Solving Differential Equations in R (book) - BVP examples

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Abstract

This vignette contains the R-examples of chapter 12 from the book:

Soetaert, K., Cash, J.R. and Mazzia, F. (2012). Solving Differential Equations in R. that will be published by Springer.

Chapter 12. Solving Boundary Value Problems in R.

Here the code is given without documentation. Of course, much more information about each problem can be found in the book.

Keywords: partial differential equations, initial value problems, examples, R.

1. A simple BVP Example

```
prob7 <- function(x, y, pars) {
 list(c( y[2],
        1/eps * (-x*y[2] + y[1] - (1+eps*pi*pi)*
             cos(pi*x) - pi*x*sin(pi*x))))
}
eps  <- 0.1
sol <- bvptwp(yini = c(y = -1, y1 = NA),
             yend = c(1, NA), func = prob7,
             x = seq(-1, 1, by = 0.01))
prob7_2 <- function(x, y, pars) {
 list(1/eps * (-x*y[2] + y[1] - (1+eps*pi*pi)*
             cos(pi*x) - pi*x*sin(pi*x)))
}
sol1 <- bvptwp(yini = c(y = -1, y1 = NA),
             yend = c(1, NA), func = prob7_2,
             order = 2, x = seq(-1, 1, by = 0.01))
head(sol, n=3)
```

```
         x          y          y1
[1,] -1.00 -1.0000000 0.001699844
[2,] -0.99 -0.9994887 0.100558398
[3,] -0.98 -0.9979891 0.199338166
```

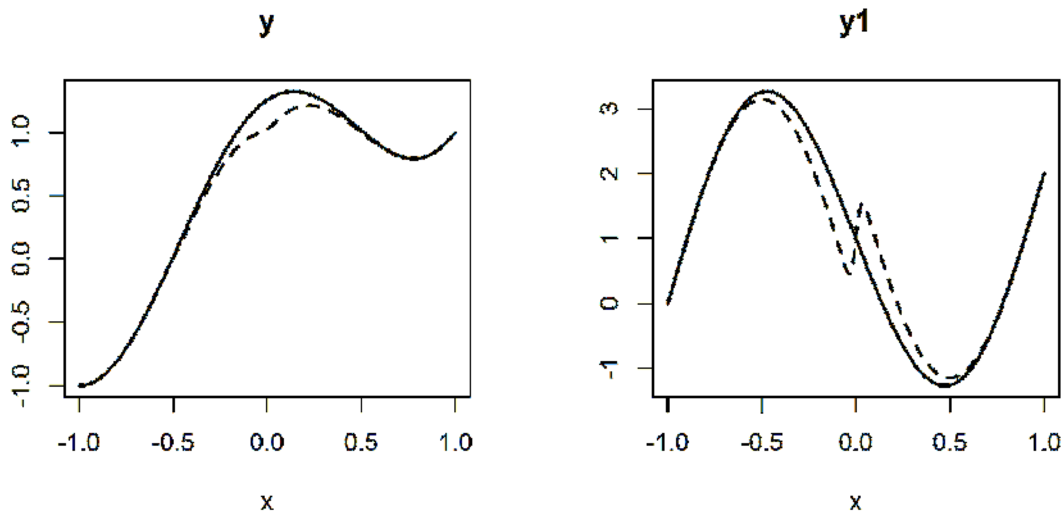

Figure 1: Solution of the test problem 7. See book for more information.

```
eps <-0.0005
sol2 <- bvptwp(yini = c(y = -1, y1 = NA),
              yend = c(1, NA), func = prob7,
              x =  seq(-1, 1, by=0.01))

plot(sol, sol2, col = "black", lty = c("solid", "dashed"),
     lwd = 2)
```

