Rate expressions in biogeochemistry: detritus mineralization by bacteria

Exercises Accompanying the Course Reaction Transport Modelling in the Hydrosphere

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Modelling detritus mineralization by bacteria

In class you have seen how to write rate expressions for ecological interactions: you need to distinguish between compartments that are actively performing the task (the "worker"), and compartments that are taken up as a result (the "resource"). This exercise is meant to make you think about these different roles that compartments may play.

You already made the conceptual diagram for this problem. Now you need to find rate expressions for each of the flows. If you have time, you can also implement the model in R.
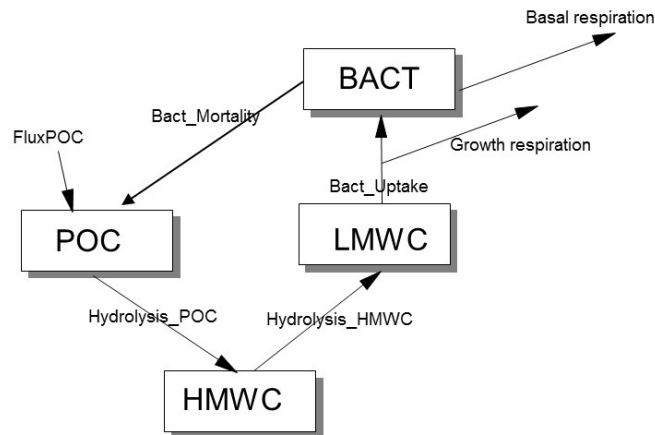
Problem formulation

Figure 1: Conceptual diagram of the detritus model.

Detritus in the marine system is degraded by the action of heterotrophic bacteria. This is not a one-step process: bacteria cannot 'eat' detritus! You will make a model that is closer to the reality of the process.

The model considers that particulate detritus (POC) is first hydrolysed by the action of bacterial exoenzymes to high-molecular-weight dissolved organic carbon (HMWC). This in turn is attacked by bacterial enzymes to yield low-molecular-weight dissolved organic carbon (LMWC), which can then be taken up by the bacteria (BACT) to grow on it. The conceptual diagram of this model is shown in Figure 1.

Tasks

- Create the mass balance equations for this model.
- Find suitable rate expressions for the fluxes. For ecological or biogeochemical interactions, think which compartment is the "worker" and which is the "resource". The units of the parameters may provide guidance as to which rate expressions you may want to implement.

The parameters are:

parameter	value	Description	units
rPOC	0.75	rate constant of hydrolysis of POC	d^{-1}
rHMWC	0.5	rate constant of hydrolysis of HMWC	d^{-1}
rup	2	uptake rate constant of LMWC by bacteria	d^{-1}
ksPOC	0.10	Monod ct for POC hydrolysis	$mol\ C\ m^{-3}$
ksHMWC	0.005	Monod ct for HMWC hydrolysis	$mol\ C\ m^{-3}$
ksLMWC	0.0005	Monod ct for LMWC uptake by bacteria	$mol\ C\ m^{-3}$
rBas	0.1	basal respiration rate constant	d^{-1}
pResp	0.5	fraction of LMWC uptake respired	-
rClos	50	quadratic mortality rate constant for bacteria	$(mol\ C\ m^{-3})^{-1}\ d^{-1}$
fluxPOC	0.0005	constant influx of POC	$mol\ C\ m^{-3}\ d^{-1}$

- Check the dimensionality of your model.

If you have time

- Use the model template file *RTM_0D.Rmd* to implement this model.[1]

- The initial conditions are: POC = 0.1, HMWC = 0.005, LMWC = 0.00015, BACT = 0.005, all in $mol\ C\ m^{-3}$.

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[1] You can obtain this file from Rstudio: File → new File → Rmarkdown → from template → RTM_0D. Save this file under a different name. Do not forget to change the heading of this file.

