# The FESDIA package - early diagenetic modelling of the C, N, P, Fe and S cycle

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## FESDIA

```
require(FESDIA)
```

The FESDIA package contains functions to generate diagenetic profiles, describing the cycles of C, N, O2, Fe, S and P. It is based on the OMEXDIA model (Soetaert et al., 1996a, b), extended with P, S, Fe dynamics.

The model describes seventeen state variables, in 100 layers:

- 2 fractions of organic carbon (FDET,SDET): fast and slow decaying, solid substance.
- Oxygen (O2), dissolved substance.
- Nitrate (NO3), dissolved substance.
- Nitrite (NO2), dissolved substance.
- Ammonia (NH3), dissolved substance.
- Dissolved inorganic carbon (DIC), dissolved substance
- Iron 2+ (Fe), dissolved substance
- Sulphide (H2S), dissolved substance
- Methane (CH4), dissolved substance
- Phosphate (PO4), dissolved substance
- Alkalinity (ALK), dissolved substance
- Iron hydroxides (FeOH3), solid substance
- Iron-bound P (FeP), P bound to iron oxides, solid substance
- Ca-bound P (CaP), apatite, solid substance
- Adsorbed P (Pads), solid substance

Time is expressed in days, and space is expressed in centimeters.

Concentrations of liquids and solids are expressed in [nmol/cm3 liquid] and [nmol/cm3 solid] respectively (Note: this is the same as [mmol/m3 liquid] and [mmol/m3 solid]).

Compared to the OMEXDIA model, FESDIA includes the following additions:

- simple phosphorus, iron and sulphur dynamics
- long-distance H2S and CH4 oxidation, e.g. by cable bacteria or worms associated with chemosynthetic bacteria
- allowing boundary conditions with water overlying sediment or exposure to the air.
- external conditions set either with time-variable forcings or as constant parameters
- bottom water conditions either imposed or dynamically modeled
- possibility to include sediment perturbation events
- vertical profiles of porosity, irrigation, bioturbation either set with parameters or inputted as data.

The model is implemented in fortran (for speed) and linked to R (for flexibility).

# The package

The FESDIA package contains functions to generate (a time series of) 1-D diagenetic profiles. It can either be run in dynamic mode, or the steady-state solution can be estimated. It contains several utility functions, e.g. to help in extracting information on the model output, or to estimate mass budgets. It contains functions to perturb sediment properties, e.g. mimicking resuspension or deposition events.

The main functions allow to solve the model to steady state (*FESDIAsolve*), to run it dynamically (*FESDIAdyna*), or to add perturbations (*FESDIAperturb*) to dynamic simulations (this is discussed in another vignette)..

## Steady-state solution, function FESDIAsolve

Function *FESDIAsolve* finds the steady-state solution of the FESDIA model. Its arguments are:

```
args(FESDIAsolve)
```

```
function (parms = list(), yini = NULL, gridtype = 1, Grid = NULL,
    porosity = NULL, bioturbation = NULL, irrigation = NULL,
    surface = NULL, diffusionfactor = NULL, dynamicbottomwater = FALSE,
    ratefactor = NULL, calcpH = FALSE, verbose = FALSE, method = NULL,
    times = c(0, 1e+06), ...)
NULL
```

here *parms* is a list with a subset of the FESDIA parameters (see appendix for what they mean and their default values). If unspecified, then the default parameters are used.

The *gridtype* by default assumes a cartesian grid (*gridtype = 1*), but can be 1D cylindrical (*gridtype = 2*) or spherical (*gridtype = 3*). An irregular grid can be seleceted by specifying the surface areas at the interface through argument *surface*. In a cartesian grid the surface area remains constant.

The vertical profiles that can be imposed as a vector are: *porosity*, *bioturbation irrigation*, *surface* (surface areas of box interfaces) and *diffusionfactor* (multiplication factor to estimate effective sediment diffusion based on molecular diffusion).

*dynamicbottomwater*, when set to TRUE will also explicitly model the bottom water concentrations.

*ratefac* is a multiplication factor, that is multiplied with all biogeochemical rates. It is included here for consistency with *FESDIAdyna*.

## Dynamic run, function FESDIAdyna

Function *FESDIAdyna* runs the FESDIA model for a specific time interval and produces output at requested times. Its arguments are:

```
args(FESDIAdyna)
```

```
function (parms = list(), times = 0:365, spinup = NULL, yini = NULL,
    gridtype = 1, Grid = NULL, porosity = NULL, bioturbation = NULL,
    irrigation = NULL, surface = NULL, diffusionfactor = NULL,
    dynamicbottomwater = FALSE, CfluxForc = NULL, FeOH3fluxForc = NULL,
    CaPfluxForc = NULL, O2bwForc = NULL, NO3bwForc = NULL, NO2bwForc = NULL,
    NH3bwForc = NULL, FebwForc = NULL, H2SbwForc = NULL, SO4bwForc = NULL,
    CH4bwForc = NULL, PO4bwForc = NULL, DICbwForc = NULL, ALKbwForc = NULL,
    wForc = NULL, biotForc = NULL, irrForc = NULL, rFastForc = NULL,
    rSlowForc = NULL, pFastForc = NULL, MPBprodForc = NULL, gasfluxForc = NULL,
    HwaterForc = NULL, ratefactor = NULL, calcpH = FALSE, verbose = FALSE,
    ...)
NULL
```

The functions to run the model dynamically also allow for several external conditions to be either constants or to vary in time. Thus, they can be set by a parameter or as a forcing function.

These conditions are:

- the flux of carbon, CaP and FeP (*Cflux, CaPflux, FeOH3flux*), forcings *CfluxForc, CaPfluxForc, FeOH3fluxForc*),

- the bottom water concentrations (*O2bw, NO2bw, NO3bw, NH3bw, H2Sbw, PO4bw, DICbw, ALKbw*), forcings *O2bwForc, NO3bwForc, NO2bwForc, NH3bwForc, ODUbwForc, PO4bwForc, DICbwForc, ALKbwForc*)
- the sedimentation, bioturbation and bio-irrigation rates (*w, biot, irr*), (*wForc, biotForc, irrForc*)
- the decay rates of organic matter (*rFast, rSlow*) and the fraction fast organic matter present in the flux (*pFast*), forcings (*rFastForc, rSlowForc, pFastForc*)
- the microphytobenthos production rate (*MPBprod*), (*MPBprodForc*)
- the air-sea exchange rate when exposed to the air (*gasflux*), (*gasfluxForc*)
- the height of the overlying water (*Hwater*), (*HwaterForc*), used only if *dynamicbottomwater* is *TRUE*.
- *ratefac* is a (time series or a constant) multiplication factor, that is multiplied with all biogeochemical rates. It can be used to impose temperature dependency.

These forcing functions are either prescribed as a list that either contains a data series (*list (data = ...)*) or as a list that specifies a periodic signal, defined by the amplitude (*amp*), *period*, *phase*, a coefficient that defines the strength of the periodic signal (*power*) and the minimum value (*min*) : the default settings are: *list(amp = 0, period = 365, phase = 0, pow = 1, min = 0)*. The mean value in the sine function is given by the corresponding parameter.

For instance, for the C flux, the seasonal signal would be defined as: $max(min, Cflux*(1+(amp*sin((times-phase)/period*2*pi))^pow)$.

## Perturbation run, function FESDIAperturb

```
args(FESDIAperturb)
```

```
function (parms = list(), times = 0:365, spinup = NULL, yini = NULL,
    gridtype = 1, Grid = NULL, porosity = NULL, bioturbation = NULL,
    irrigation = NULL, surface = NULL, diffusionfactor = NULL,
    dynamicbottomwater = FALSE, perturbType = "mix", perturbTimes = seq(from = 0,
        to = max(times), by = 365), perturbDepth = 5, concfac = 1,
    CfluxForc = NULL, FeOH3fluxForc = NULL, CaPfluxForc = NULL,
    O2bwForc = NULL, NO3bwForc = NULL, NO2bwForc = NULL, NH3bwForc = NULL,
    FebwForc = NULL, H2SbwForc = NULL, SO4bwForc = NULL, CH4bwForc = NULL,
    PO4bwForc = NULL, DICbwForc = NULL, ALKbwForc = NULL, wForc = NULL,
    biotForc = NULL, irrForc = NULL, rFastForc = NULL, rSlowForc = NULL,
    pFastForc = NULL, MPBprodForc = NULL, gasfluxForc = NULL,
    HwaterForc = NULL, ratefactor = NULL, verbose = FALSE, ...)
NULL
```

Three types of perturbations are possible (argument *perturb*):

- *mixing* straightens the profiles over a certain depth
- *erosion* removes part of the surficial sediment
- *deposition* adds sediment on top.

These perturbations are implemented as events, and need input of the perturbation times (*perturbTimes*), and the depth (*perturbDepth*). For deposition events, the factor of increase/decrease of the solid fraction concentrtion can also be inputted (*concfac*).

## Accessory functions

The default values of the parameters, and their units can be interrogated:

```
P  <- FESDIAparms()
head(P)
```

```
##                  parms       units                description
## Cflux     4.566210e+02 nmolC/cm2/d total organic C deposition
## pFast     9.000000e-01           -   part FDET in carbon flux
## FeOH3flux 1.000000e+00  nmol/cm2/d   deposition rate of FeOH3
## CaPflux   0.000000e+00  nmol/cm2/d     deposition rate of CaP
## rFast     6.849315e-02          /d            decay rate FDET
## rSlow     1.369863e-04          /d            decay rate SDET
```

Note: some parameters only apply if the bottom water concentration is modeled dynamically; they comprise the *dilution* of the bottom water (nudging to bottom water concentration), the height of the bottom water (*Hwater*), and the sinking rate of the solid constituents (C, FeP, FeOH3) (parameters *Cfall*, *FePfall* and *FeOH3fall*).