2. A More Complex BVP Example

```
swirl <- function (t, Y, eps)  {
  with(as.list(Y),
    list(c((g*f1 - f*g1)/eps,
           (-f*f3 - g*g1)/eps))
      )
}
eps  <- 0.001
x    <- seq(from = 0, to = 1, length = 100)
yini <- c(g = -1, g1 = NA, f = 0, f1 = 0, f2 = NA, f3 = NA)
yend <- c(1, NA, 0, 0, NA, NA)
Soltwp <- bvptwp(x = x, func = swirl, order = c(2, 4),
                 par = eps, yini = yini, yend = yend)

pairs(Soltwp, main = "swirling flow III, eps=0.001")


diagnostics(Soltwp)
```

```
--------------------
solved with  bvptwp
--------------------
  Integration was successful.

  1 The return code                               : 0
  2 The number of function evaluations            : 28507
  3 The number of jacobian evaluations            : 3179
  4 The number of boundary evaluations            : 84
  5 The number of boundary jacobian evaluations   : 66
  6 The number of steps                           : 18
  7 The number of mesh resets                     : 1
  8 The maximal number of mesh points             : 1000
  9 The actual number of mesh points              : 199
 10 The size of the real work array               : 280660
 11 The size of the integer work array            : 14018


--------------------
conditioning pars
--------------------

  1 kappa1  : 12601.34
  2 gamma1  : 818.5373
  3 sigma   : 36.8086
  4 kappa   : 13175.8
  5 kappa2  : 574.46
```