Modelling detritus mineralization by bacteria — Answers

Mass balances

Based on the conceptual diagram in Figure 1, the mass balance equations are:

$$\frac{dPOC}{dt} = FluxPOC - HydrolysisPOC + BactMortality$$

$$\frac{dHMWC}{dt} = HydrolysisPOC - HydrolysisHMWC$$

$$\frac{dLMWC}{dt} = HydrolysisHMWC - BactUptake$$

$$\frac{dBACT}{dt} = BactUptake - GrowthRespiration - BasalRespiration - BactMortality$$

Rate expressions

For the rate expressions, it is important to realise that bacteria are doing ALL the work to dissolve POC into smaller (HMWC) and smaller (LMWC) chunks, until they eventually take up the resource. Thus they are the worker for HydrolysisPOC, HydrolysisHMWC and BactUptake:

$$HydrolysisPOC = rPOC \times \frac{POC}{(POC + ksPOC)} \times BACT$$

$$HydrolysisHMWC = rHMWC \times \frac{HMWC}{(HMWC + ksHMWC)} \times BACT$$

$$BactUptake = rup \times \frac{LMWC}{(LMWC + ksLMWC)} \times BACT$$

Not all LMWC taken up by the bacteria yields new bacterial biomass. Part of this uptake is used to generate the energy required for biomass synthesis, which is done by respiration. This is called "activity respiration", and it is represented by the rate *GrowthRespiration*:

$$GrowthRespiration = pResp \times BactUptake$$

In addition, there is basal respiration (also called "maintenance respiration"), which provides energy for the basic body functions but does not lead to growth of the bacterial biomass:

$$BasalRespiration = rBas \times BACT$$

The parameter that defines the bacterial mortality has units of $(mol\ C\ m^{-3})^{-1}\ d^{-1}$, while the bacterial mortality should have units of $mol\ C\ m^{-3}\ d^{-1}$. This means that we need to multiply the mortality parameter with a concentration squared to obtain the correct units for the flux. Thus, the rate expression for the mortality is:[2]

$$BactMortality = rClos \times BACT^2$$

Modelers often use a quadratic mortality for small organisms that grow very fast and whose predator also grows very fast, so that the predator has high concentration if the prey has high concentration and vice versa.

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[2]The description of the parameter as a "quadratic mortality ct" also gives this idea away.

R-implementation

Here is the R-code for the model:

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

# state variables, units = mmolC/m3
state <- c(POC = 100, HMWC = 5, LMWC = 0.15, BACT = 5)

# parameters
parms <- c(
  rPOC = 0.75,     # [d-1]
  rHMWC = 0.5,     # [d-1]
  rup = 2,         # [d-1]
  ksPOC = 100,     # [mmolC.m-3]
  ksHMWC = 5,      # [mmolC.m-3]
  ksLMWC = 0.5,    # [mmolC.m-3]
  rbas = 0.1,      # [d-1]
  ploss = 0.5,     # [-]
  rclos = 0.05,    # [(mmolC.m-3)-1.d-1]
  fluxPOC = 0.5    # [mmolC.m-3.d-1]
)

# Model function
DetBact <- function(t, state, params) {
  with (as.list(c(state, params)), {

    # Rate expressions - all in units of [mmolC/m3/day]
    HydrolysisPOC = rPOC * POC / (POC + ksPOC) * BACT
    HydrolysisHMWC = rHMWC * HMWC / (HMWC + ksHMWC) * BACT
    UptakeLMWC = rup * LMWC/(LMWC + ksLMWC) * BACT
    BasalResp = rbas * BACT
    ActivityResp = UptakeLMWC * ploss
    MortBact = rclos * BACT^2

    # Mass balances [molC/m3/day]
    dPOC.dt  <-  fluxPOC - HydrolysisPOC + MortBact
    dHMWC.dt <-  HydrolysisPOC - HydrolysisHMWC
    dLMWC.dt <-  HydrolysisHMWC - UptakeLMWC
    dBACT.dt <-  UptakeLMWC - BasalResp - ActivityResp - MortBact

    list(c(dPOC.dt, dHMWC.dt, dLMWC.dt, dBACT.dt),
         totalC = POC + HMWC + LMWC + BACT)
  })

