One-dimensional model

template markdown file for 1-D models without porosity

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Contents

Introduction

This template file contains a simple one-dimensional reaction-transport model describing the dynamics of oxygen (O2) and biochemical oxygen demand (BOD), both expressed in units of mol/m3, in a river that is in contact with the air.

The model domain is divided into a grid with N equally sized boxes (N=100).

Both BOD and O2 are *vectors* with a length of N. They represent the concentrations of the state variables in the *center* of the boxes.

With regard to the reaction, a simple first-order decay of BOD that is limited by oxygen is assumed. This reaction consumes both BOD and O2. O2 is also exchanged with the atmosphere.

The species are modeled with the following boundary conditions:

- BOD: imposed flux at the upstream (flux.up) and imposed concentration boundary downstream (C.down).
- O2: imposed concentration upstream (C.up), zero-gradient boundary downstream (default, need not be specified).

The partial derivatives related to transport are approximated with function tran.1D from the ReacTran package. The steady-state and dynamic solutions are obtained using functions from the rootSolve and deSolve package. The latter two packages are loaded together with ReacTran.

Model definition

```
require(ReacTran)  # package with solution methods - includes deSolve, rootSolve

# model grid
Length <- 1000                                  # [m]
N      <- 100                                   # [-] number of boxes
Grid   <- setup.grid.1D(L = Length, N = N)      # grid of N equally-sized boxes

# Modeled state variables
SVnames <- c("O2", "BOD")

# initial conditions - state variables are defined in the middle of grid cells
O2      <- rep(0.1,   times = N)                # [molO2/m3]
BOD     <- rep(0.001, times = N)                # [molO2/m3]

# the initial state of the system is described as a vector with all state variables (2*N)
yini   <- c(O2, BOD)

# model parameters
pars <- c(
  D        = 100,    # [m2/d]      dispersion coefficient
  v        = 10,     # [m/d]       advection velocity
  rDecay   = 0.05 ,  # [/d]        first-order decay constant of BOD
  kO2      = 0.001,  # [mol/m3]    half-saturation O2 concentration for decay
  inputBOD = 10,     # [mol/m2/d]  BOD input rate upstream
  BODdown  = 0.1,    # [mol/m3]    BOD concentration downstream
  O2up     = 0.25 ,  # [mol/m3]    O2 concentration upstream
  satO2    = 0.3  ,  # [mol/m3]    saturation concentration of Oxygen
  k        = 0.1     # [/d]        reaeration coefficient
)


# Model function
BOD1D <-function(t, state, pars) {  # state is a long vector
  with (as.list(pars),{

  # The vectors of the state variables O2 and BOD are
  # "extracted" from the LONG vector state passed to the function as input.
    O2  <- state[   1 :   N ]   # first N elements in O2
    BOD <- state[(N+1):(2*N)]   # second N elements in BOD

  # Transport - tran.1D solves the spatial derivatives
    # note: for O2: zero-gradient boundary downstream (default), not specified
    tranO2  <- tran.1D(C = O2,
                       C.up = O2up,          # imposed conc upstream,
                       D = D, v = v,         # dispersion, advection
                       dx = Grid)            # Grid

    tranBOD <- tran.1D(C       = BOD,
                       flux.up = inputBOD,  # imposed boundary flux
                       C.down  = BODdown,   # imposed boundary concentration
                       D = D, v = v,        # dispersion, advection
```

```
                     dx = Grid)           # Grid

  # rate expressions [mol/m3/d]
    Decay     <- rDecay * BOD * O2/(O2+kO2)   # BOD decay, limited by O2
    Aeration  <- k * (satO2-O2)               # air-water exchange of O2

  # Time-derivatives: dC/dt = transport + production-consumption [mol/m3/d]
    dO2dt   <- tranO2$dC  - Decay  + Aeration
    dBODdt  <- tranBOD$dC - Decay

  # return vector of time-derivatives and ordinary variables as a list
  list(c(dO2dt, dBODdt),      # derivatives (same order as state variable definition)

    # the ordinary variables
    Decay        = Decay,             # 1D rates (vector)
    Aeration     = Aeration,
    MeanDecay    = mean(Decay),       # mean decay rate
    MeanAeration = mean(Aeration),    # mean aeration rate

    # ordinary variables used for budgetting (per m2 cross-sectional area)
    TotalDecay    = sum(Decay*Grid$dx), # decay integrated over the domain,   mol/m2/d
    TotalAeration = sum(Aeration*Grid$dx),

    BODinflux = tranBOD$flux.up,     # BOD flux INto the system upstream,     mol/m2/d
    BODefflux = tranBOD$flux.down,   # BOD flux OUT of the system downstream, mol/m2/d
    O2influx = tranO2$flux.up,       # O2 flux INto the system upstream,      mol/m2/d
    O2efflux = tranO2$flux.down)     # O2 flux OUT of the system downstream,  mol/m2/d
  })
}
```