## Budgets

Once the model is solved, it is possible to calculate budgets of the C, N, P, S, Fe and O2 cycle (*FESDIAbudgetC*, *FESDIAbudgetN*, *FESDIAbudgetP*, *FESDIAbudgetS*, *FESDIAbudgetFe*, *FESDIAbudgetO2*).

```
std <- FESDIAsolve()
print(FESDIAbudgetC(std))
```

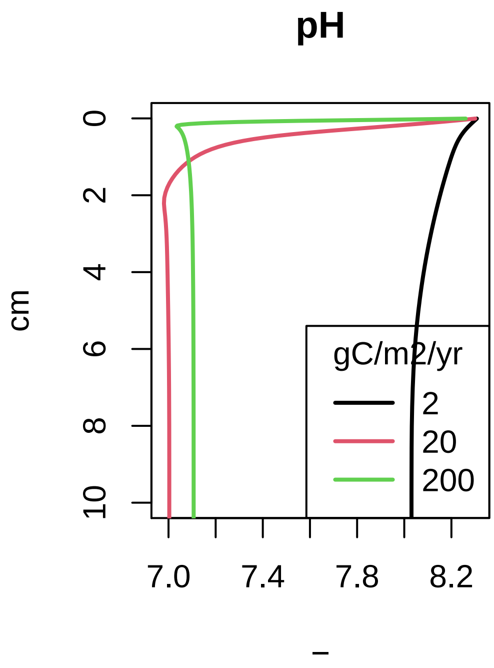
```
## $Fluxes
##                  FDET         SDET           DIC           CH4 CinCaP CaCO3 ARAG        Total
## surface  4.109589e+02 4.566210e+01 -456.61647919 -4.379898e-08      0     0    0 4.525330e-03
## bottom  1.001633e-191 1.168446e-71    0.00452533  8.891745e-30      0     0    0 4.525330e-03
## perturb  0.000000e+00 0.000000e+00    0.00000000  0.000000e+00      0     0    0 0.000000e+00
## netin    4.109589e+02 4.566210e+01 -456.62100452 -4.379898e-08      0     0    0 9.729705e-12
## 
## $Rates
##             OxicMineralisation Denitrification IronReduction SulphateReduction Methanogenesis
## nmolC/cm2/d           426.9966        9.340614     0.7385786          18.91766      0.6275274
##             TotalMineralisation CH4oxidation CH4oxid.dist CH4oxidAOM MPBDICuptake MPBFDETproduction
## nmolC/cm2/d             456.621    0.0169016            0  0.2968621            0                 0
##             MPBResp CaPprecipitation CaPdissolution CaCO3dissolution ARAGdissolution
## nmolC/cm2/d       0                0              0                0               0
##             CaCO3production
## nmolC/cm2/d               0
## 
## $Losses
## [1] 0.00452533
## 
## $dC
##           Ext           DET           DIC           CaP           CH4           MPB         CaCO3
##  4.525373e-03  0.000000e+00  1.358558e-11  0.000000e+00 -4.382230e-08  0.000000e+00  0.000000e+00
##          ARAG        Burial           sum
##  0.000000e+00 -4.525330e-03  1.617803e-14
##
## $Delta
## [1] 9.750213e-12
##
## $Fluxmat
##              Ext     DET         DIC CaP       CH4 MPB CaCO3 ARAG       Burial
## Ext       0.0000 456.621   0.0000000   0 0.0000000   0     0    0 0.000000e+00
## DET       0.0000   0.000 456.3072408   0 0.3137637   0     0    0 1.168446e-71
## DIC     456.6165   0.000   0.0000000   0 0.0000000   0     0    0 4.525330e-03
## CaP       0.0000   0.000   0.0000000   0 0.0000000   0     0    0 0.000000e+00
## CH4       0.0000   0.000   0.3137637   0 0.0000000   0     0    0 0.000000e+00
## MPB       0.0000   0.000   0.0000000   0 0.0000000   0     0    0 0.000000e+00
## CaCO3     0.0000   0.000   0.0000000   0 0.0000000   0     0    0 0.000000e+00
## ARAG      0.0000   0.000   0.0000000   0 0.0000000   0     0    0 0.000000e+00
## Burial    0.0000   0.000   0.0000000   0 0.0000000   0     0    0 0.000000e+00
```

## pH calculation

pH can be calculated after the solution has been found, both for steady-state and dynamic runs. Plotting of these pH profiles has to be done with the default plotting functions.

### Steady-state pH profile

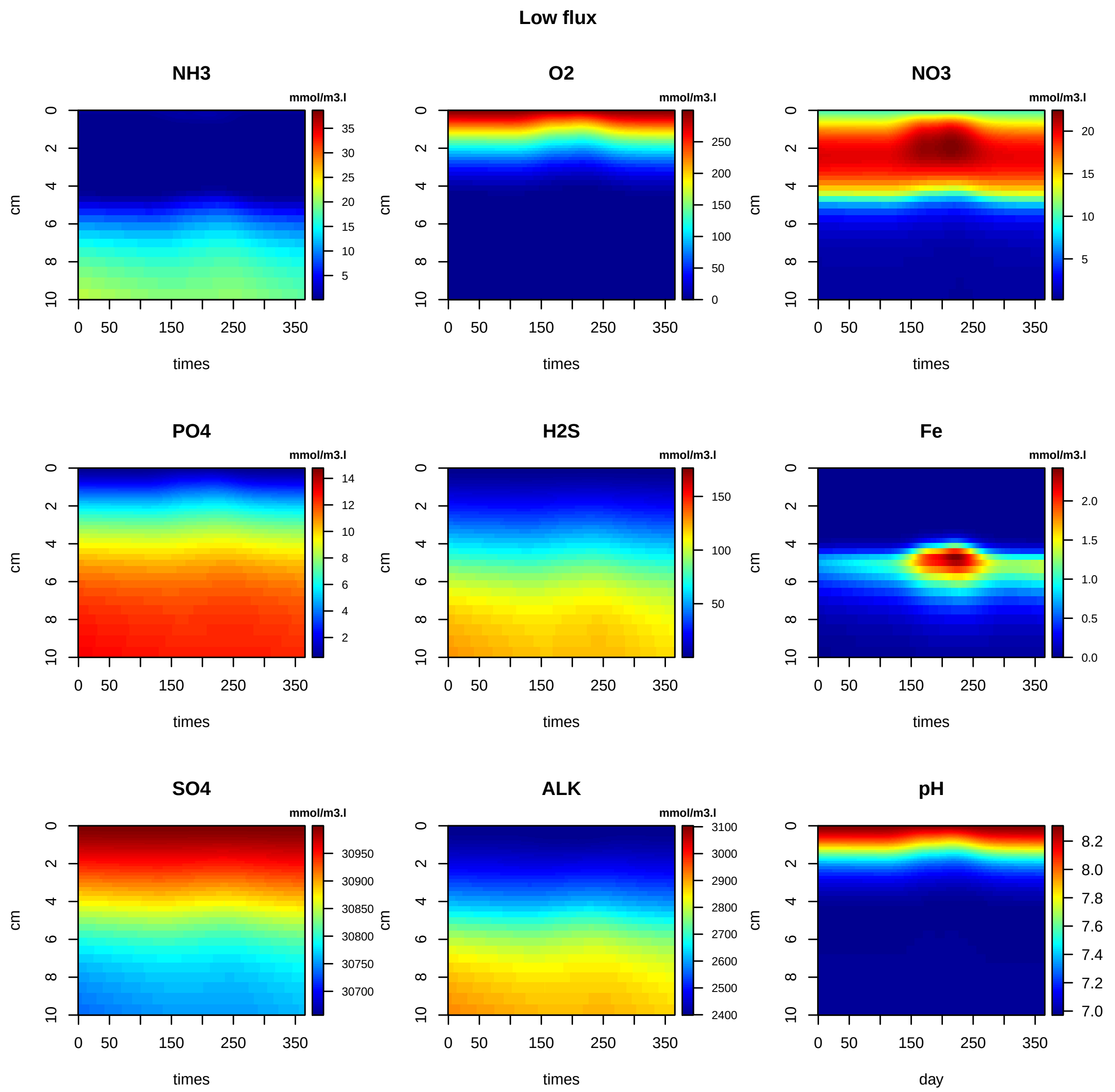
```
std  <- FESDIAsolve(parms = list(Cflux = 2*1e5/12/365))
std2 <- FESDIAsolve(parms = list(Cflux = 20*1e5/12/365))
std3 <- FESDIAsolve(parms = list(Cflux = 200*1e5/12/365))
pH  <- FESDIApH(std)
pH2 <- FESDIApH(std2)
pH3 <- FESDIApH(std3)
matplot(x = cbind(pH, pH2, pH3), y = FESDIAdepth(std), ylim = c(10,0),
  main = "pH", ylab= "cm", type = "l", xlab = "-", lwd = 2, lty = 1)
legend("bottomright", legend = c(2,20,200), title = "gC/m2/yr",
  lty=1, col = 1:3, lwd = 2)
```



### Dynamic pH solutions

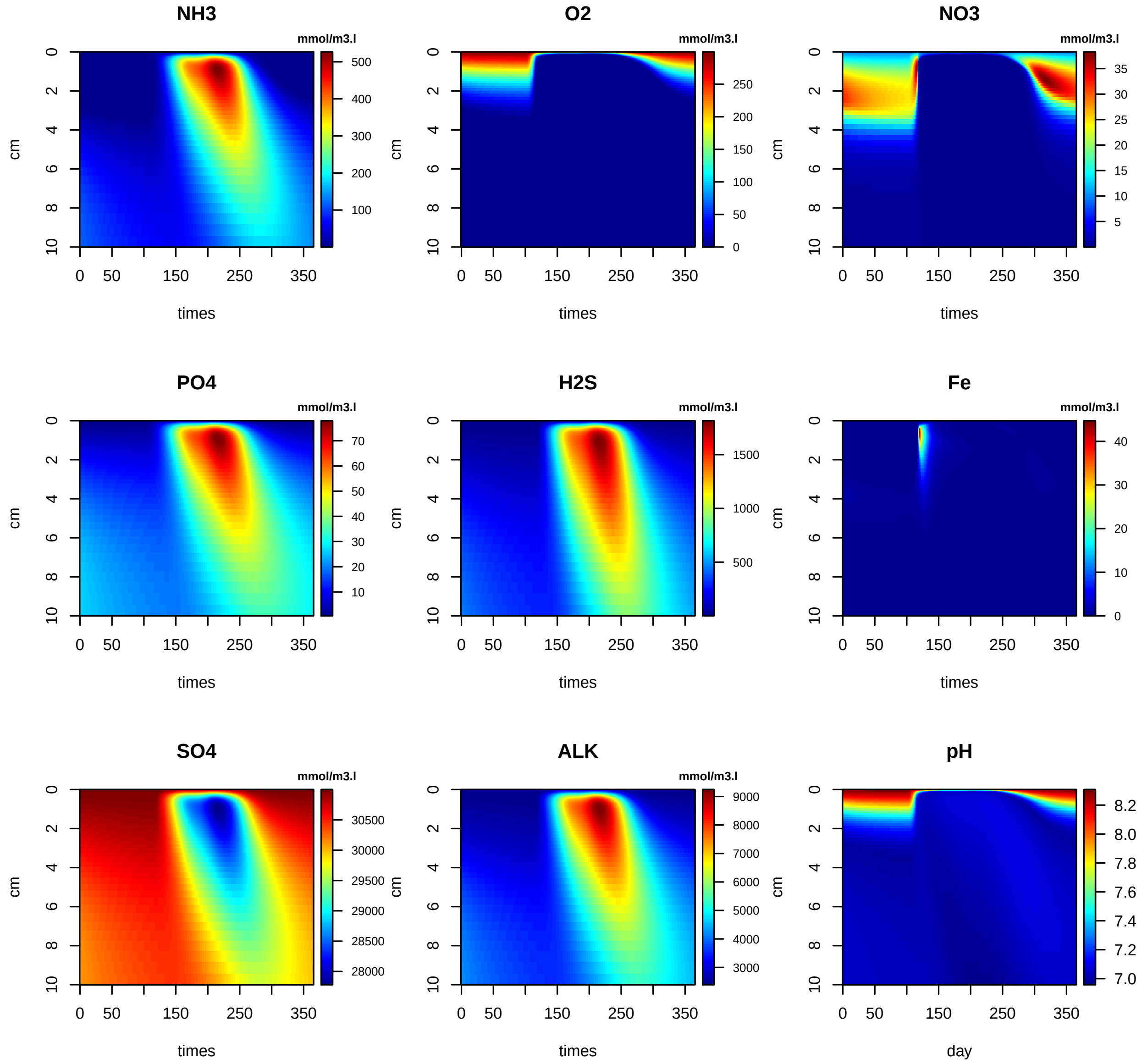
```
Cflux2 <- cbind (time = c(0, 100,  150,  175, 200, 250, 365),
                flux = c(1, 1,    1000, 800, 1200, 10, 1))
Cflux1 <- Cflux3 <- Cflux2
Cflux1[,2] <- Cflux1[,2]/10
Cflux3[,2] <- Cflux3[,2]*10

out1 <- FESDIAdyna(parms = list(pFast = 0.9), CfluxForc = list(data = Cflux1),
                   spinup = 0:365, times = 0:365)
out2 <- FESDIAdyna(parms = list(pFast = 0.9), CfluxForc = list(data = Cflux2),
                   spinup = 0:365,  times = 0:365)
out3 <- FESDIAdyna(parms = list(pFast = 0.9), CfluxForc = list(data = Cflux3),
                   spinup = 0:365, times = 0:365)
pH1 <- FESDIApH(out1)
pH2 <- FESDIApH(out2)
pH3 <- FESDIApH(out3)
```

```
par(oma = c(0,0,2,0))
image2D(out1, ylim = c(10, 0), mfrow = c(3, 3),
    which = c("NH3", "O2", "NO3", "PO4", "H2S", "Fe", "SO4", "ALK"))
image2D(pH1, ylim = c(10,0), y = FESDIAdepth(out1), x = out1[,1],
       clab = "", xlab = "day", ylab = "cm", main = "pH")
title(main = "Low flux", outer = TRUE)
```



```
image2D(out3, ylim = c(10, 0),
  mfrow = c(3, 3), which = c("NH3", "O2", "NO3", "PO4", "H2S", "Fe", "SO4", "ALK"))
plot3D::image2D(pH3, ylim = c(10,0), y = FESDIAdepth(out3), x = out3[,1],
       clab = "", xlab = "day", ylab = "cm", main = "pH")
title(main = "High flux", outer = TRUE)
```

