NPZD model: Nutrients, Phytoplankton, Zooplankton and Detritus in a Marine Bay

Exercises Accompanying the Course Reaction Transport Modelling in the Hydrosphere

Karline Soetaert and Lubos Polerecky, Utrecht University

March 2021

Problem formulation

The NPZD model is a monument in biological oceanography and limnology. It provides a simplified description for nutrient cycling in the water column in which only four state variables are described: Nutrients (N), Phytoplankton (P), Zooplankton (Z) and Detritus (D).

In the marine environment, the limiting nutrient is typically dissolved inorganic nitrogen (DIN). In freshwater environments, dissolved inorganic phosphorus (DIP) is typically used as the limiting nutrient.

The NPZD model is a "real-life" model, in the sense that it is actively used in research: it forms the biological heart of most biogeochemical modules in present-day ocean circulation models.

In this exercise, you start by making an NPZD model, which you will then extend to a NPZD2 model by including *two* detritus fractions (hence the "D2").

The conceptual scheme of the NPZD model is given in Figure 1.

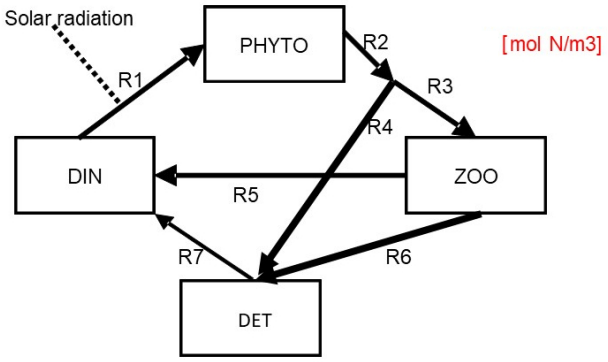


Figure 1: Conceptual diagram of an NPZD model.

Assumptions of the NPZD model

The following assumptions are made:

- All state variables are expressed in $mol\ N\ m^{-3}$.
- DIN is the limiting nutrient.
- Solar radiation (light) is a forcing function that drives photosynthesis, and it changes seasonally.

- A fraction of the light is photosynthetically active radation (PAR). PAR decreases exponentially with water depth (with the extinction coefficient of 0.05 m^{-1}). The algae perceive — on average — the PAR in the *middle* of the water column.[1]
- Nitrogen uptake is limited by light availability and nutrient availability. Nutrient and light limitation are both described with a type II functional response (Michaelis-Menten, or Monod kinetics). Total limitation is calculated as the *product* of nitrogen and light limitation.
- The food intake by zooplankton (i.e., by grazing on the phytoplankton) is governed by a type II functional response.
- A fixed fraction *pFaeces* of total food intake by zooplankton is lost as faeces.
- Zooplankton excretes ammonium at a rate described by the first-order kinetics.
- Zooplankton mortality is modelled as a quadratic function of zooplankton biomass. Tip: the units of the mortality parameter give a hint as to how such a function looks like.
- Mineralization of detritus is a first-order process.

Tasks

Step 1. Create the NPZD model

- Start by creating the mass balance equations based on the flow scheme above.
- Create suitable rate expressions for each of the flows, based on the assumptions given above. For ecological interactions you will need to think which component is the "worker" and which component is the "resource".
- The following table lists the values and units of the parameters used:

Parameter	Value	Description	Units
depth	10	water depth	m
rUptake	1.0	Nitrogen uptake rate constant	d^{-1}
ksPAR	140	Monod ct for light limitation	$\mu Einst\ m^{-2}s^{-1}$
ksDIN	1×10^{-3}	Monod ct for nutrient limitation	$mol\ N\ m^{-3}$
rGrazing	1.0	Grazing rate constant	d^{-1}
ksGrazing	1×10^{-3}	Monod ct for grazing	$mol\ N\ m^{-3}$
pFaeces	0.3	Part of ingestion to faeces	$-$
rMortality	400	Mortality rate constant	$(mol\ N\ m^{-3})^{-1}d^{-1}$
rExcretion	0.1	Excretion rate constant (to DIN)	d^{-1}
rMineralisation	0.05	Mineralisation rate constant	d^{-1}