}
```
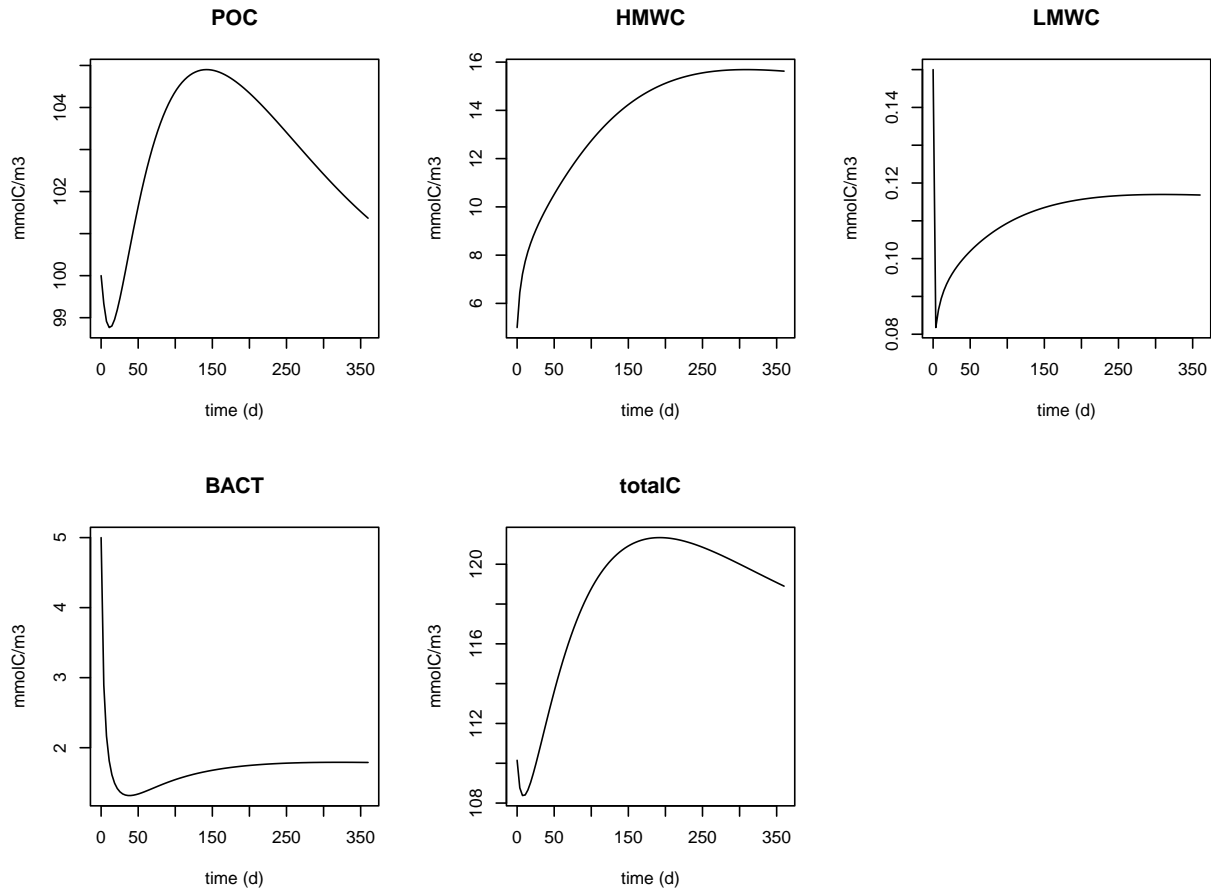
And the model solution:

```r
# output times
outtimes <- seq(from = 0, to = 360, length.out = 100)  # run the model for 360 days

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

```
# visualise output
plot(out, xlab="time (d)", ylab="mmolC/m3")
```

POC

HMWC

LMWC

BACT

totalC

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