High flux



## Properties of solutions

There are functions to retrieve several properties of the solution:

- *FESDIAdepth*, *FESDIAdx*, *FESDIAgrid* retrieve the sediment depths, layer thicknesses and grid of *FESDIA* model solutions.
- *FESDIAbiot*, *FESDIApor*, *FESDIAirr* retrieve the bioturbation, porosity, and irrigation profiles of *FESDIA* model solutions.
- *FESDIA0D* and *FESDIA1D* return the output variables of the solution as a vector or data.frame. For dynamic runs, the output is averaged over the mean of the run. *FESDIA1D* always returns the sediment depth and the porosity as the first two columns.

```
head(FESDIAdepth(std))
```

```
## [1] 0.00498923 0.01530360 0.02631242 0.03806243 0.05060354 0.06398901
```

```
head(FESDIA1D(std), n = 3)
```

```
##            x       por     FDET     SDET       O2      NO3        NO2       NH3      DIC
## 1 0.00498923 0.8934027 15551.22 18170.32 299.7282 10.02519 0.01554555 0.9979468 2100.445
## 2 0.01530360 0.8801069 14220.97 18018.58 299.1634 10.07880 0.04655839 0.9936467 2101.370
## 3 0.02631242 0.8664113 12992.01 17874.01 298.5584 10.13770 0.07836972 0.9888813 2102.359
##            Fe    FeOH3          H2S   SO4          CH4       PO4      FeP CaP         Pads      ALK
## 1 0.001127354 678365.0 5.606366e-10 31000 5.835650e-13 0.5027497 149502.3   0 3.331114e-86 2399.925
## 2 0.003180364 678339.0 1.717357e-09 31000 1.103246e-12 0.5083401 149503.8   0 3.331114e-86 2399.770
## 3 0.005082877 678315.4 2.946140e-09 31000 1.339171e-12 0.5141716 149505.4   0 3.329544e-86 2399.603
##         TOC DICprodMin DINprodMin DIPprodMin O2prod  Oxicmin Denitrific  Feredmin       BSRmin
## 1 0.5161863   127.3867   19.22818   1.201761      0 126.9661  0.1068066 0.3138317 6.676649e-07
## 2 0.5154750   133.0253   20.07929   1.254956      0 132.5852  0.1121928 0.3279043 6.951890e-07
## 3 0.5148157   137.5823   20.76714   1.297946      0 137.1262  0.1167798 0.3393278 7.166850e-07
##           Methmin   nitri1    nitri2     Anammox    Feoxid      H2Soxid      CH4oxid          AOM
## 1 2.194141e-08 19.89257 0.3098772 0.001551363 0.1013699 8.401930e-11 4.722594e-09 5.427155e-13
## 2 2.284593e-08 19.80673 0.9280657 0.004626260 0.2854346 2.568852e-10 8.911372e-09 1.026019e-12
## 3 2.355235e-08 19.71160 1.5621621 0.007749836 0.4552607 4.397974e-10 1.079516e-08 1.245429e-12
##           FeSprod FePadsorp FePdesorp CaPprod CaPdiss Padsorb H2Soxsurf CH4oxsurf O2distConsump
## 1 6.320357e-16 0.3410478 0.2766567       0       0       0         0         0             0
## 2 5.461819e-15 0.3448269 0.2890763       0       0       0         0         0             0
## 3 1.497487e-14 0.3487705 0.2991607       0       0       0         0         0             0
##     ALKprod    DICprodCH4 MPBCprod MPBuptakeNO3 MPBuptakeNH3 MPBuptakePO4 MPBuptakeDIC
## 1 -19.30096 -6.247567e-09        0            0            0            0            0
## 2 -18.59125 -2.510566e-09        0            0            0            0            0
## 3 -18.00688 -9.797681e-10        0            0            0            0            0
```

```
FESDIAparms(std, which = "Cflux")
```

```
##         parms       units                description
## Cflux 45.6621 nmolC/cm2/d total organic C deposition
```

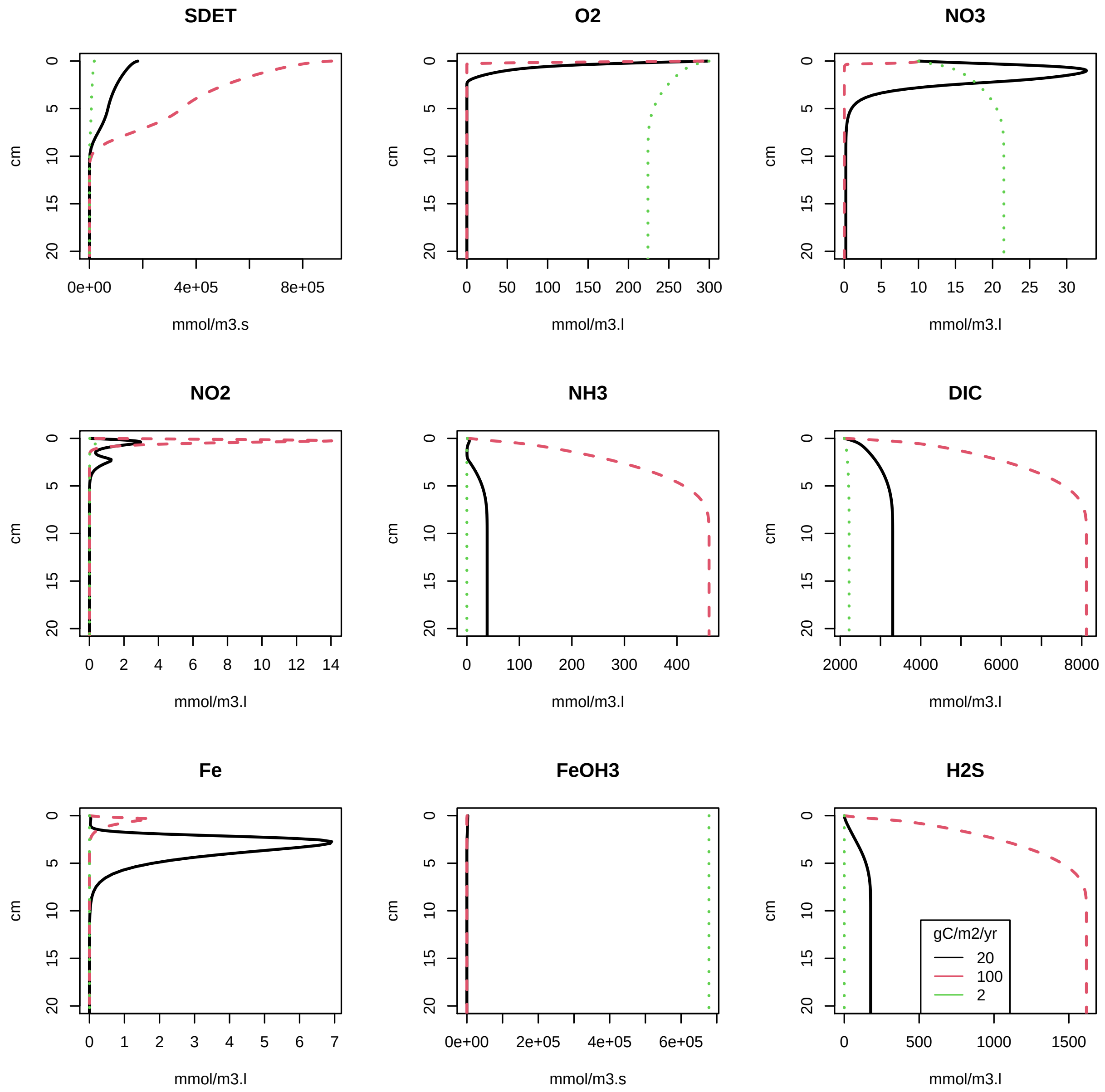
# Steady-state applications

The function *FESDIAsolve* solves for a steady-state condition.