- The initial conditions of the state variables (SV) are:

SV	value	Units
DIN	0.010	$mol\ N\ m^{-3}$
PHYTO	0.0005	$mol\ N\ m^{-3}$
ZOO	0.0003	$mol\ N\ m^{-3}$
DET	0.005	$mol\ N\ m^{-3}$

- Implement the model in R, using the R+markdown file *RTM_npzd.Rmd* to start with (this file already contains the statement that estimates the light intensity as a function of the time of the year and the depth of the water column).[2] First, change the heading and rename this file to *NPZD.Rmd*.

[1] This corresponds well to the average light intensity through the water-column.

[2] You can download this file from Rstudio: File → new File → Rmarkdown → from template → RTM_npzd.

- Run the model and inspect the output.

Step 2. NPZD2 — expand the NPZD model with sediment detritus

First copy the file that implements the NPZD model and rename it as *NPZD2.Rmd*. (The "D2" means that there will be eventually two types of detritus).

- Redraw the conceptual diagram by adding bottom detritus. Add the new flows.
  - What are suitable units for bottom detritus?
  - What are the units of the new flows?
- Assume that both algae and detritus sink with a sinking velocity of 1 $m\ d^{-1}$. Upon entering the sediment, the algae die and add to bottom detritus.
- Bottom detritus mineralizes with the same rate constant as suspended detritus; DIN released by this process is immediately exchanged with the entire water column (i.e., well-mixed water column).
- Find suitable initial conditions for the bottom detritus. You may use trial and error; the bottom detritus concentration should not show any long-term trends, rather its dynamics should be repeated annually.
- Implement this model in R and run the model.
- At the last day of the simulation, where do we find most of the organic matter — in the water or in the sediment? (tip: out[nrow(out),] shows the values on the last day).
- Compare N contents in the different model compartments as a function of time. Where is most of the N stored during the summer and winter seasons?

Answers: The NPZD model

State variables in this model are expressed in $mol\ N\ m^{-3}$.

- In the DIN uptake flux the worker is the PHYTOplankton, while both DIN and Light are rate limiting resources.
- In the Grazing flux, the ZOOplankton does the work while the PHYToplankton is the limiting resource.
- Faeces can only be produced if there is grazing; a fixed part of what is ingested ($pFaeces$) is expelled as faeces. That is, only the part $1 - pFaeces$ leads to an *increase* in the ZOOplankton biomass.
- $Grazing - FaecesProduction$ is used for the growth of the zooplankton.
- For the mortality of the zooplankton, a second-order kinetics is used ($mortalityRate \times ZOO \times ZOO$). This is often done for small organisms that are predated upon by other small organisms. It is then implicitly assumed that the predator fluctuates together with the prey. Thus, if the prey concentration is low, there will be few predators and the predation pressure will also be low. If there are many prey, there will also be many predators, so the predation pressure will be very high.