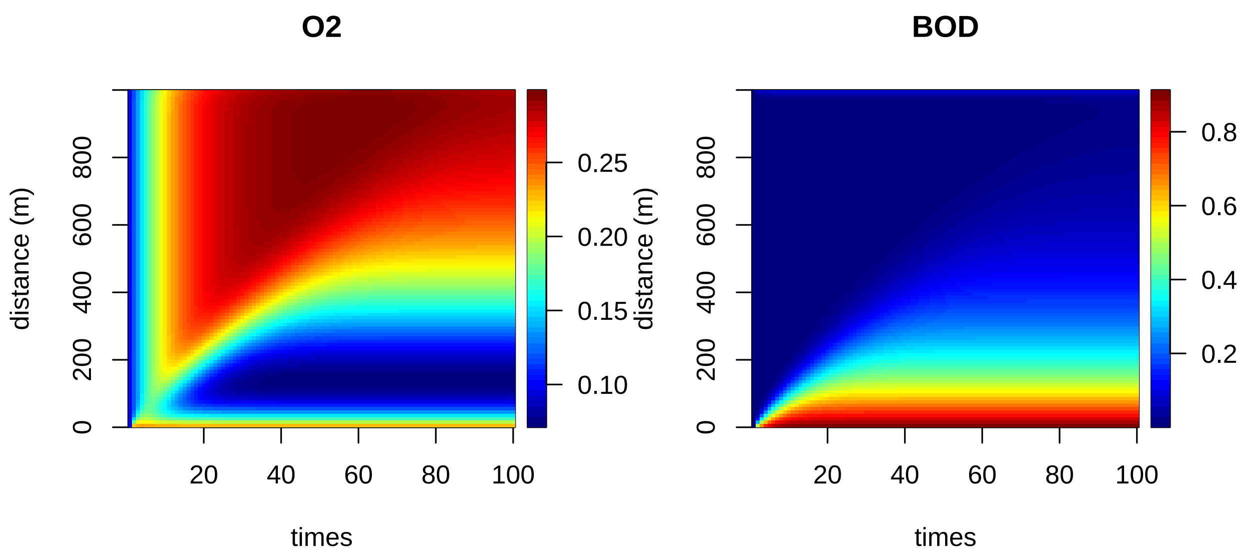
Model solution

Dynamic solution

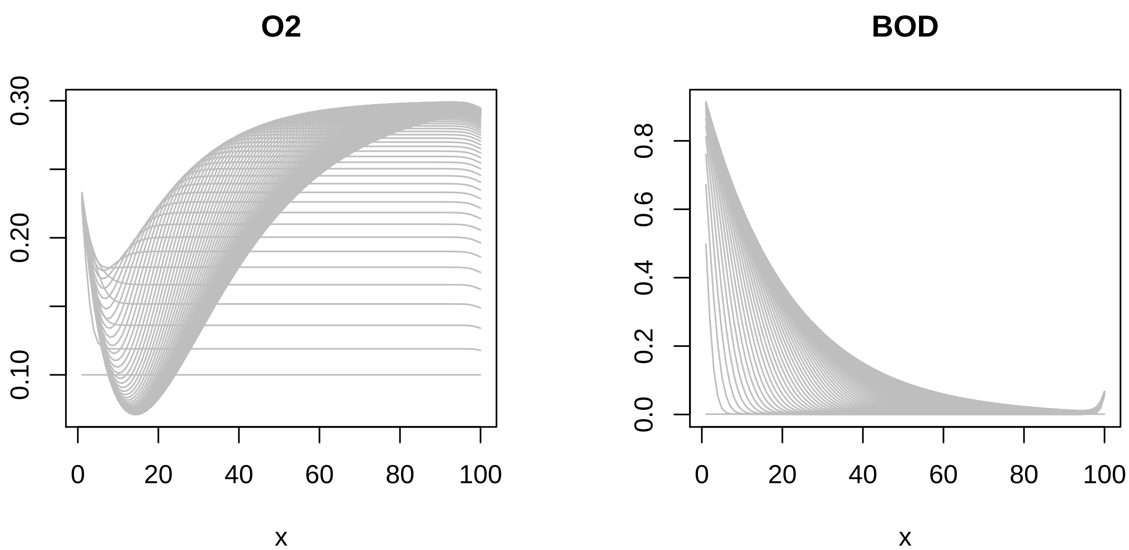
```
outtimes <- seq(from = 1, to = 100, length.out = 100)   # output times

# ode.1D integrates the 1D model
# It needs the number (nspec) and names of species, and the dimension (dimens).
out <- ode.1D(y = yini, parms = pars, func = BOD1D, times = outtimes,
              names = SVnames, nspec = length(SVnames), dimens = N)
```

Output the solution as an image, time plot, and lines.