## Simple applications

In the frst example, we run the model for different carbon deposition rates (expressed in *nmolC/cm2/d*) and plot the results using *rootSolve*'s *plot* function.

```
convert <- 1e5/12/365
STD1 <- FESDIAsolve ()
STD2 <- FESDIAsolve (parms = list(Cflux = 100*convert))
STD3 <- FESDIAsolve (parms = list(Cflux = 2*convert))
plot(STD1, STD2, STD3, lwd = 2, which = 2:10)
legend("bottom", legend = c(20, 100, 2), lty = 1, col = 1:3, title = "gC/m2/yr")
```

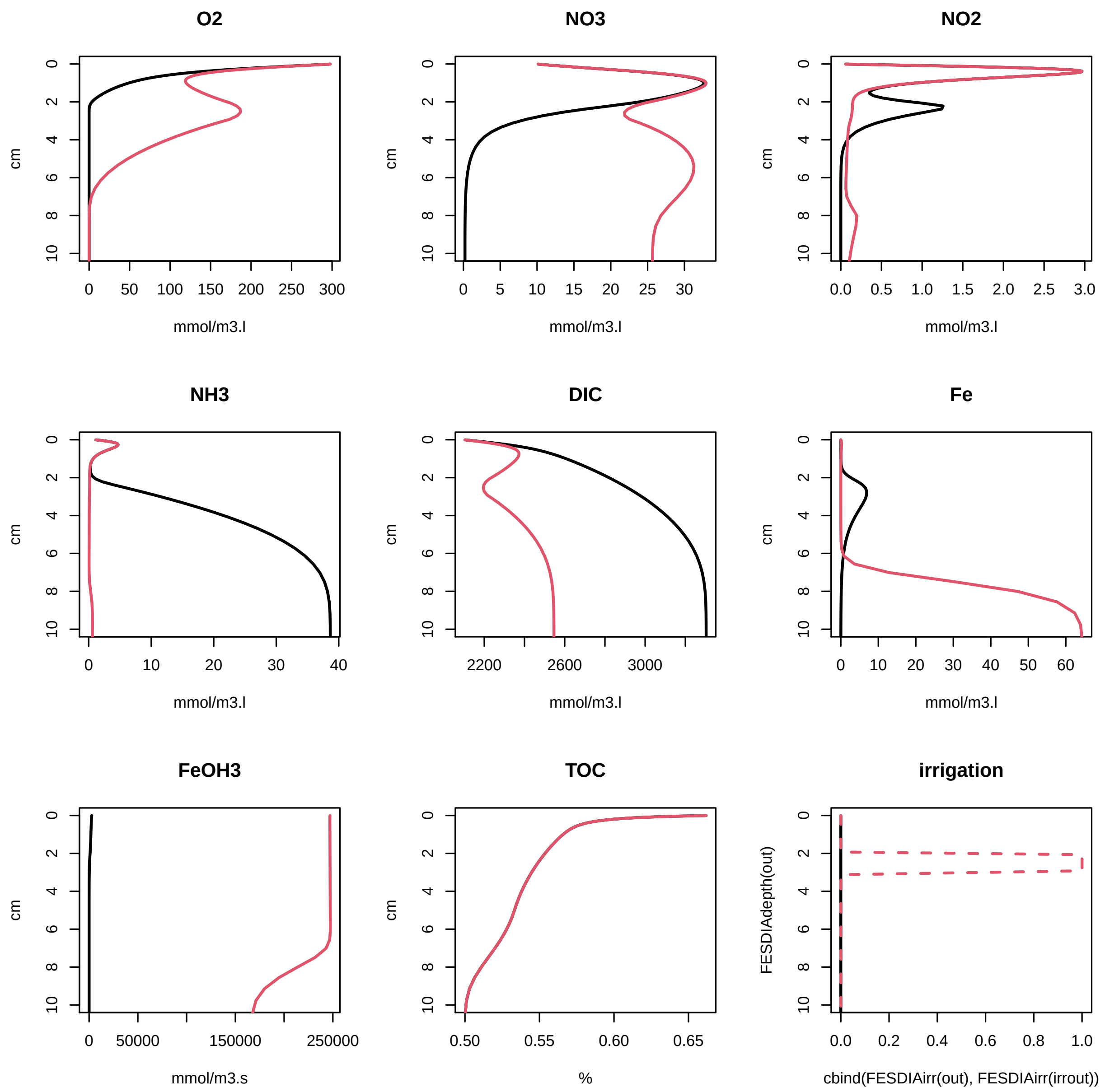


## User-inputted profiles

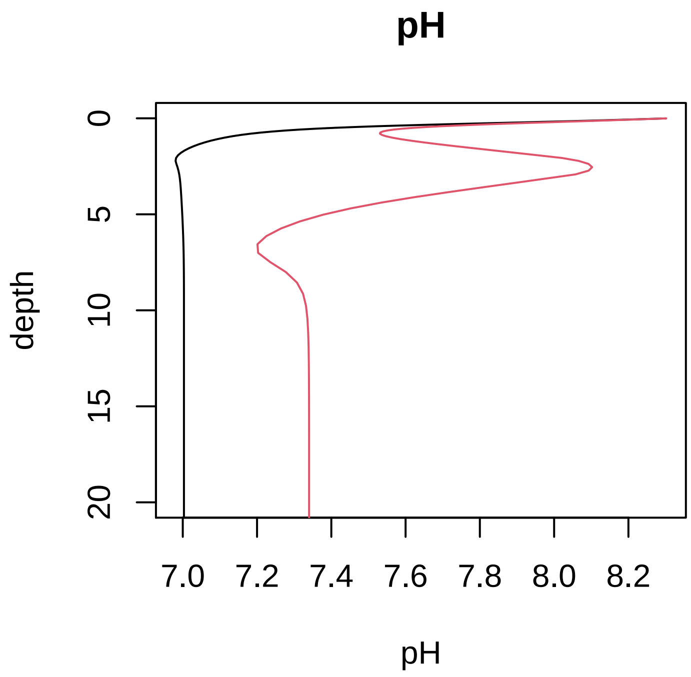
By default porosity, bioturbation, and bio-irrigation profiles are generated based on parameter settings. However, it is possible to directly impose profiles for these quantities.

In the following example, an irrigation profile is generated where there is substantial irrigation only in a certain section of the sediment ([2-3 cm]).

```
Grid <- FESDIAgrid()
Irr <- rep(0, Grid$N)
Irr[Grid$x.mid > 2 &  Grid$x.mid < 3] <- 1
out <- FESDIAsolve()
irrout <- FESDIAsolve(irrigation = Irr)
plot(out, irrout,
     ylim = c(10, 0), lty = 1, lwd = 2, which = c(3:9))
plot(out, irrout,
     ylim = c(10, 0), lty = 1, lwd = 2, which = c("TOC"), mfrow = NULL)
matplot(x=cbind(FESDIAirr(out), FESDIAirr(irrout)), y = FESDIAdepth(out),
     ylim = c(10, 0), type = "l", lty = 1:2, lwd = 2, main = "irrigation")
```



```
pH <- cbind(FESDIApH(out), FESDIApH(irrout))
matplot(x = pH, y = FESDIAdepth(out), ylim = c(20,0),
        type = "l", main = "pH", lty = 1, ylab = "depth")
```



### Microphytobenthos production

MPB is modeled in a straightforward way, by imposing the maximal (unlimited) oxygen production rate (parameter *MPBprod*), an exponential decay parameter (*kMPB*), describing light penetration, and nutrient and DIC limitation, modeled by a Monod equations, with parameters *kNH3upt*, *kPO4upt* and *kDICupt* respectively.

The larger the MPB production rate, the more difficult it becomes to find a solution. Difficult cases can be solved by ramping up the solution, using previous solutions as initial guesses for the next solution.

```
out1 <- FESDIAsolve(parms = c(por0 = 0.5, MPBprod = 0))
out2 <- FESDIAsolve(parms = c(por0 = 0.5, MPBprod = 1e2), yini = out1$y)
out2b <- FESDIAsolve(parms = c(por0 = 0.5, MPBprod = 1e3), yini = out2$y)
out2c <- FESDIAsolve(parms = c(por0 = 0.5, MPBprod = 5e3), yini = out2b$y, method = "mixed")
out2d <- FESDIAsolve(parms = c(por0 = 0.5, MPBprod = 8e3), yini = out2c$y, method = "mixed")
out3 <- FESDIAsolve(parms = c(por0 = 0.5, MPBprod = 1e4), yini = out2d$y, method = "mixed")
out4 <- FESDIAsolve(parms = c(por0 = 0.5, MPBprod = 5e4), yini = out3$y, method = "mixed")
out5 <- FESDIAsolve(parms = c(por0 = 0.5, MPBprod = 1e5), yini = out4$y, method = "mixed")
PH1 <- FESDIApH(out1)
PH2 <- FESDIApH(out2)
PH3 <- FESDIApH(out3)
PH4 <- FESDIApH(out4)
PH5 <- FESDIApH(out5)
```

```
plot(out1, out2, out3, out4, out5,  ylim = c(10, 0),
    lty = 1, lwd = 2, which = c(4,5:7), mfrow = c(2, 3))
legend("center", col = 1:5, title = "prod, mmol/m3/d", legend = c(0, 1e2, 1e4,  5e4, 1e5), lty = 1)
plot(out1, out2, out3, out4, out5, ylim = c(3, 0),
  lty = 1, lwd = 2, which = 3, mfrow = NULL)
```

```r
matplot(x = cbind(PH1, PH2, PH3, PH4, PH5), y = FESDIAdepth(out1), type = "l",
     ylim = c(3, 0), lty = 1, lwd = 2, main = "pH", ylab = "", xlab = "")
```

```r
pH <- cbind(FESDIApH(out1),FESDIApH(out2),FESDIApH(out3),FESDIApH(out4))
par(mfrow = c(1,2))
matplot(x = pH, y = FESDIAdepth(out1), ylim = c(2,0),
        type = "l", main = "pH", lty = 1, lwd = 2, ylab = "depth")
matplot(x = pH, y = FESDIAdepth(out1), ylim = c(10,0),
        type = "l", main = "pH", lty = 1, lwd = 2, ylab = "depth")
```

```r
FESDIAbudgetO2(out1, out2, out3, out4)
FESDIAbudgetC (out1, out2, out3, out4, which = "Rates")
```

## Dry flats (but moist sediment)

When flats are dry, the exchange is governed by a piston velocity. The exchange of substances at the upper interface can take on two modes: exchange with water overlying the sediment or exchange with the atmosphere.

When the parameter *gasflux*, or forcing function *gasfluxForc* is 0, this means that the sediment is submersed. When they have a positive value, equal to the piston velocity, (units [cm/d]), this means that the sediment is exposed to the air. In that case, only oxygen and DIC are exchanged with the air at the upper interface, while there is no exchange for NH3, NO3, NO2, PO4, … Deposition of the two carbon fractions and of FeOH3, CaP continues.

```r
out    <- FESDIAsolve()
outdry <- FESDIAsolve(parms = list(gasflux = 1e2), yini = out$y)

plot(out1, outdry, ylim = c(10, 0), lty = 1, lwd = 2,
     which = c("O2","NO3","NH3","PO4","FeP","TOC"))
legend("center", col = 1:2, title = "exchange", legend = c("water","dry"), lty = 1)

print(FESDIAbudgetO2(outdry))
print(FESDIAbudgetN(outdry))
```

## Long distance oxidation

Parameters *rSurfH2Sox*, *rSurfCH4ox*,*ODUoxdepth* and *ODUoxatt* define the deep H2S or CH4 oxidation rate consuming oxygen from the surface layer.

The larger the oxidation rate, the more difficult it becomes to find a solution, so difficult cases can be solved by ramping up the solution, using previous solutions as initial guesses for the next solution.

It also helps to run the model dynamically to steady-state.

This will only be effective if sufficient H2S is formed, so the Carbon flux is sufficiently high.