Model implementation

```
require(deSolve)  # package with solution methods
```

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

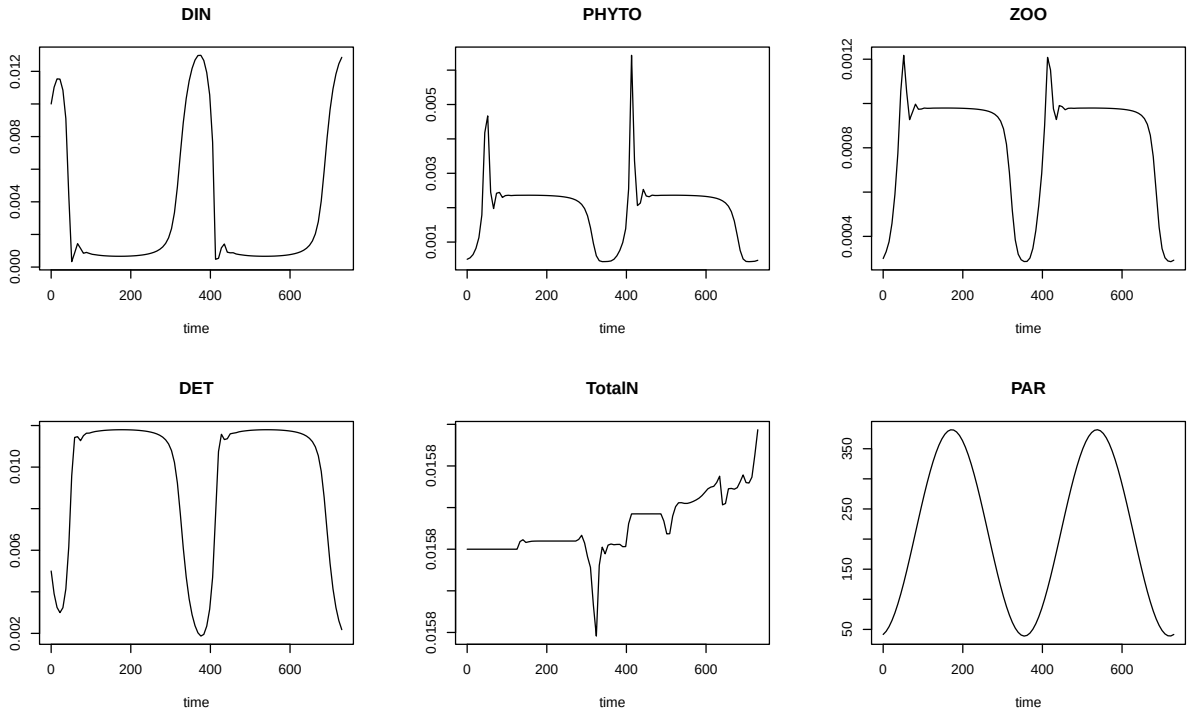
```
# state variables, units = molN/m3
state  <- c(DIN = 0.010, PHYTO = 0.0005, ZOO = 0.0003, DET = 0.005)

# parameters
parms <- c(
  depth           = 10,        # [m] depth of the bay
  rUptake         = 1.0,       # [/day]
  ksPAR           = 140,       # [uEinst/m2/s]
  ksDIN           = 1.e-3,     # [molN/m3]
  rGrazing        = 1.0,       # [/day]
  ksGrazing       = 1.e-3,     # [molN/m3]
  pFaeces         = 0.3,       # [-]
  rExcretion      = 0.1,       # [/day]
  rMortality      = 400,       # [/(molN/m3)/day]
  rMineralisation = 0.05       # [/day]
)

#================================================================================
# Model formulation
#================================================================================

NPZD <- function(t, state, parameters) {
 with(as.list(c(state, parameters)),{

    # Forcing function = Light a sine function
    # light = (540+440*sin(2*pi*t/365-1.4)), 50% of light is PAR
    # spring starts on day 81 (22 March)
    # We calculate the PAR in the middle of the water column; extinction coefficient = 0.05/m
    PAR <- 0.5*(540+440*sin(2*pi*(t-81)/365))*exp(-0.05*depth/2)

    # Rate expressions - all in units of [molN/m3/day]
```

```
    DINuptake      <- rUptake * PAR/(PAR+ksPAR) * DIN/(DIN+ksDIN)*PHYTO
    Grazing        <- rGrazing * PHYTO/(PHYTO+ksGrazing)*ZOO
    Faeces         <- pFaeces * Grazing
    ZooGrowth      <- (1-pFaeces) * Grazing
    Excretion      <- rExcretion * ZOO
    Mortality      <- rMortality * ZOO * ZOO
    Mineralisation <- rMineralisation * DET

    # Mass balances [molN/m3/day]
    dDIN      <- Mineralisation + Excretion - DINuptake
    dPHYTO    <- DINuptake - Grazing
    dZOO      <- ZooGrowth - Excretion - Mortality
    dDET      <- Mortality - Mineralisation + Faeces
    TotalN    <- DIN+PHYTO+ZOO+DET              # [molN/m3]

    return (list(c(dDIN, dPHYTO, dZOO, dDET),   # the derivatives
                 TotalN = TotalN, PAR = PAR)  # ordinary output variables
           )
    })
}  # end of model equations
```

