

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.
UseR series, Springer, 248 pp.
www.springer.com/statistics/computational+statistics/book/978-3-642-28069-6
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

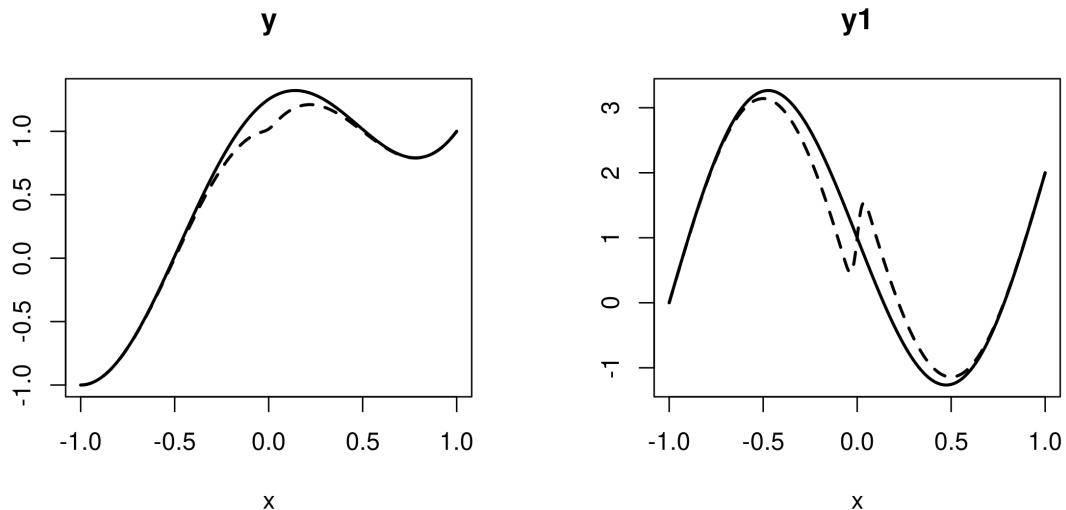


Figure 1: Solution of the test problem 7. See book for more information.

```
[2,] -0.99 -0.9994887 0.100558398
[3,] -0.98 -0.9979891 0.199338166
```

```
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