Three parameters determine the long distance oxidation:

```r
FESDIAparms(which = c("rSurfH2Sox", "rSurfCH4ox","ODUoxdepth", "ODUoxatt"))
```

```
##              parms units                            description
## rSurfH2Sox     0    /d      Max rate H2S oxidation with BW O2
## rSurfCH4ox     0    /d      Max rate CH4 oxidation with BW O2
## ODUoxdepth     5    cm Max depth H2S/CH4 oxidation with BW O2
## ODUoxatt       1   /cm        depth attenuation ODU oxidation
```

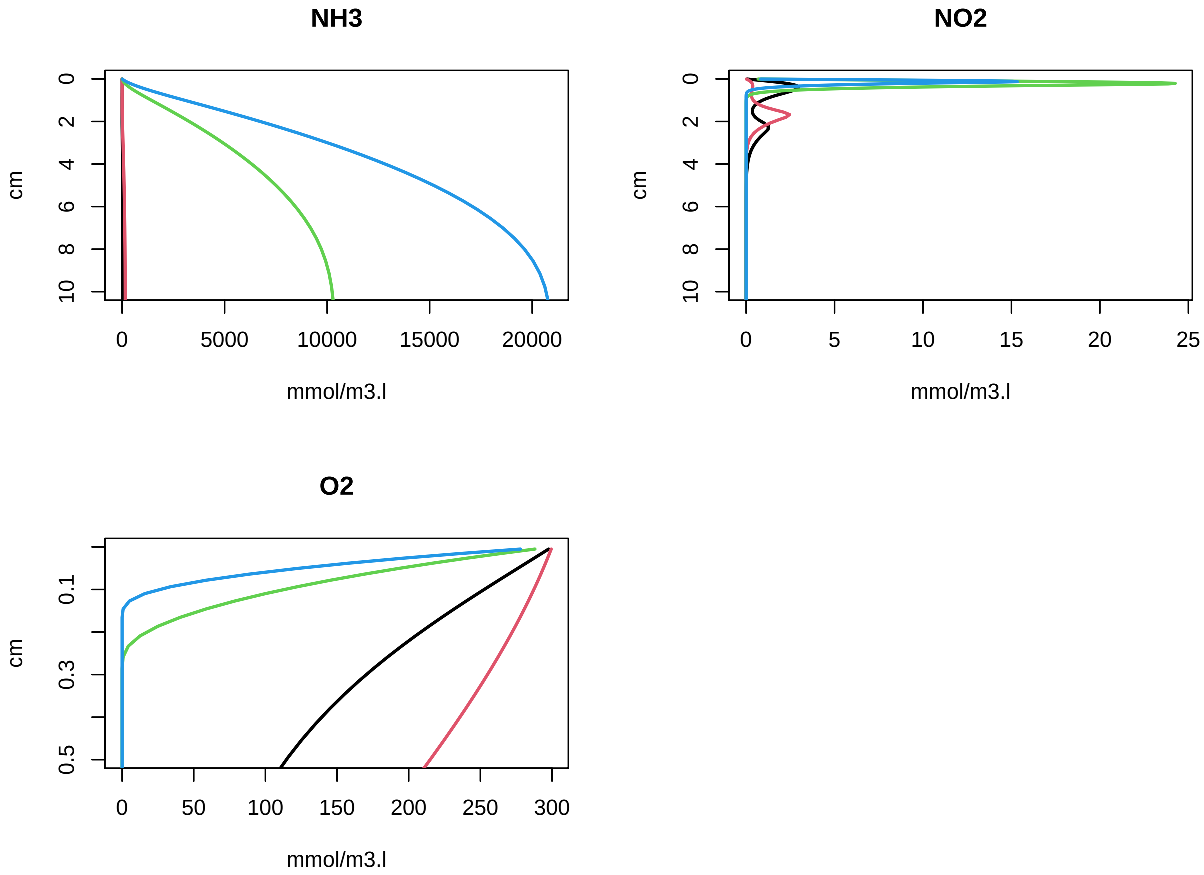
*rSurfH2Sox* and *rSurfCH4ox* set the maximal rate, while *ODUoxdepth* and *ODUoxatt* determine the shape of the rate, maximal in an upper layer with thickness *ODUoxdepth* and then going to 0 with an attenuation rate *ODUoxatt*.

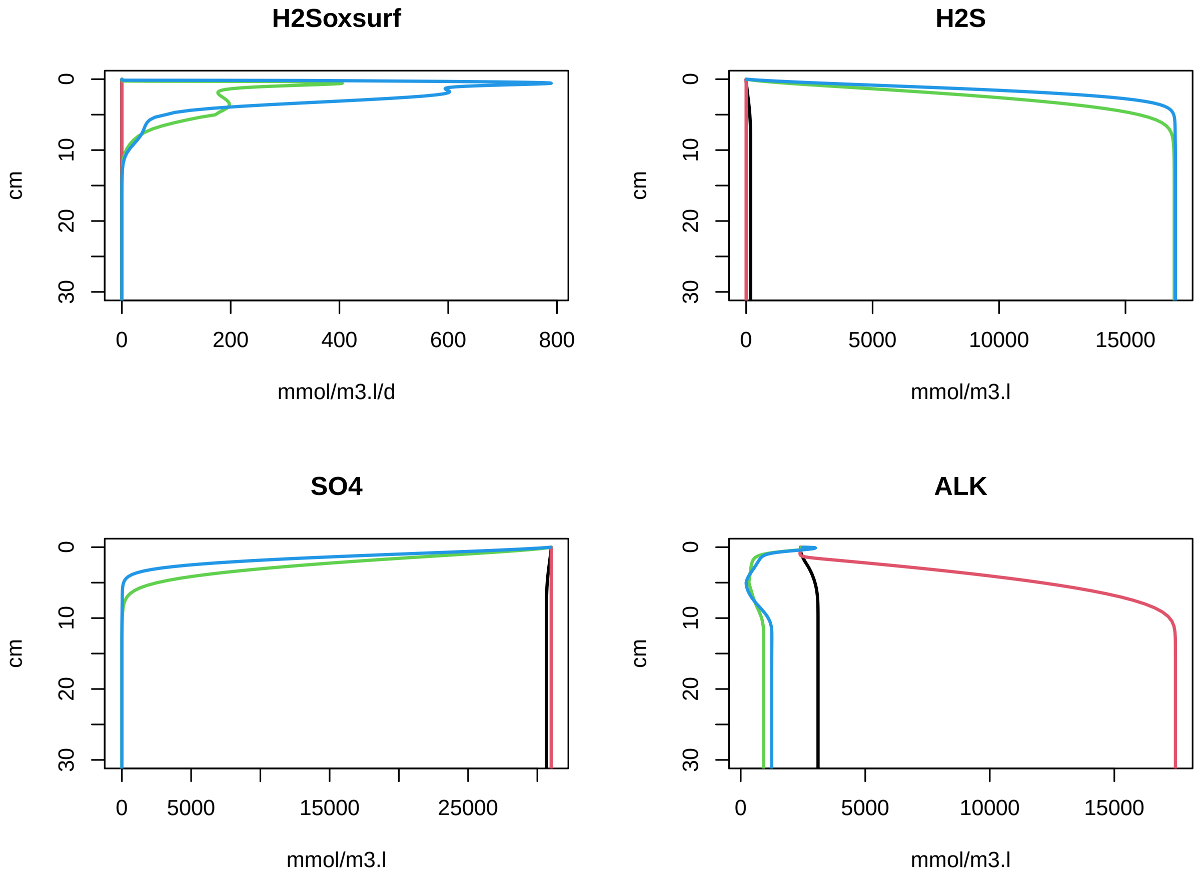
As an examples, runs are created that vary the surface rate as well as the depth of the oxidation:

```
P <- FESDIAparms(as.vector = TRUE)
P["rSurfH2Sox"]   <- 1
P["pFast"]        <- 0.2   # mmolFeOH3/m3 half-sat FeOH3 in iron red
P["rSlow"]        <- 1e-5
P["kinFeOH3"]     <- 0.1
P["kinNO3anox"]   <- 0.1
P["FeOH3flux"]   <- 100
#P["ODUoxdepth"] <- 10
p0 <- p1 <- p2 <- p3 <- P

p1["Cflux"] <- 100
p2["Cflux"] <- 5000
p3["Cflux"] <- 10000 #; p3["ODUoxdepth"] <- 10

out0<- FESDIAsolve()
out0b   <- FESDIAdyna (parms = p0, yini = out0$y,          times = c(0,1e8))
out0b   <- FESDIAdyna (parms = p0, yini = out0b[2,2:1701], times = c(0,1e8))
out0c   <- FESDIAsolve(parms = p0, yini = out0b[2,2:1701], method = "mixed")

out1ini <- FESDIAsolve(parms = list(Cflux = 100))
out1a   <- FESDIAdyna (parms = p1, yini = out1ini$y,       times = c(0,1e10))
out1a   <- FESDIAdyna (parms = p1, yini = out1a[2,2:1701], times = c(0,1e10))
out1    <- FESDIAsolve(parms = p1, yini = out1a[2,2:1701], method = "runsteady")

out2ini <- FESDIAsolve(parms = list(Cflux = 5000))
out2a <- FESDIAdyna(parms = p2, yini = out2ini$y, times = c(0,1e10))
out2 <- FESDIAsolve(parms = p2, yini = out2a[2,2:1701], method = "runsteady")


out3ini <- FESDIAsolve(parms = list(Cflux = 10000))
out3a   <- FESDIAdyna(parms = p3, yini = out3ini$y, times = c(0,1e10))
out3    <- FESDIAsolve(parms = p3, yini = out3a[2,2:1701], method = "runsteady")
```

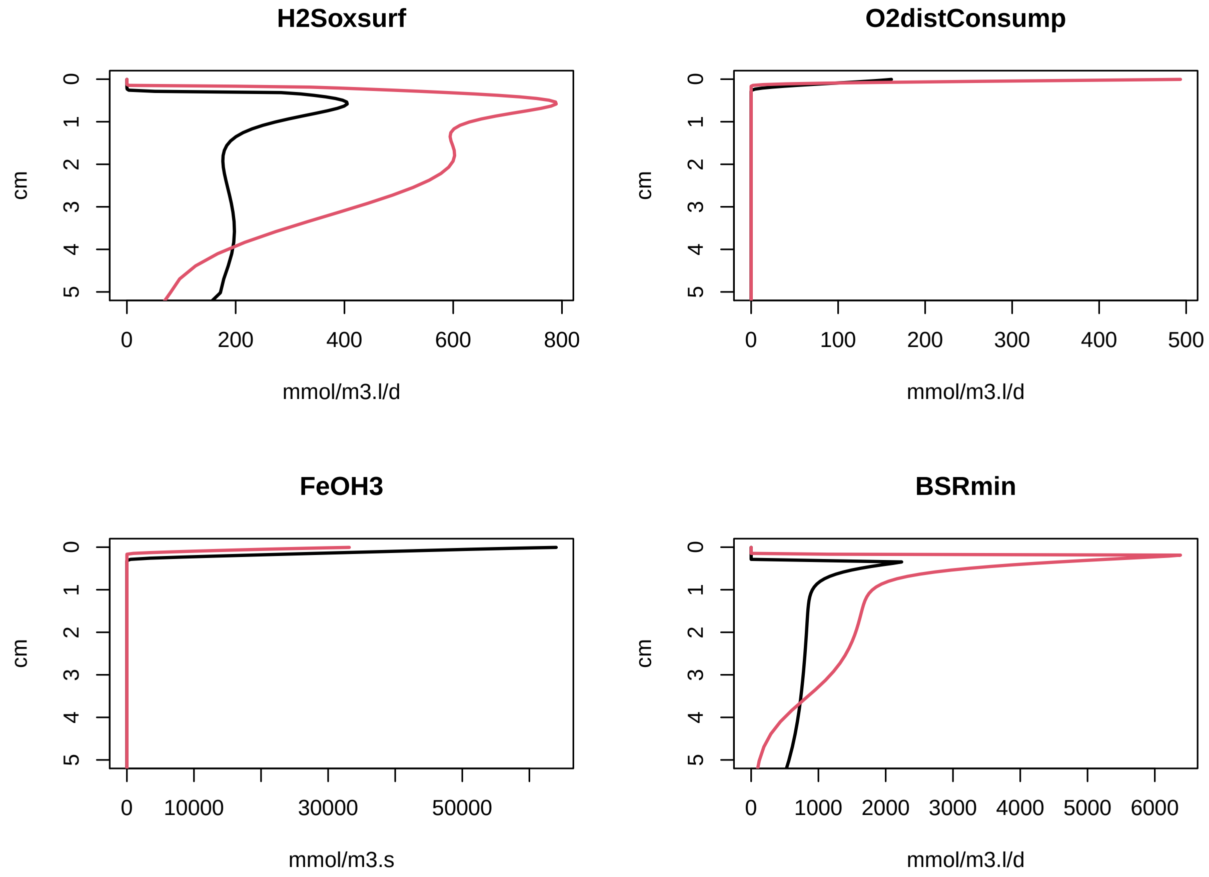
This makes no sense for the pH and alkalinity profiles.

```
plot(out0, out1, out2, out3, ylim = c(10, 0),
     lty = 1, lwd = 2, which = c(6,5), mfrow = c(2,2))
plot(out0,out1, out2, out3, ylim = c(0.5, 0),
     lty = 1, lwd = 2, which = 3, mfrow = NULL)
plot(out0,out1, out2, out3, ylim = c(30, 0),
     lty = 1, lwd = 2, which = c("H2Soxsurf", "H2S", "SO4", "ALK"))
```


