.hypo*res.11.4[nrow(res.11.4),"C.ZOO.Hypo"])-
                        (param$h.epi*res.11.4[1,"C.ZOO.Epi"]+
                           param$h.hypo*res.11.4[1,"C.ZOO.Hypo"])),
             POMD    = param$A/1e6*param$alpha.N.POM*
                       ((param$h.epi*res.11.4[nrow(res.11.4),"C.POMD.Epi"]+
                           param$h.hypo*res.11.4[nrow(res.11.4),"C.POMD.Hypo"])-
                        (param$h.epi*res.11.4[1,"C.POMD.Epi"]+
                           param$h.hypo*res.11.4[1,"C.POMD.Hypo"])),
             POMI    = param$A/1e6*param$alpha.N.POM*
                       ((param$h.epi*res.11.4[nrow(res.11.4),"C.POMI.Epi"]+
                           param$h.hypo*res.11.4[nrow(res.11.4),"C.POMI.Hypo"])-
                        (param$h.epi*res.11.4[1,"C.POMI.Epi"]+param$h.hypo*res.11.4[1,"C.POMI.Hypo"])),
             POMDsed = param$A/1e6*param$alpha.N.POM*
                         (res.11.4[nrow(res.11.4),"D.POMD.Hypo"]-res.11.4[1,"D.POMD.Hypo"]),
             POMIsed = param$A/1e6*param$alpha.N.POM*
                         (res.11.4[nrow(res.11.4),"D.POMI.Hypo"]-res.11.4[1,"D.POMI.Hypo"]))

print("Input (tN)")
print(signif(F.in.N,3))
print("Output (tN)")
print(signif(F.out.N,3))
print(signif(sum(F.out.N),3))
print("Accumulation (tN)")
print(signif(Acc.N,3))
print(signif(sum(Acc.N),3))

print("Input - Output - Accumulation:")
print(sum(F.in.N)-sum(F.out.N)-sum(Acc.N))
```

```
## [1] "Input (tN)"
## NO3
## 158
## [1] "Output (tN)"
##     NO3     NH4     ALG     ZOO    POMD    POMI
## 122.000   4.920   6.410   1.580   2.780   0.764
## [1] 138
```

```
## [1] "Accumulation (tN)"
##     NO3     NH4     ALG     ZOO    POMD    POMI POMDsed POMIsed
##  -0.790  -6.600  -0.235  -0.386   0.456   0.139   0.169   8.590
## [1] 1.35
## [1] "Input - Output - Accumulation:"
## [1] 17.90208
```