Model run

We run the model for 2 years.

```
outtimes <- seq(from = 0, to = 2*365, length.out = 100)
out <- ode(y = state, parms = parms, func = NPZD, times = outtimes)  # solution
plot(out, mfrow=c(2,3))
```



The NPZD2 model

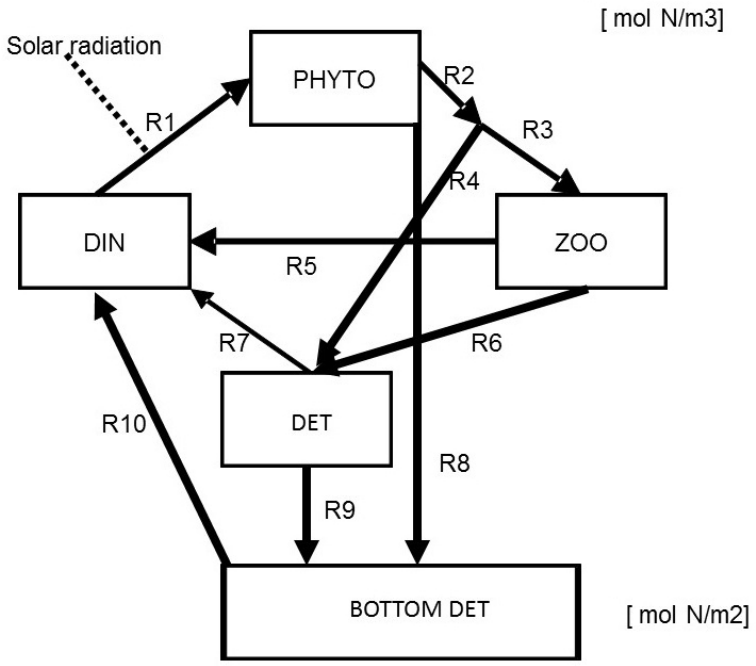


Figure 2: Concentual diagram of the NPZD2 model (includes bottom detritus).

Figure 2 shows the conceptual diagram that includes both the free-floating and bottom detritus fractions.

It is most logical to express the pelagic (water) constituents per volume of water, i.e., in $mol\ N\ m^{-3}$, while the benthic (sediment) constituents are best expressed per surface of sediment, i.e., in $mol\ N\ m^{-2}$.

Consequently, most rates featuring in the mass balance of pelagic state variables are in $mol\ N\ m^{-3}\ d^{-1}$, while the rates for the benthic state variable are in $mol\ N\ m^{-2}\ d^{-1}$.

An exception is the sinking of phytoplankton and detritus:

$$R8 = sinkVelocity \times PHYTO$$

$$R9 = sinkVelocity \times DET$$

With *sinkVelocity* expressed in $m\ d^{-1}$, the fluxes R8 and R9 are expressed in $mol\ N\ m^{-2}\ d^{-1}$.

For the mass balance equations of phytoplankton and detritus, we will need to convert between volumetric (m^{-3}) and areal (m^{-2}) units.

Consequently, the mass balances for the phytoplankton and pelagic and bottom detritus are:

$$\frac{dPHYTO}{dt} = R1 - R2 - R8/depth$$

$$\frac{dDET}{dt} = R4 + R6 - R7 - R9/depth$$

$$\frac{dBOT\_DET}{dt} = R8 + R9 - R10$$

The mineralisation rate of bottom detritus is expressed as

$$R10 = rMineralisation \times BOT\_DET$$

and has units of $mol\ N\ m^{-2}\ d^{-1}$. This will need to be converted to units of $mol\ N\ m^{-3}\ d^{-1}$ to update the mass balance of pelagic DIN.