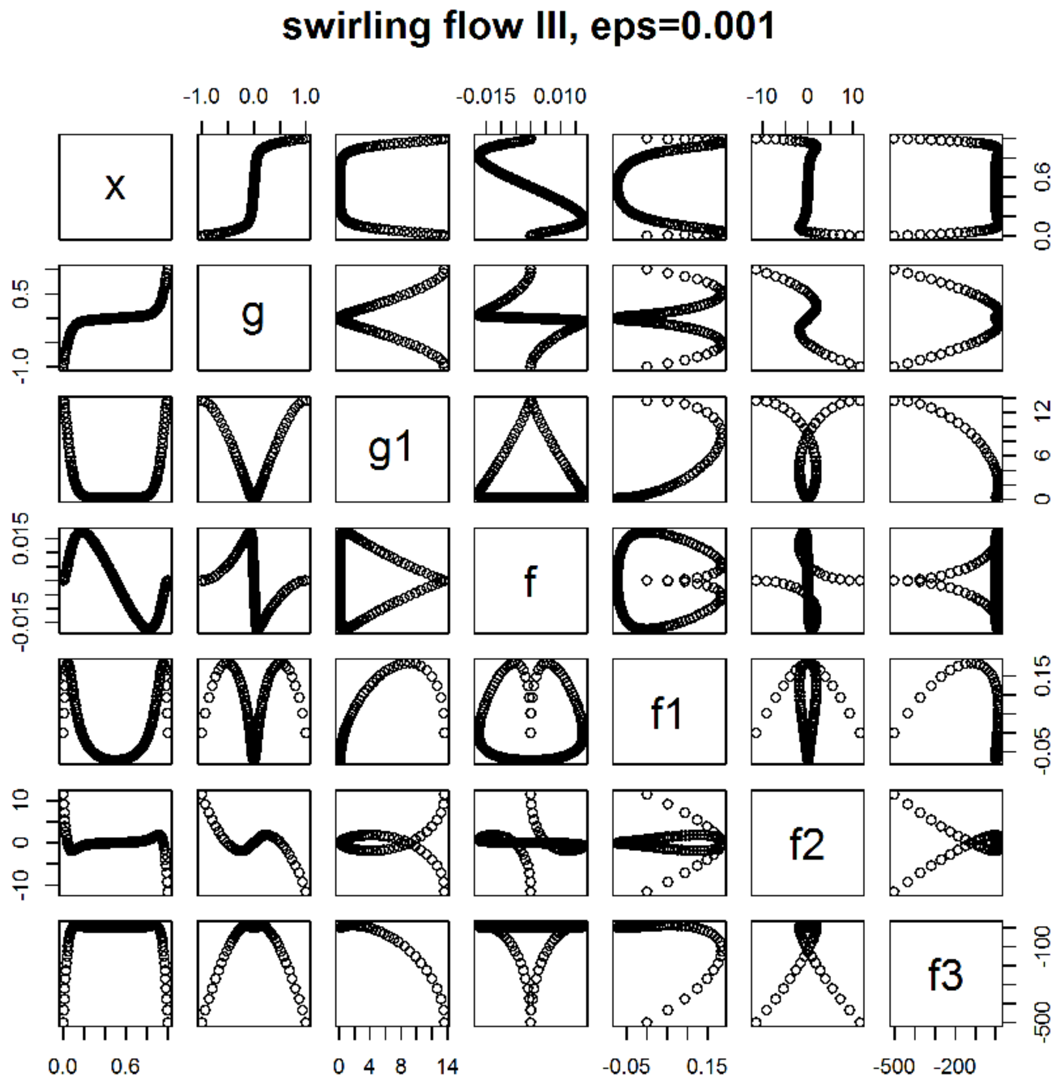

Figure 2: The swirling flow III problem. See book for explanation.

3. Complex Initial or End Conditions

```
musn <- function(x, Y, pars) {
  with (as.list(Y),  {
    du <- 0.5 * u * (w - u) / v
    dv <- -0.5 * (w - u)
    dw <- (0.9 - 1000 * (w - y) - 0.5 * w * (w - u))/z
    dz <- 0.5 * (w - u)
    dy <- -100 * (y - w)
    return(list(c(du, dv, dw, dz, dy)))
  })
}
bound <- function(i, Y, pars) {
  with (as.list(Y), {
    if (i == 1) return (u - 1)
    if (i == 2) return (v - 1)
    if (i == 3) return (w - 1)
    if (i == 4) return (z + 10)
    if (i == 5) return (w - y)
 })
}
xguess <- seq(0, 1, length.out = 5)
yguess <- matrix(ncol = 5,
                data = (rep(c(1, 1, 1, -10, 0.91), 5)))
rownames(yguess) <- c("u", "v", "w", "z", "y")
xguess
```

```
[1] 0.00 0.25 0.50 0.75 1.00
```

```
yguess
```

```
    [,1]   [,2]   [,3]   [,4]   [,5]
u   1.00   1.00   1.00   1.00   1.00
v   1.00   1.00   1.00   1.00   1.00
w   1.00   1.00   1.00   1.00   1.00
z -10.00 -10.00 -10.00 -10.00 -10.00
y   0.91   0.91   0.91   0.91   0.91
```

```
Sol <- bvptwp(x = x, func = musn, bound = bound,
              xguess = xguess, yguess = yguess,
              leftbc = 4, atol = 1e-10)
yguess <- matrix(ncol = 5, data = (rep(c(1,1,1, 10, 0.91), 5)))
rownames(yguess) <- c("u", "v", "w", "z", "y")
Sol2<- bvpcol(x = x, func = musn, bound = bound,
              xguess = xguess, yguess = yguess,
              leftbc = 4, atol = 1e-10)
```

```
plot(Sol, Sol2, which = "y", lwd = 2)
```

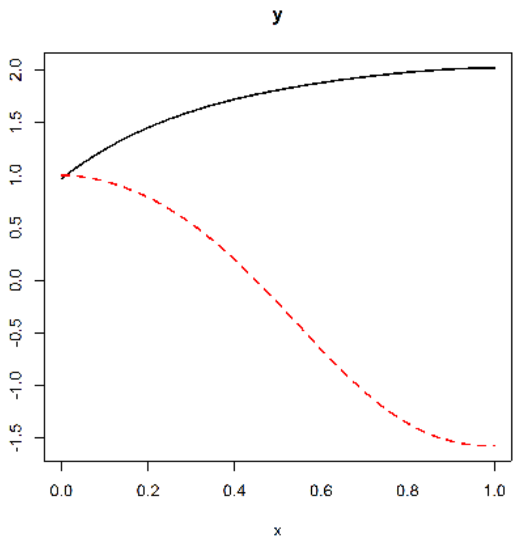

Figure 3: The musn problem. See book for explanation.