NH3
cm
0
2
4
6
8
10
0
5000
10000
15000
20000
mmol/m3.l
NO2
cm
0
2
4
6
8
10
0
5
10
15
20
25
mmol/m3.l
O2
cm
0.1
0.3
0.5
0
50
100
150
200
250
300
mmol/m3.l



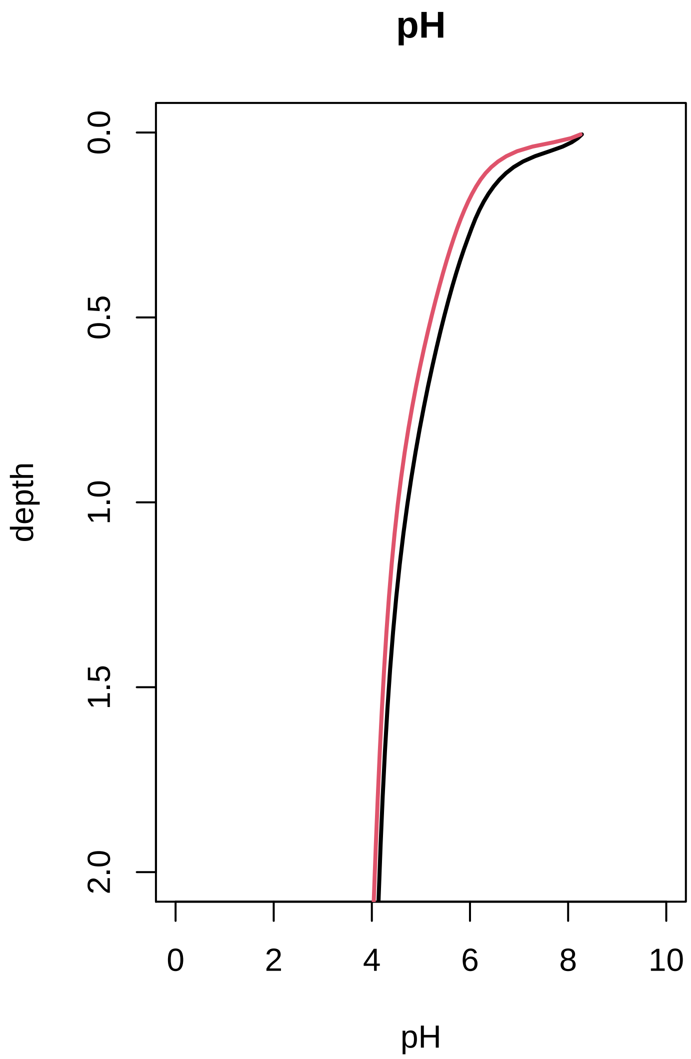
```
plot(out2, out3, ylim = c(5, 0), lty = 1, lwd = 2,
  which = c("H2Soxsurf", "O2distConsump", "FeOH3", "BSRmin"))
```



```r
FESDIAbudgetO2(out0, out1, out2, out3, which = "Fluxes")
```

```
##                 [,1]          [,2]     [,3]     [,4]
## O2surf     506.7625  1.229427e+02 2573.932 4757.927
## O2deep       0.0000 1.626905e-229    0.000    0.000
## O2perturb    0.0000  0.000000e+00    0.000    0.000
## O2net      506.7625  1.229427e+02 2573.932 4757.927
```

```r
pH <- cbind(FESDIApH(out2),FESDIApH(out3))
matplot(x = pH, y = FESDIAdepth(out1), ylim = c(2,0), xlim = c(0,10),
        type = "l", main = "pH", lty = 1, lwd = 2, ylab = "depth")
```

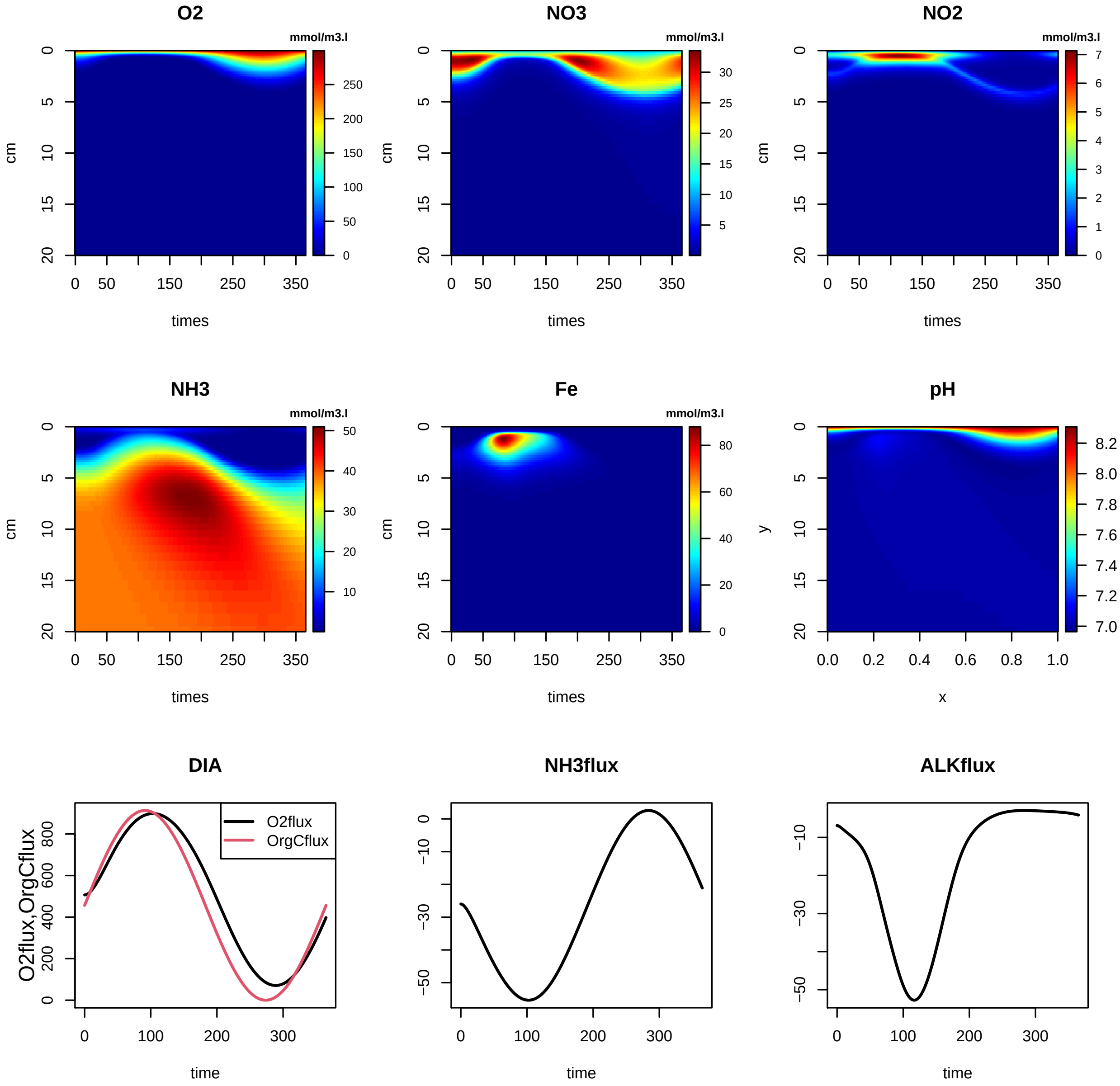


# Dynamic runs with sinusoidal forcing

## Carbon input

In the first dynamic run, a sinusoidal variation in time is used for the C flux, with amplitude = 1, the other parameters are left equal to the default.

```
DIA <- FESDIAdyna (Cflux = list(amp = 1))
pH  <- FESDIApH(DIA)

image2D(DIA, ylim = c(20, 0), which = c(3:6,8), mfrow = c(3,3))
plot3D:::image2D(pH, y = FESDIAdepth(DIA), ylim = c(20, 0), main = "pH")
matplot.0D(DIA, which = c("OrgCflux", "O2flux"), mfrow = NULL, lty = 1, lwd = 2)
plot(DIA, which = c("NH3flux", "ALKflux"), mfrow = NULL, lwd = 2)
```