Note that also the formula to calculate total nitrogen in the system needs to take into account the different units.

Model implementation

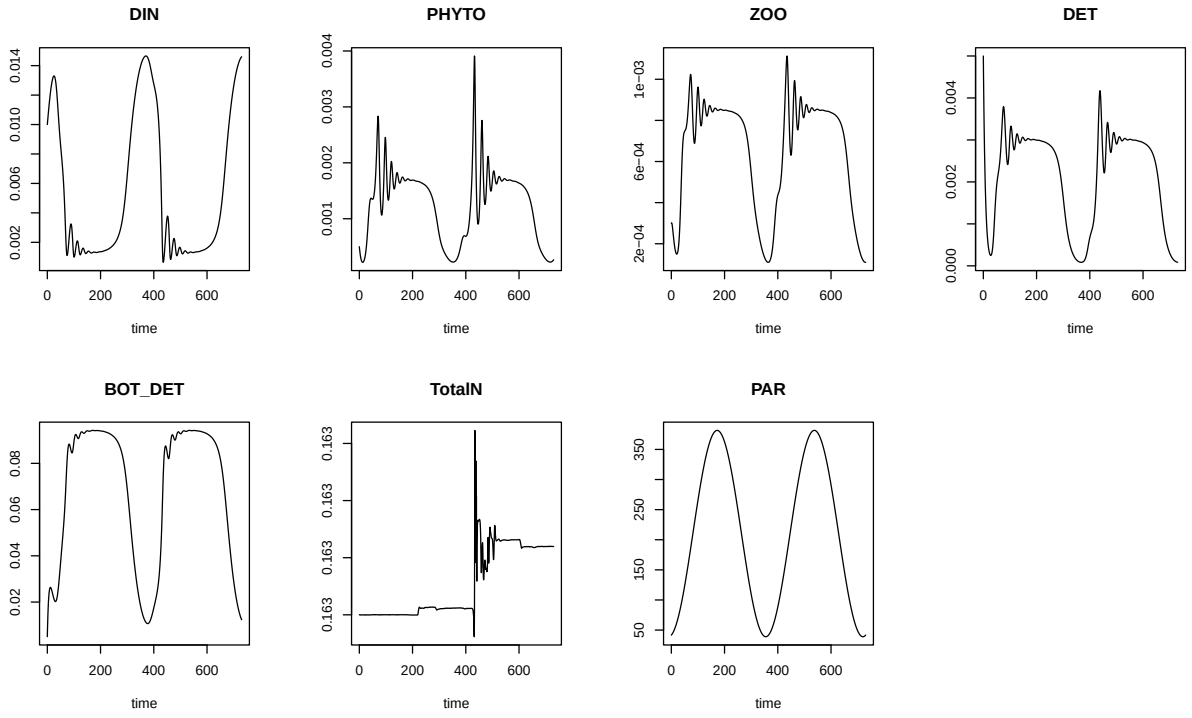
```
require(deSolve)  # package with solution methods

# state variables, units = molN/m3 or molN/m2 (BOT_DET)
state  <- c(DIN = 0.010, PHYTO = 0.0005, ZOO = 0.0003, DET = 0.005, BOT_DET = 0.005)

# parameters
parms <- c(
  depth           = 10,        # [m] depth of the bay
  rUptake         = 1.0,       # [/day]
  ksPAR           = 140,       # [uEinst/m2/s]
  ksDIN           = 1.e-3,     # [molN/m3]
  rGrazing        = 1.0,       # [/day]
  ksGrazing       = 1.e-3,     # [molN/m3]
  pFaeces         = 0.3,       # [-]
  rExcretion      = 0.1,       # [/day]
  rMortality      = 400,       # [/(molN/m3)/day]
  rMineralisation = 0.05,      # [/day]
  sinkVelocity    = 1          # [m/day]

)

#================================================================================
# Model formulation
#================================================================================

NPZD2 <- function(t, state, parameters)
 {
 with(as.list(c(state, parameters)),{

    # Forcing function = Light a sine function
    # light = (540+440*sin(2*pi*t/365-1.4)), 50% of light is PAR
    # spring starts at day 81 (22 March)
    # We calculate PAR at the middle of the water column; extinction coefficient=0.05/m
    PAR <- 0.5*(540+440*sin(2*pi*(t-81)/365))*exp(-0.05*depth/2)

   # Rate expressions - in units of [molN/m3/day] or [molN/m2/d]
    DINuptake      <- rUptake * PAR/(PAR+ksPAR) * DIN/(DIN+ksDIN)*PHYTO # molN/m3/d