4. Solving a Boundary Value Problem using Continuation

```
Prob19 <- function(x, y, eps) {
  pix = pi*x
  list(c(y[2],
      (pi/2*sin(pix/2)*exp(2*y[1])-exp(y[1])*y[2])/eps))
}
x <- seq(0, 1, by = 0.01)
eps <- 1e-2
mod1 <- bvptwp(func = Prob19, yini = c(0, NA), yend = c(0, NA),
               x = x,           par = eps)
diagnostics(mod1)
```

```
--------------------
solved with  bvptwp
--------------------
  Integration was successful.

  1 The return code                                 : 0
  2 The number of function evaluations              : 18057
  3 The number of jacobian evaluations              : 3091
  4 The number of boundary evaluations              : 40
  5 The number of boundary jacobian evaluations     : 26
  6 The number of steps                             : 29
  7 The number of mesh resets                       : 1
  8 The maximal number of mesh points               : 1000
  9 The actual number of mesh points                : 150
 10 The size of the real work array                 : 56108
 11 The size of the integer work array              : 6006


--------------------
conditioning pars
--------------------

  1 kappa1  : 125.6703
  2 gamma1  : 2.236132
  3 sigma   : 93.77898
  4 kappa   : 168.431
  5 kappa2  : 42.7607
```

```
plot(mod1,  lwd = 2)
```

```
xguess <- mod1[,1]
yguess <- t(mod1[,2:3])
```

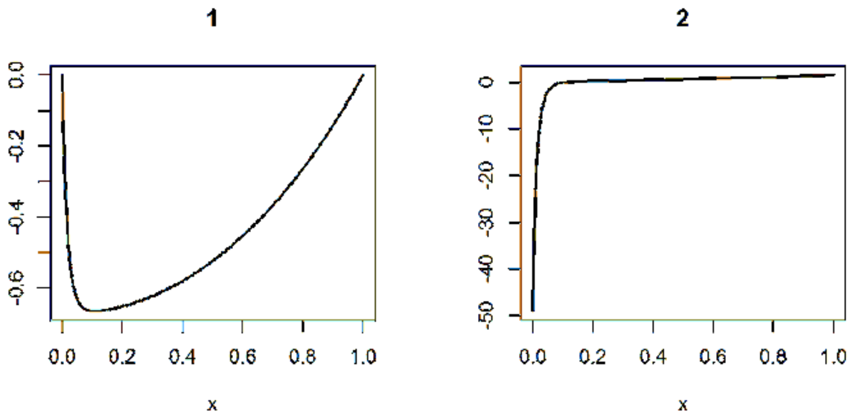

Figure 4: Solution of the test problem 19. See book for explanation.

```
eps <- 1e-3
mod2 <- bvpcol(func = Prob19, yini = c(0, NA), yend = c(0, NA),
               x = x, par = eps,
               xguess = xguess, yguess = yguess)
eps <- 1e-7
mod2 <- bvpcol(func = Prob19, yini = c(0, NA), yend = c(0, NA),
               x = x, par = eps, eps = eps, atol = 1e-4)
diagnostics(mod2)
```

```
--------------------
solved with  bvpcol
--------------------
  Integration was successful.

  1 The return code                                   : 1
  2 The number of function evaluations                : 22749
  3 The number of jacobian evaluations                : 4568
  4 The number of boundary evaluations                : 172
  5 The number of boundary jacobian evaluations       : 96
  6 The number of continuation steps                  : 10
  7 The number of succesfull continuation steps       : 10
  8 The actual number of mesh points                  : 50
  9 The number of collocation points per subinterval  : 4
 10 The number of equations                           : 2
 11 The number of components (variables)              : 2

    The problem was solved for final eps equal to     : 1e-07
```