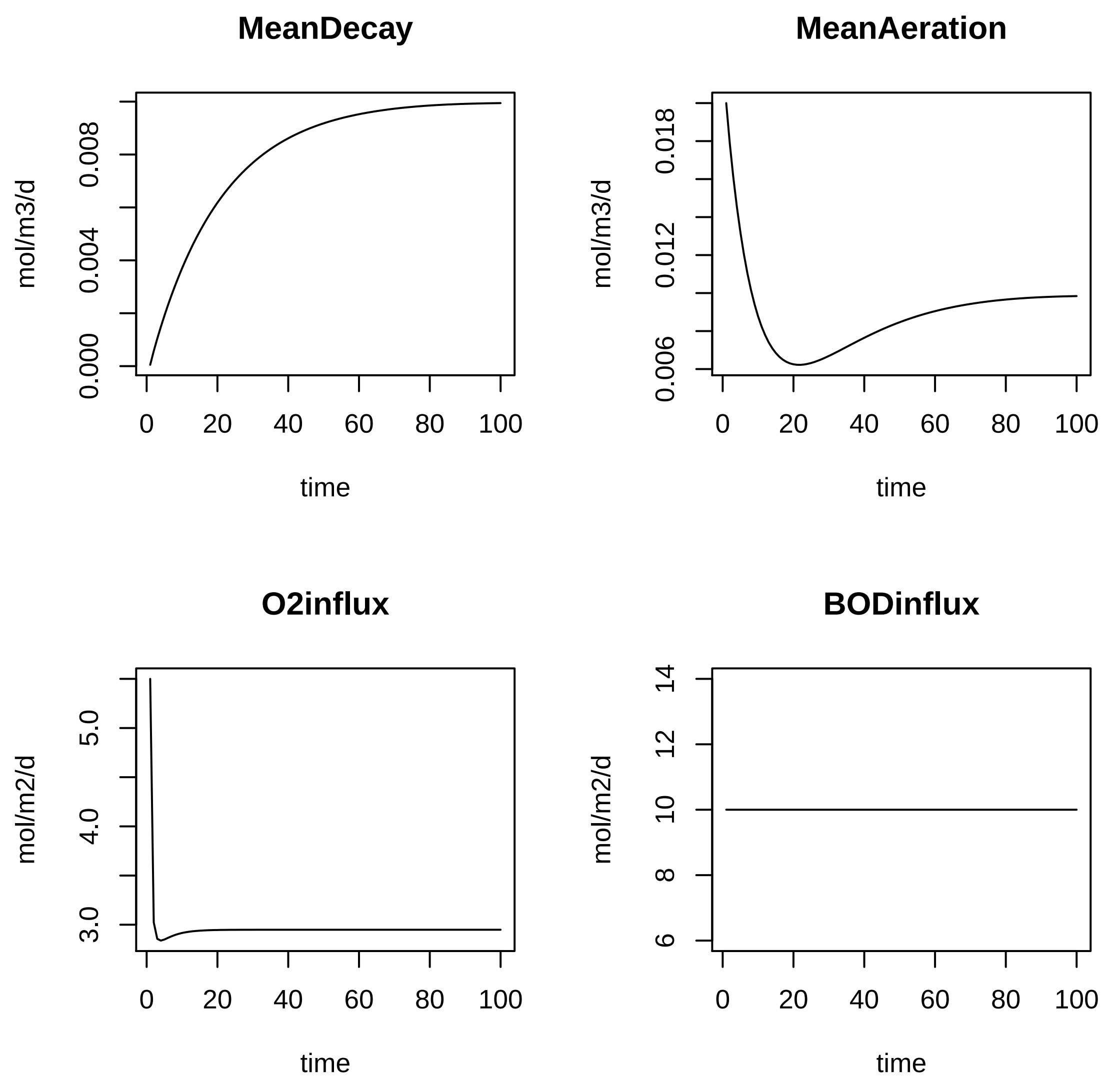
```
image(out, grid = Grid$x.mid, ylab = "distance (m)", legend = TRUE)
```




```r
# each curve represents the solution at a given time point
matplot.1D(out, type = "l", lty = 1, col = "grey")
```




```r
plot(out, which=c("MeanDecay", "MeanAeration", "O2influx", "BODinflux"),
          ylab=c("mol/m3/d","mol/m3/d","mol/m2/d","mol/m2/d"))
```