    Grazing        <- rGrazing* PHYTO/(PHYTO+ksGrazing)*ZOO             # molN/m3/d
    Faeces         <- pFaeces * Grazing                                 # molN/m3/d
    ZooGrowth      <- (1-pFaeces) * Grazing                             # molN/m3/d
    Excretion      <- rExcretion * ZOO                                  # molN/m3/d
    Mortality      <- rMortality * ZOO * ZOO                            # molN/m3/d
    Mineralisation <- rMineralisation * DET                             # molN/m3/d
    SinkDet        <- sinkVelocity * DET                                # molN/m2/d !
    SinkPhy        <- sinkVelocity * PHYTO                              # molN/m2/d !
```

```
    BotMin         <- rMineralisation * BOT_DET                          # molN/m2/d !

   # Mass balances [molN/m3/day]
    dDIN      <- Mineralisation + Excretion - DINuptake + BotMin / depth  # molN/m3/d
    dPHYTO    <- DINuptake - Grazing  - SinkPhy / depth                   # molN/m3/d
    dZOO      <- ZooGrowth - Excretion - Mortality                        # molN/m3/d
    dDET      <- Mortality - Mineralisation + Faeces - SinkDet / depth    # molN/m3/d
    dBOT_DET  <- SinkDet + SinkPhy - BotMin                               # molN/m2/d !

    TotalN <- (DIN+PHYTO+ZOO+DET)*depth + BOT_DET         # molN/m2
    # the output
    return (list(c(dDIN, dPHYTO, dZOO, dDET, dBOT_DET),   # the rates of change
                 TotalN = TotalN, PAR = PAR)              # ordinary output variable
          )
    })
  }  # end of model equations
```