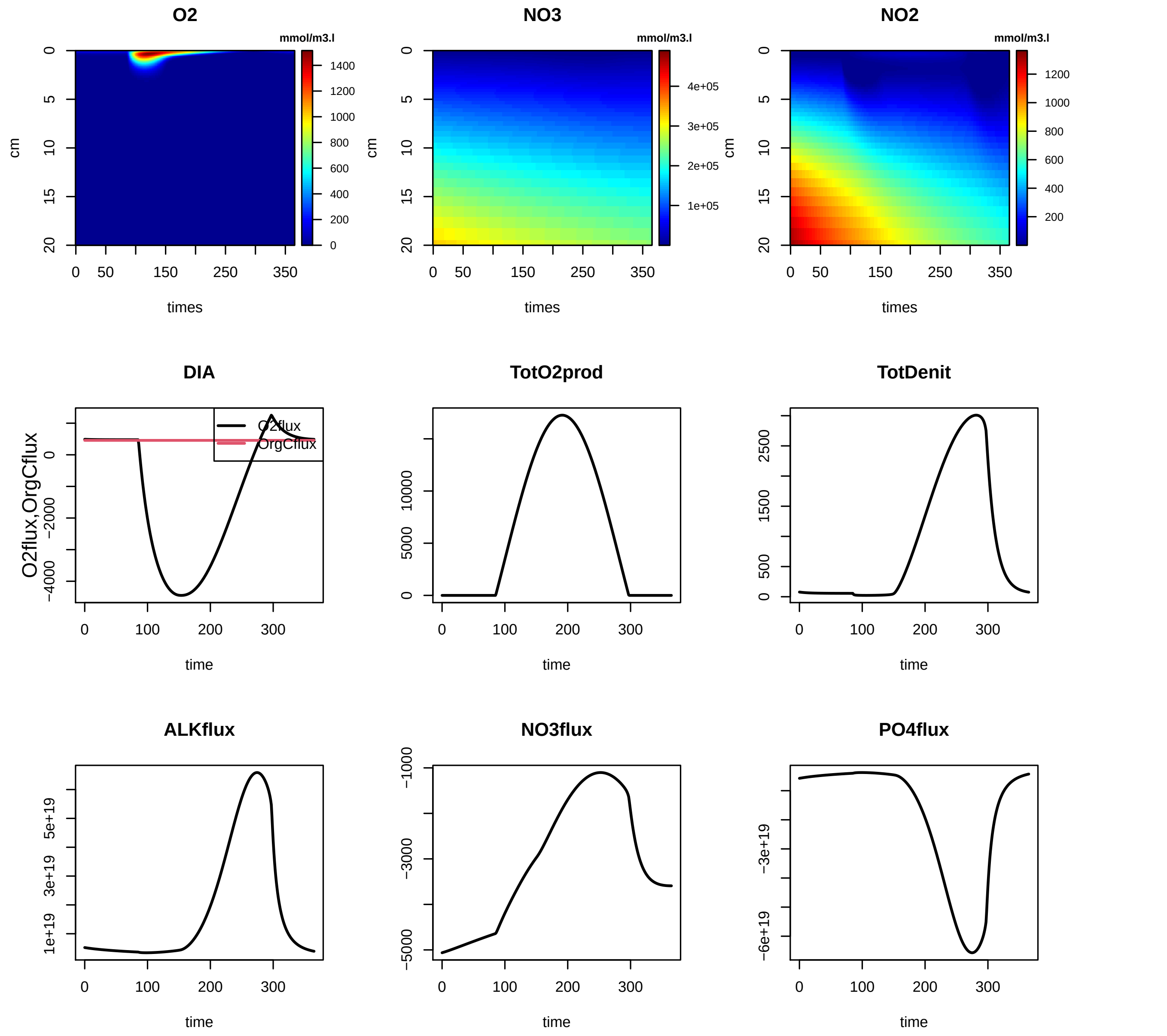


## Microphytobenthos production

### Seasonal variation

First a model is run with seasonally variable MPB production.

```
DIA <- FESDIAdyna (parms = list(MPBprod = 50000, por0 = 0.5),
      MPBprodForc = list(amp = 4, phase = 100), spinup = 0:365)
image2D(DIA, ylim = c(20, 0), which = 3:5, mfrow = c(3,3))
matplot.0D(DIA, which = c("OrgCflux", "O2flux"), mfrow = NULL, lty = 1, lwd = 2)
plot(DIA, which = c("TotO2prod", "TotDenit","ALKflux","NO3flux","PO4flux"),
  mfrow = NULL, lwd = 2)
```



```r
print(FESDIAbudgetO2(DIA))
```

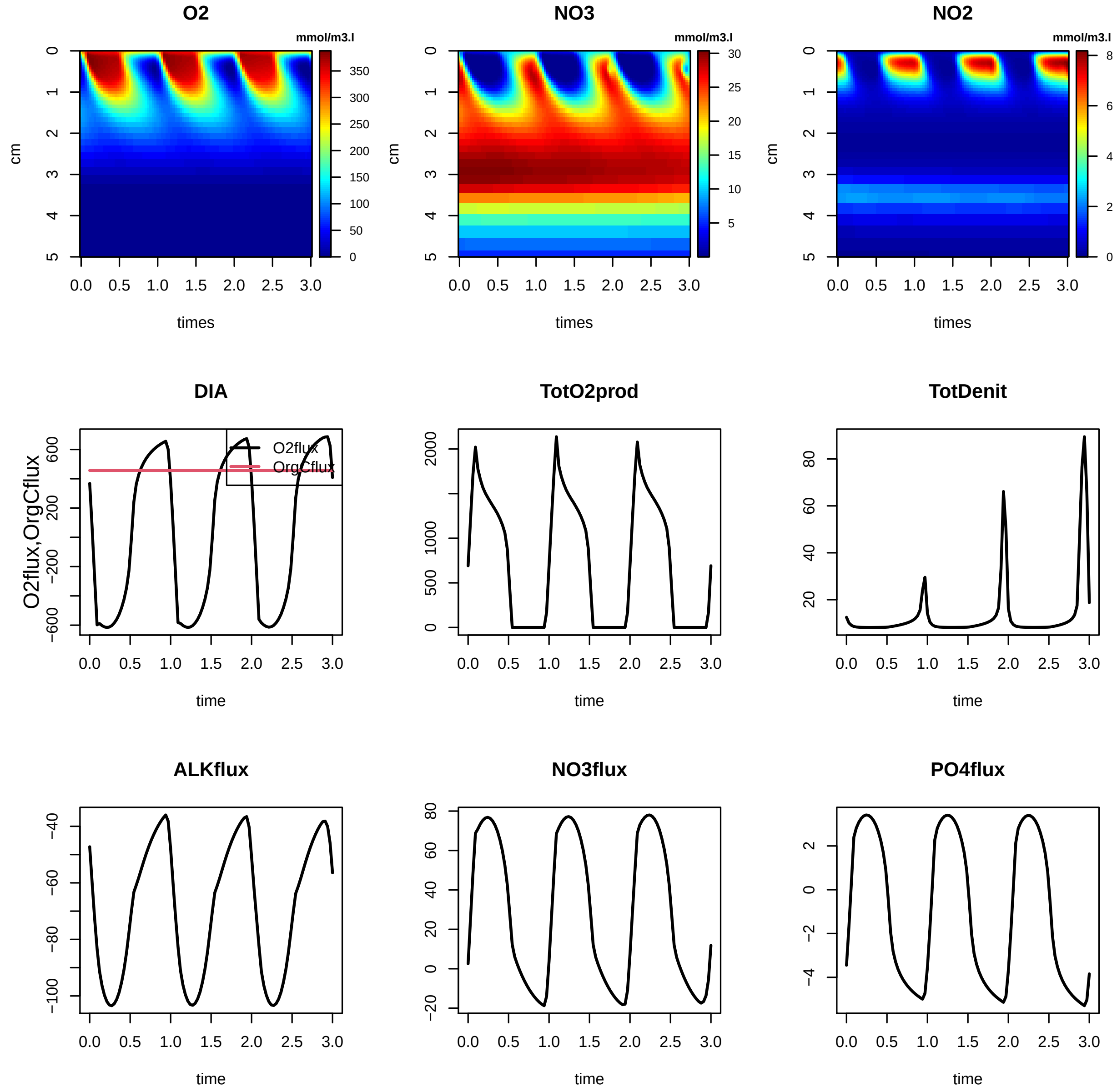
```
## $Fluxes
##                      O2
## surface  -1.167212e+03
## bottom    2.383299e-135
## perturb    0.000000e+00
## netin    -1.167212e+03
##
## $Rates
##              Nitrification FeOxidation H2Soxidation CH4oxidation H2Soxid.dist CH4oxid.dist
## nmolO2/cm2/d      891.0235   0.1479171      72.3202 0.0003065377            0            0
##              OxicMineralisation MPBO2production MPBO2respiration    Total
## nmolO2/cm2/d           5839.258        6260.641                0 13063.39
```

```
##
## $Losses
## [1] 2.383299e-135
##
## $dC
##          O2         sum
## 0.000705527 0.000705527
##
## $Delta
## [1] 11896.18
##
## $Fluxmat
##              Ext       O2      NO2      NO3      DIC      SO4     FeOH3        Burial
## Ext        0.000    0.000   0.0000   0.0000    0.000   0.0000 0.0000000  0.000000e+00
## O2      1167.212    0.000 752.5237 138.4998 5839.258 72.3202 0.1479171 2.383299e-135
## NO2        0.000    0.000   0.0000   0.0000    0.000   0.0000 0.0000000  0.000000e+00
## NO3        0.000    0.000   0.0000   0.0000    0.000   0.0000 0.0000000  0.000000e+00
## DIC        0.000 6260.641   0.0000   0.0000    0.000   0.0000 0.0000000  0.000000e+00
## SO4        0.000    0.000   0.0000   0.0000    0.000   0.0000 0.0000000  0.000000e+00
## FeOH3      0.000    0.000   0.0000   0.0000    0.000   0.0000 0.0000000  0.000000e+00
## Burial     0.000    0.000   0.0000   0.0000    0.000   0.0000 0.0000000  0.000000e+00
```

### Diurnal variation

A run with daily variable MPB production:

```
INI <- FESDIAsolve (parms = list(por0 = 0.5))

DIA <- FESDIAdyna (parms = list(MPBprod = 10000, por0 = 0.5),
                   MPBprodForc = list(amp = 4, period = 1),
                   spinup = seq(0, 10, length.out = 1000), yini = INI$y,
                   times = seq(0, 3,length.out = 100))
PH <- FESDIApH(DIA)
image2D(DIA, ylim = c(5, 0), which = 3:5, mfrow = c(3,3))
matplot.0D(DIA, which = c("OrgCflux", "O2flux"), mfrow = NULL, lty = 1, lwd = 2)
plot(DIA, which = c("TotO2prod", "TotDenit","ALKflux","NO3flux","PO4flux"), mfrow = NULL, lwd = 2)
```



```r
print(FESDIAbudgetO2(DIA))
```