Steady-state solution

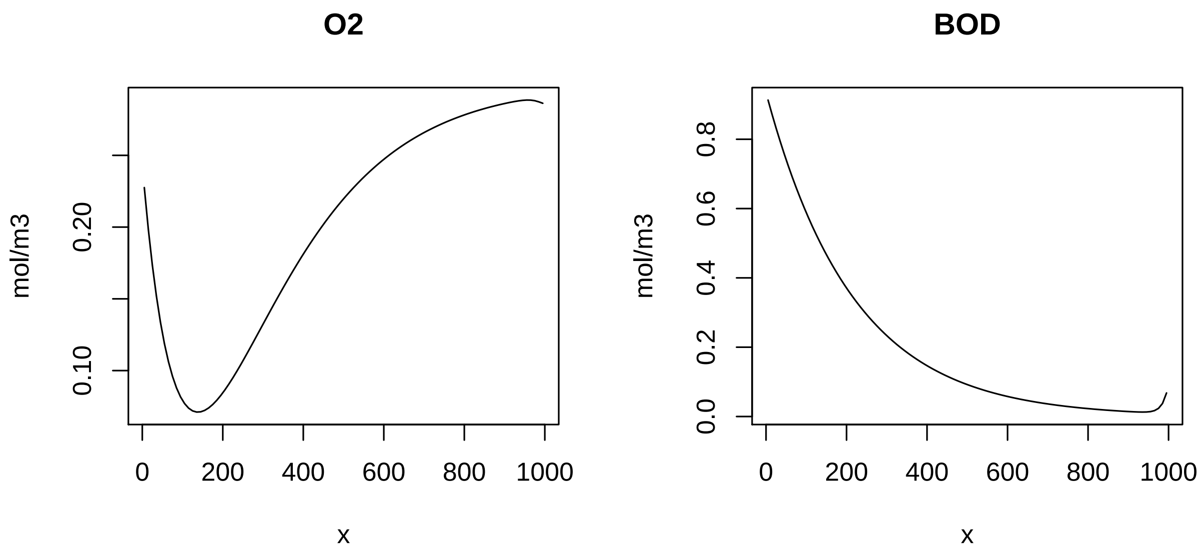
```
# find steady state solution
std <- steady.1D(y = yini, parms = pars, func = BOD1D,
          positive = TRUE,                # to ensure that the solution is positive
          names = SVnames, nspec = length(SVnames), dimens = N,
          atol = 1e-10, rtol = 1e-10)     # to increase the precision of the solution

names(std)          # std holds the state variables (y) and ordinary variables
```

```
##  [1] "y"               "Decay"          "Aeration"      "MeanDecay"
##  [5] "MeanAeration"  "TotalDecay"    "TotalAeration" "BODinflux"
##  [9] "BODefflux"     "O2influx"      "O2efflux"
```