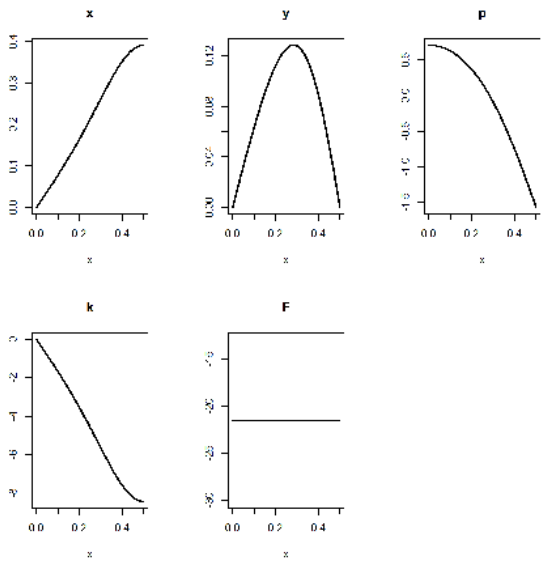

Figure 5: Solution of the elastica problem. See book for explanation.

5. BVP with Unknown Constants

5.1. Elastica Problem

```
Elastica <- function (x, y, pars) {
  list( c(cos(y[3]),
          sin(y[3]),
          y[4],
          y[5] * cos(y[3]),
          0))
}
bvpsol <- bvpcol(func = Elastica,
      yini = c(x = 0,  y = 0, p = NA,    k = 0,  F = NA),
      yend = c(x = NA, y = 0, p = -pi/2, k = NA, F = NA),
      x = seq(from = 0, to = 0.5, by = 0.01))
bvpsol[1,"F"]
```

```
        F
-21.54909
```

```
plot(bvpsol, lwd = 2)
```

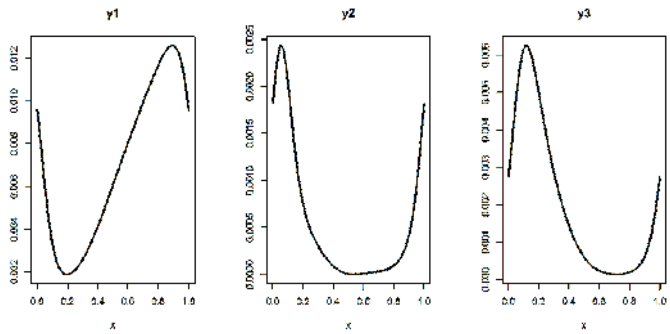

Figure 6: The measel problem. See book for explanation

5.2. Non-separated Boundary Conditions

```
measel <- function(t, y, pars)  {
  bet <- 1575 * (1 + cos(2 * pi * t))
  dy1 <- mu - bet * y[1] * y[3]
  dy2 <- bet * y[1] * y[3] - y[2] / lam
  dy3 <- y[2] / lam - y[3] / eta
  dy4 <- 0
  dy5 <- 0
  dy6 <- 0
  list(c(dy1, dy2, dy3, dy4, dy5, dy6))
}
bound <- function(i, y, pars) {
  if ( i == 1 | i == 4) return( y[1] - y[4])
  if ( i == 2 | i == 5) return( y[2] - y[5])
  if ( i == 3 | i == 6) return( y[3] - y[6])
}
mu  <- 0.02 ; lam <- 0.0279 ; eta <- 0.1
x <- seq(from = 0, to = 1, by = 0.01)
Sola <- bvpshoot(func = measel, bound = bound,
    x = x, leftbc = 3, atol = 1e-12, rtol = 1e-12,
    guess = c(y1 = 1, y2 = 1, y3 = 1, y4 = 1, y5 = 1, y6 = 1))
yguess <- matrix(ncol = length(x), nrow = 6, data = 1)
rownames(yguess) <- paste("y", 1:6, sep="")
Sol  <- bvptwp  (func = measel, bound = bound,
          x = x, leftbc = 3, xguess = x, yguess = yguess)
max(abs(Sol[1,-1] - Sol[nrow(Sol),-1]))
```

```
[1] 0
```

```
plot(Sol, lwd = 2, which = 1:3, mfrow = c(1, 3))
```