Model run

We run the model for 2 years.

```
# output times
outtimes <- seq(from = 0, to = 2*365, length.out = 1000)

# solve this model, using the ode function from deSolve
out <- ode(y = state, parms = parms, func = NPZD2, times = outtimes)  # solution

# visualise output
plot(out, mfrow=c(2,4))
```



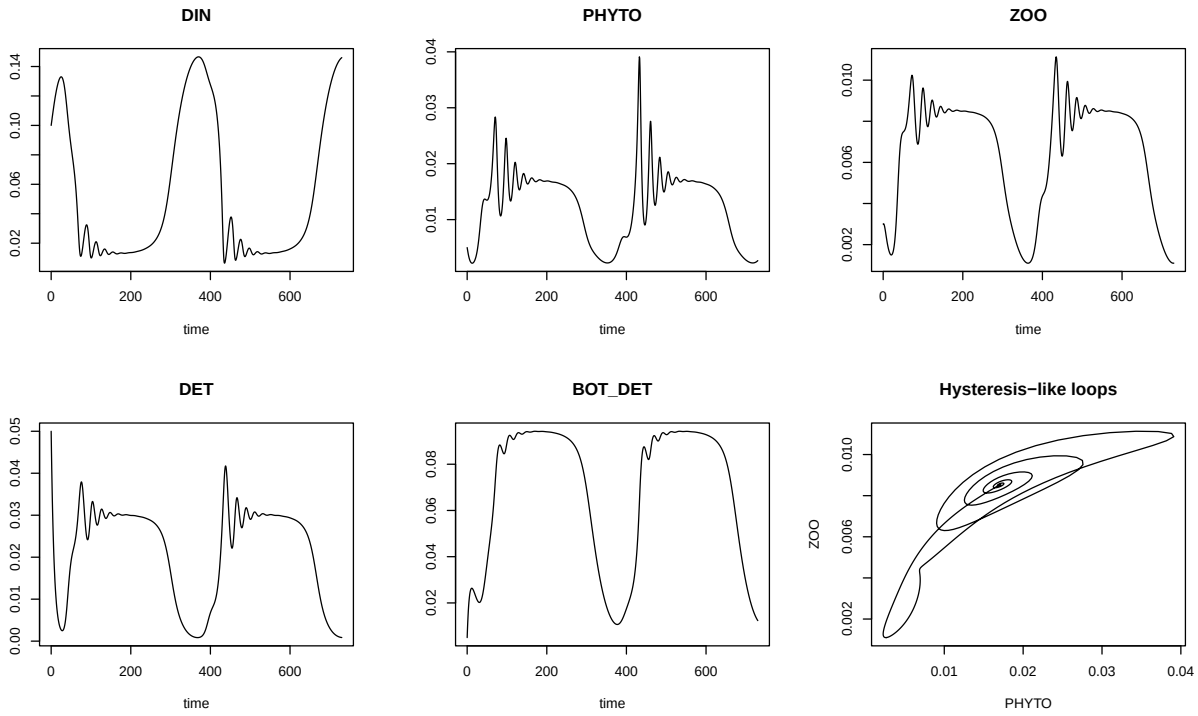
Now we compare the amounts of organic matter in the pelagic vs. benthic compartment at the end of the simulation. Note that we multiply the pelagic state variables by *depth* so that the amounts are comparable (all are expressed in $mol\ N\ m^{-2}$).

```
last <- out[nrow(out),]
c(pelagic = sum(last[3:5]*parms["depth"]), benthic = last["BOT_DET"])
```

```
##         pelagic benthic.BOT_DET
##     0.004624478     0.012350506
```

Now, we visualize the areal concentrations of N ($mol\ N\ m^{-2}$) for all state variables, to illustrate how N is distributed among the different compartments throughout the year. Additionally, we plot the PHYTOplankton biomass against the ZOOplankton biomass (only for the second year) to show that although they appear to follow each other *closely* when plotted against time, they are *not* linearly proportional to each other. Instead, there is a time delay in the response of the ZOOplankton to the change in the PHYTOplankton, which results in hysteresis-like loops.

```
out.areal <- out
out.areal[,2:5] <- out.areal[,2:5] * parms[["depth"]]
plot(out.areal, mfrow=c(2,3), which=1:5)
N <- length(outtimes)
plot(out.areal[round(N/2):N,"PHYTO"], out.areal[round(N/2):N,"ZOO"],
     type="l", xlab="PHYTO", ylab="ZOO", main="Hysteresis-like loops")
```



We see that most of the N in the system is in the "non-living" components. During the summer, it is mostly in the "dead" organic matter, which is due to the limited rate of mineralization and the subsequent limitation of growth by DIN. In the winter, it is mostly in the inorganic form (DIN), which is due to growth limitation by low availability of light.

References

R Core Team (2020). R: A language and environment for statistical computing. R Foundation for Statistical Computing, Vienna, Austria. URL https://www.R-project.org/.

Karline Soetaert, Thomas Petzoldt, R. Woodrow Setzer (2010). Solving Differential Equations in R: Package deSolve. Journal of Statistical Software, 33(9), 1–25. URL http://www.jstatsoft.org/v33/i09/ DOI 10.18637/jss.v033.i09