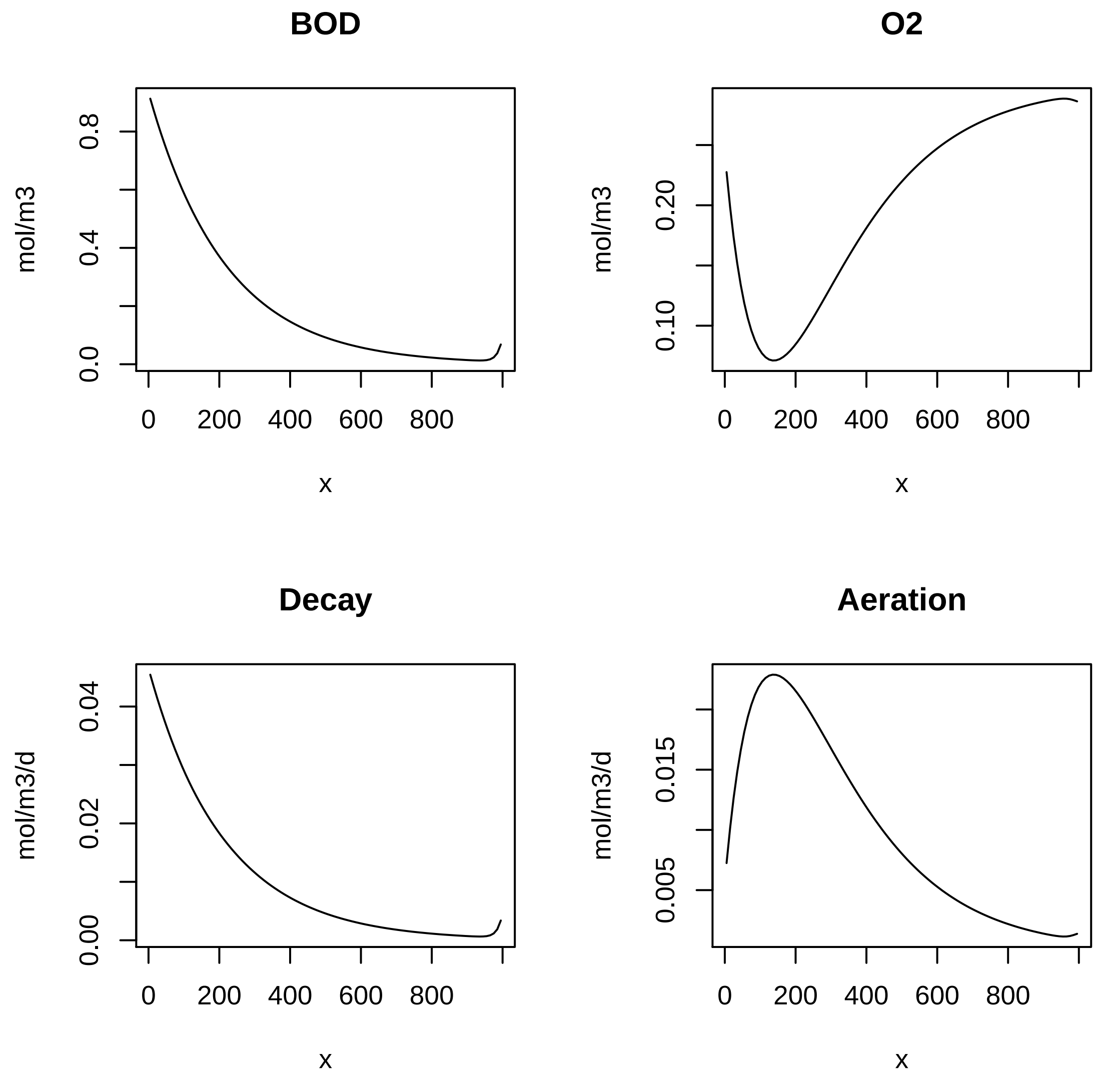
```
head(std$y, n = 2)  # std$y contains the state variables (matrix)
```

```
##               O2       BOD
## [1,] 0.2275553 0.9130921
## [2,] 0.1984315 0.8716390
```

```r
plot(std, grid = Grid$x.mid, ylab = "mol/m3") # plot the state variables
```




```r
plot(std, grid = Grid$x.mid,
     which=c("BOD", "O2", "Decay", "Aeration"),  # plot state variables and reaction rates
     ylab =c("mol/m3","mol/m3","mol/m3/d", "mol/m3/d"))
```



Budgetting:

```
toselect <- c("TotalDecay", "TotalAeration", "O2influx", "O2efflux", "BODinflux", "BODefflux")
BUDGET   <- std[toselect]
unlist(BUDGET)
```

```
##    TotalDecay TotalAeration      O2influx      O2efflux     BODinflux
##     9.9598947     9.8737590     2.9488942     2.8627584    10.0000000
##     BODefflux
##     0.0401053
```

```
# should be same
BUDGET$BODinflux - BUDGET$BODefflux
```

```
## [1] 9.959895
```

```
BUDGET$TotalDecay
```

```
## [1] 9.959895
```

```
# should be ~0
BUDGET$O2influx - BUDGET$O2efflux -BUDGET$TotalDecay + BUDGET$TotalAeration
```

```
## [1] 0
```

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/.

Soetaert Karline (2009). rootSolve: Nonlinear root finding, equilibrium and steady-state analysis of ordinary differential equations. R-package version 1.6

Soetaert Karline, 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

Soetaert, Karline and Meysman, Filip, 2012. Reactive transport in aquatic ecosystems: Rapid model prototyping in the open source software R Environmental Modelling & Software, 32, 49-60.