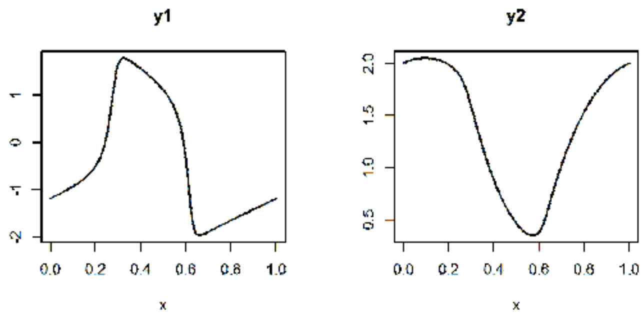

Figure 7: The nerve impulse problem. See book for explanation.

5.3. Unknown Integration Interval

```
nerve <- function (x, y, p)
  list(c(3 * y[3] * (y[1] + y[2] - 1/3 * (y[1]^3) -1.3),
        (-1/3) * y[3] * (y[1] - 0.7 + 0.8 * y[2]) ,
        0,
        0,
        0)
  )
bound <- function(i, y, p) {
 if (i ==1) return (-y[3]* (y[1] - 0.7 + 0.8*y[2])/3 -1)
 if (i ==2) return (y[1] - y[4] )
 if (i ==3) return (y[2] - y[5] )
 if (i ==4) return (y[1] - y[4] )
 if (i ==5) return (y[2] - y[5] )
}
xguess <- seq(0, 1, by = 0.1)
yguess <- matrix(nrow = 5, ncol = length(xguess), data = 5.)
yguess[1,] <- sin(2 * pi * xguess)
yguess[2,] <- cos(2 * pi * xguess)
rownames(yguess) <- c("y1", "y2", "T", "y1ini", "y2ini")
Sol  <- bvptwp(func = nerve, bound = bound,
              x = seq(0, 1, by = 0.01),leftbc = 3,
              xguess = xguess, yguess = yguess)
Sol[1,]
```

```
       x        y1        y2         T     y1ini     y2ini
0.000000 -1.183453  2.004203 10.710808 -1.183453  2.004203
```

```
plot(Sol, lwd = 2, which = c("y1", "y2"))
```

6. Integral Constraints

```
integro <- function (t, u, p)
  list(c(u[2], -p*exp(u[1]), u[2]))
yini <- c(u1 = 1, u2 = NA, I = 0)
yend <- c(NA, NA, 1)
x    <- seq(from = 0, to = 1, by = 0.01)
out <- bvpcol (yini = yini, yend = yend, func = integro,
               x = x, parms = 0.5)
```

7. Sturm-Liouville Problems

```
Sturm <- function(x, y, p) {
   dy1 <- y[2]
   dy2 <- -y[3] * y[1]
   dy3 <- 0.
   list( c(dy1, dy2, dy3))
}
yini <- c(y = 0, dy = 1,  lambda = NA)
yend <- c(y = 0, dy = NA, lambda = NA)
x    <- seq(from = 0, to = pi,  by = pi/10)
S1 <- bvpshoot(yini = yini, yend = yend, func = Sturm,
               parms = 0, x = x)
(lambda1 <- S1[1, "lambda"])
```

```
lambda
     1
```

```
ana <- function(x, lambda) sin(x*sqrt(lambda))/sqrt(lambda)
max (abs(S1[,2]-ana(S1[,1],lambda1)))
```

```
[1] 8.987562e-08
```