```

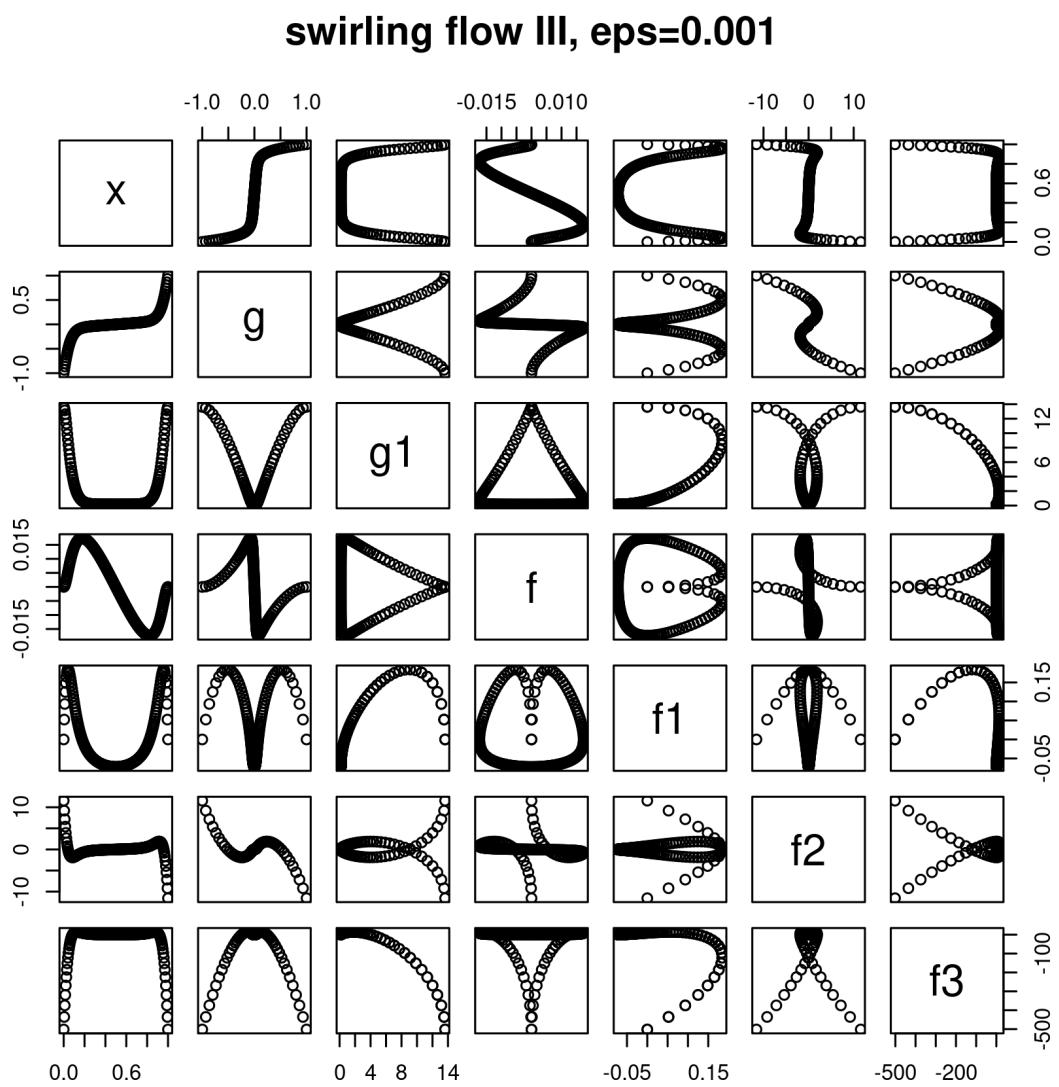


Figure 2: The swirling flow III problem. See book for explanation.

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)

```

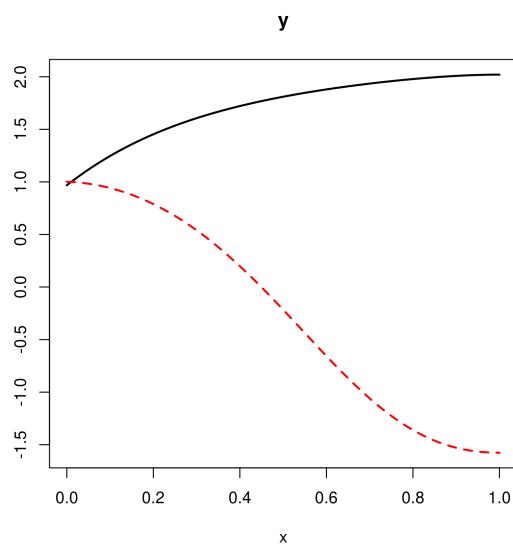


Figure 3: The musn problem. See book for explanation.

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   : 125.6702
  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])

```

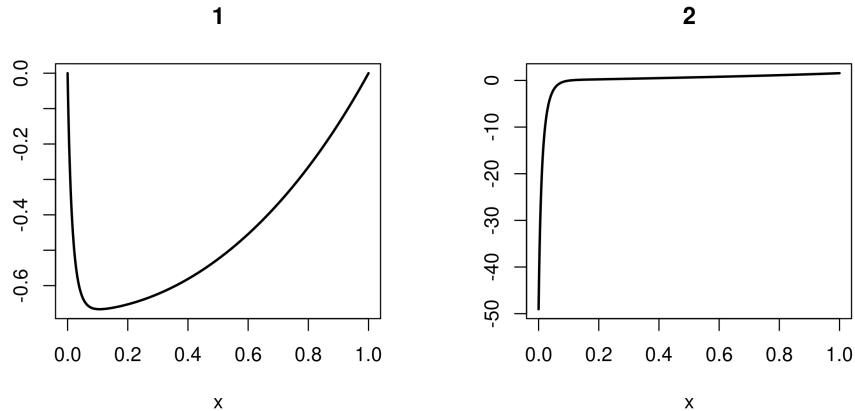


Figure 4: Solution of the test problem 19. See book for explanation.

```

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 : 22537
  3 The number of jacobian evaluations : 4568
  4 The number of boundary evaluations : 170
  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

```

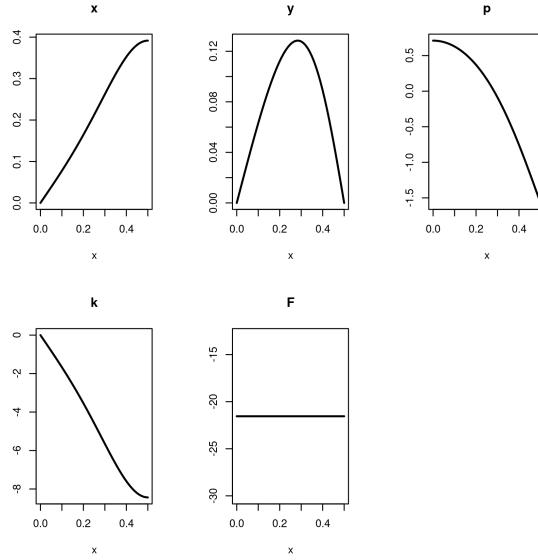


Figure 5: Solution of the elastica problem. See book for explanation.

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)
```

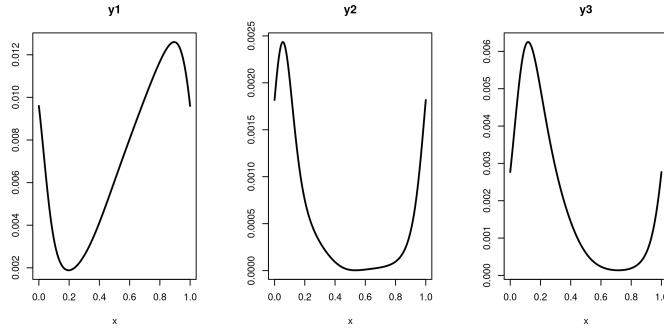


Figure 6: The measles problem. See book for explanation

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))

```

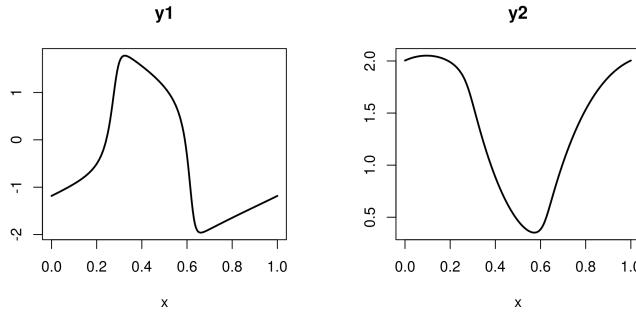


Figure 7: The nerve impulse problem. See book for explanation.

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
0.0000000 -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] 8.987612e-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
0.099   0.028   0.127

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))

```

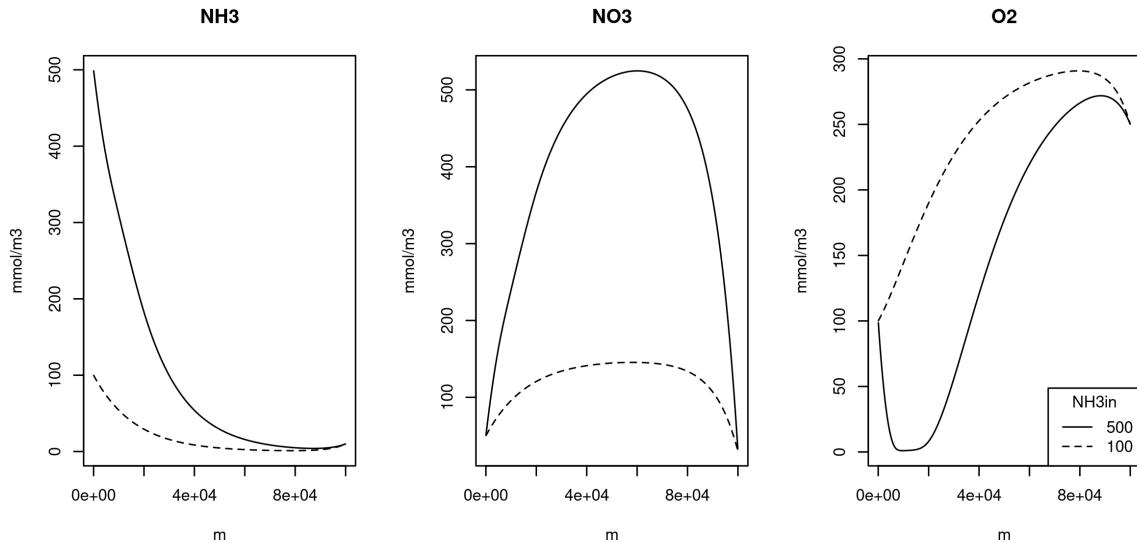


Figure 8: The estuarine problem. See book for explanation.

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