8. A Reaction Transport Problem

```
N    <- 1000
Grid <- setup.grid.1D(N = N, L = 100000)
v <- 1000; D <- 1e7; O2s <- 300;
NH3in <- 500; O2in <- 100; NO3in <- 50
r <- 0.1; k <- 1.; p <- 0.1
Estuary <- function(t, y, parms)  {
 NH3 <- y[1:N]
 NO3 <- y[(N+1):(2*N)]
 O2  <- y[(2*N+1):(3*N)]
 tranNH3<- tran.1D (C = NH3, D = D, v = v,
             C.up = NH3in, C.down = 10,  dx = Grid)$dC
 tranNO3<- tran.1D (C = NO3, D = D, v = v,
             C.up = NO3in,  C.down = 30,  dx = Grid)$dC
 tranO2 <- tran.1D (C = O2 , D = D, v = v,
             C.up = O2in, C.down = 250, dx = Grid)$dC

 reaeration <- p * (O2s - O2)
 r_nit      <- r * O2 / (O2 + k) * NH3

 dNH3    <- tranNH3 - r_nit
 dNO3    <- tranNO3 + r_nit
 dO2     <- tranO2  - 2 * r_nit + reaeration

 list(c(  dNH3, dNO3, dO2 ))
}
print(system.time(
std <- steady.1D(y = runif(3 * N), parms = NULL,
             names=c("NH3", "NO3", "O2"),
             func = Estuary, dimens = N,
             positive = TRUE)
))

  user  system elapsed
  0.12    0.00    0.12

NH3in <- 100
std2 <- steady.1D(y = runif(3 * N), parms = NULL,
             names=c("NH3", "NO3", "O2"),
             func = Estuary, dimens = N,
             positive = TRUE)

plot(std, std2, grid = Grid$x.mid, ylab = "mmol/m3",
     xlab = "m", mfrow = c(1,3), col = "black")
legend("bottomright", lty = 1:2, title = "NH3in",
      legend = c(500, 100))
```

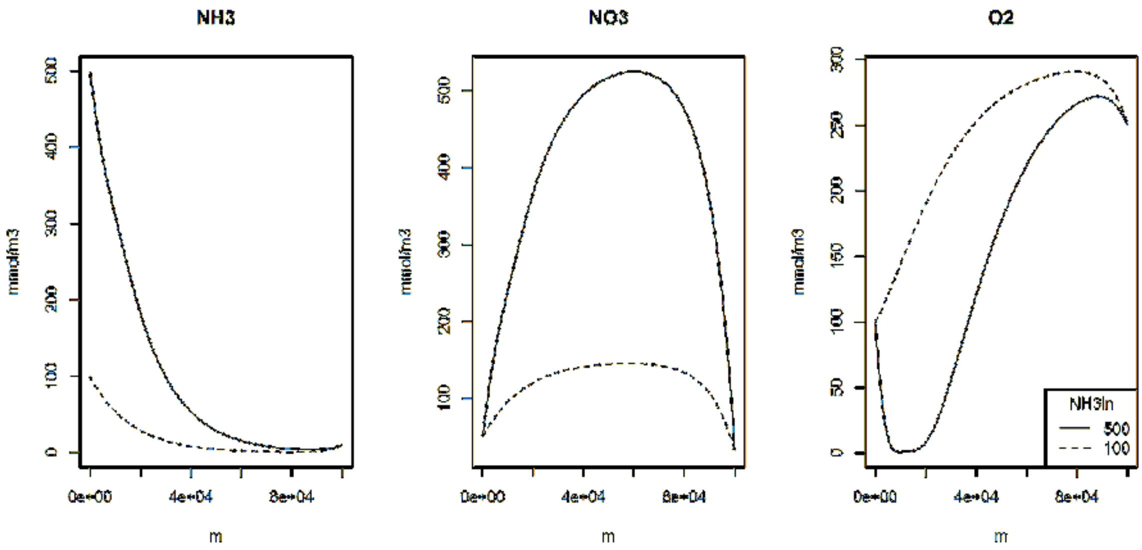

Figure 8: The estuarine problem. See book for explanation.

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