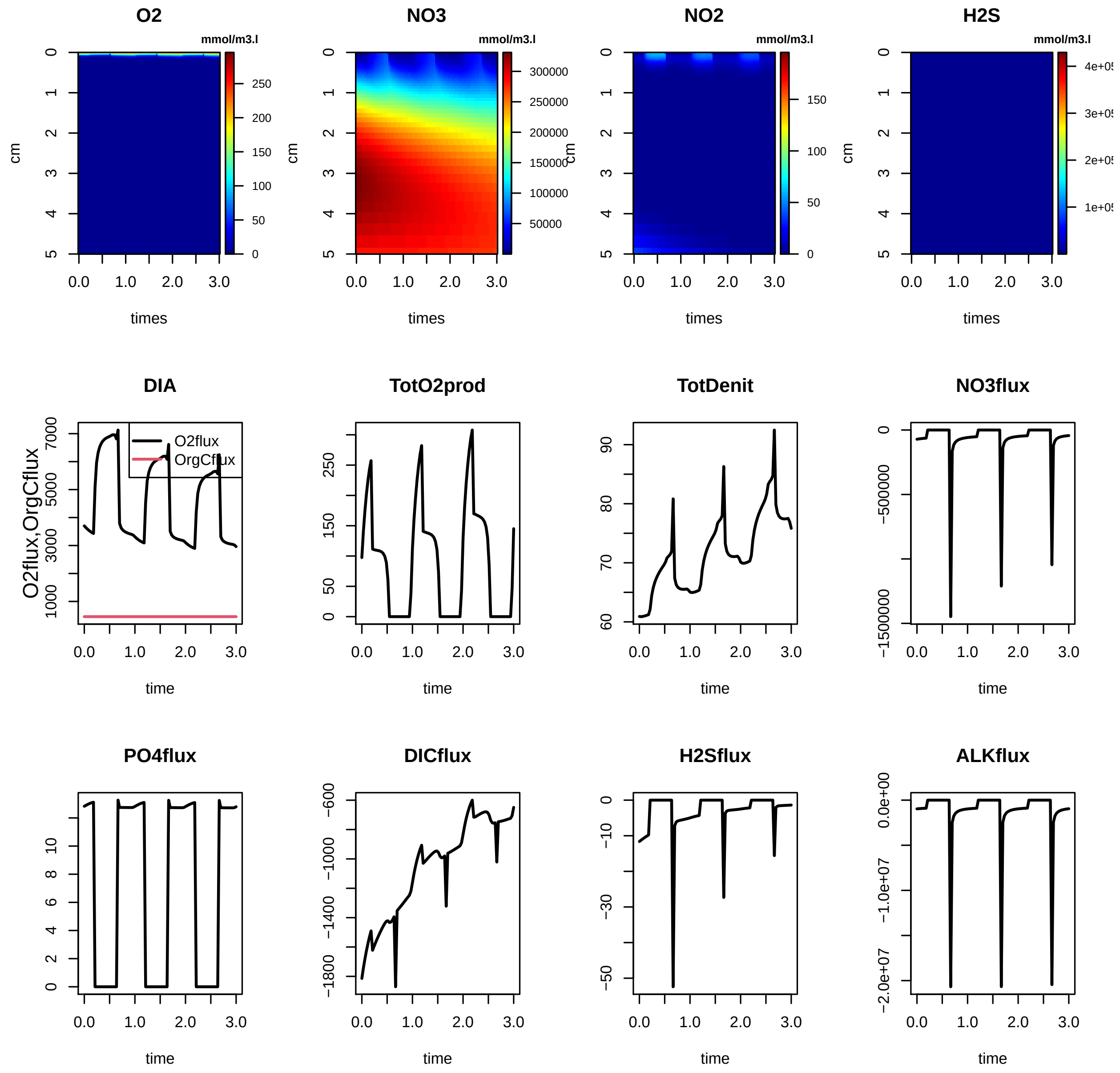
```
## $Fluxes
##                    O2
## surface  3.684513e+01
## bottom  2.433981e-138
## perturb  0.000000e+00
## netin    3.684513e+01
##
## $Rates
##                Nitrification FeOxidation H2Soxidation CH4oxidation H2Soxid.dist CH4oxid.dist
## nmolO2/cm2/d         90.4969   0.4385311     7.596695   0.02023508            0            0
##                OxicMineralisation MPBO2production MPBO2respiration    Total
## nmolO2/cm2/d               799.89        736.6921                0 1635.134
```

```
##
## $Losses
## [1] 2.433981e-138
##
## $dC
##        O2       sum
## -8.339827 -8.339827
##
## $Delta
## [1] 1671.98
##
## $Fluxmat
##        Ext        O2      NO2      NO3      DIC      SO4     FeOH3        Burial
## Ext      0  36.84513  0.00000  0.00000   0.0000 0.000000 0.0000000  0.000000e+00
## O2       0   0.00000 71.50817 18.98872 799.9102 7.596695 0.4385311 2.433981e-138
## NO2      0   0.00000  0.00000  0.00000   0.0000 0.000000 0.0000000  0.000000e+00
## NO3      0   0.00000  0.00000  0.00000   0.0000 0.000000 0.0000000  0.000000e+00
## DIC      0 736.69208  0.00000  0.00000   0.0000 0.000000 0.0000000  0.000000e+00
## SO4      0   0.00000  0.00000  0.00000   0.0000 0.000000 0.0000000  0.000000e+00
## FeOH3    0   0.00000  0.00000  0.00000   0.0000 0.000000 0.0000000  0.000000e+00
## Burial   0   0.00000  0.00000  0.00000   0.0000 0.000000 0.0000000  0.000000e+00
```

### Microphytobenthos production with sediments falling dry

Sediments are imposed to be exposed to the air by giving *gasfluxForc* a value other than 0, as in following example.

```
F <- 1e3
gasflux <- data.frame(time = c(0, 0.19999, 0.2, 0.6, 0.6661, 1.19999, 1.2, 1.6, 1.6661, 2.19999, 2.2, 2
                flux = c(0,  0,      F,   F,   0,      0      , F,   F,   0,      0      ,F,   F,   0,
DIA <- FESDIAdyna (parms = list(MPBprod = 10000),
             MPBprodForc = list(amp = 4, period = 1), gasfluxForc = list(data = gasflux),
             spinup = seq(0, 3, length.out = 100), times = seq(0, 3, length.out = 100))
image2D(DIA, ylim = c(5, 0), which = c(3:5,10),  mfrow = c(3,4))
matplot.0D(DIA, which = c("OrgCflux", "O2flux"), mfrow = NULL, lty = 1, lwd = 2)
plot(DIA, which = c("TotO2prod", "TotDenit","NO3flux","PO4flux","DICflux","H2Sflux","ALKflux"), mfrow =
```



```r
print(FESDIAbudgetO2(DIA))
```

```
## $Fluxes
##                      O2
## surface  4.587212e+03
## bottom  8.018354e-154
## perturb  0.000000e+00
## netin    4.587212e+03
##
## $Rates
##               Nitrification FeOxidation H2Soxidation CH4oxidation H2Soxid.dist CH4oxid.dist
## nmolO2/cm2/d      356.7857    3634.164   0.01280528     519.9763            0            0
##               OxicMineralisation MPBO2production MPBO2respiration    Total
## nmolO2/cm2/d            100.3121        89.30625                0 4700.558
```

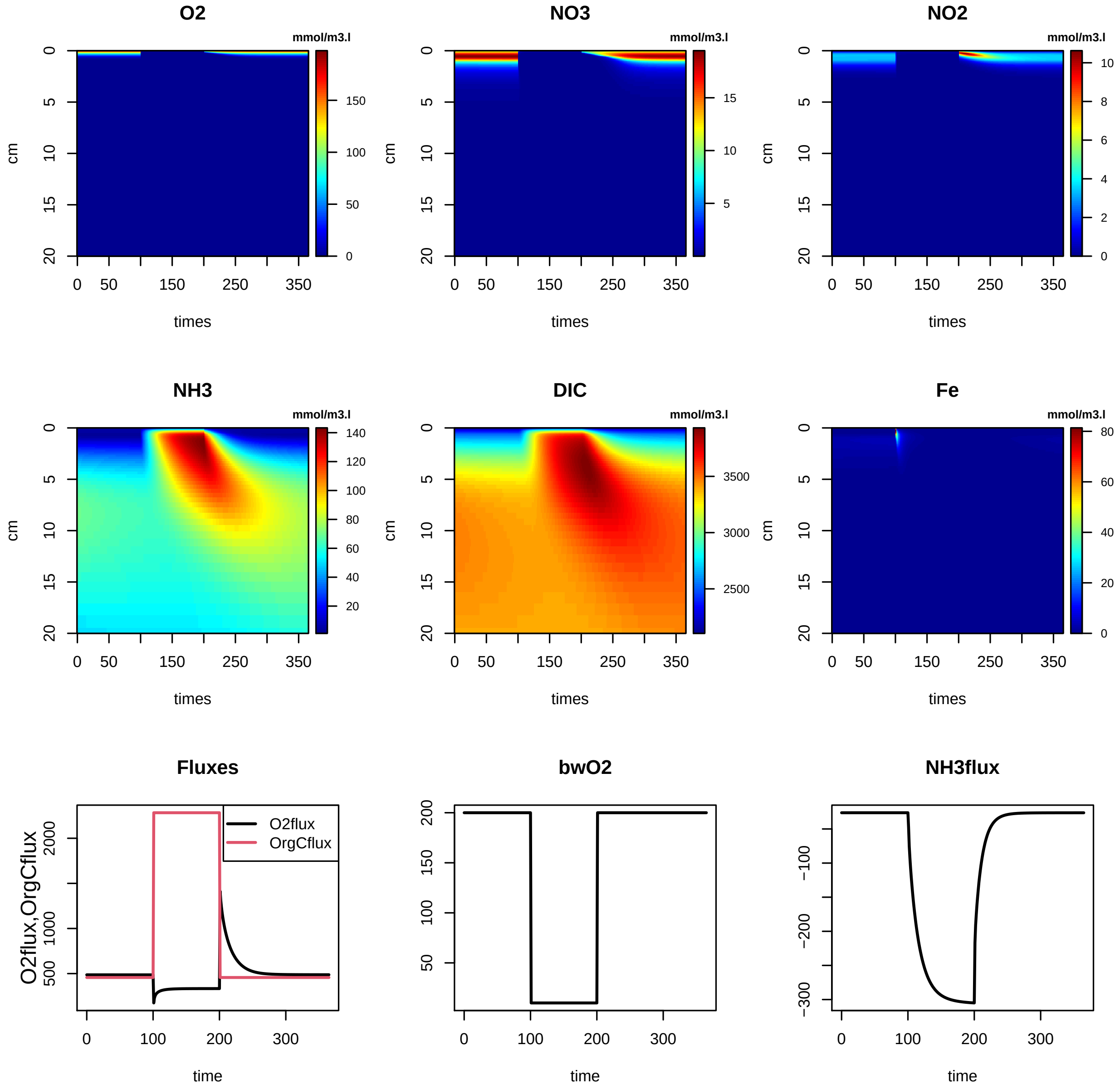
```
##
## $Losses
## [1] 8.018354e-154
##
## $dC
##      O2     sum
## 1.16945 1.16945
##
## $Delta
## [1] 9287.769
##
## $Fluxmat
##        Ext         O2      NO2      NO3      DIC        SO4    FeOH3        Burial
## Ext      0 4587.21183   0.0000  0.00000   0.0000 0.00000000    0.000  0.000000e+00
## O2       0    0.00000 324.6535 32.13221 620.2884 0.01280528 3634.164 8.018354e-154
## NO2      0    0.00000   0.0000  0.00000   0.0000 0.00000000    0.000  0.000000e+00
## NO3      0    0.00000   0.0000  0.00000   0.0000 0.00000000    0.000  0.000000e+00
## DIC      0   89.30625   0.0000  0.00000   0.0000 0.00000000    0.000  0.000000e+00
## SO4      0    0.00000   0.0000  0.00000   0.0000 0.00000000    0.000  0.000000e+00
## FeOH3    0    0.00000   0.0000  0.00000   0.0000 0.00000000    0.000  0.000000e+00
## Burial   0    0.00000   0.0000  0.00000   0.0000 0.00000000    0.000  0.000000e+00
```

# dynamic runs with forcing function time series

## Carbon flux and bottom water concentrations

We can also impose a time-series. Here we impose this for the carbon flux, and for the Oxygen bottom water concentration.

```
fluxforcdat <- data.frame(time = c(0, 100, 101, 200, 201, 365),
                          flux = c(20, 20, 100, 100, 20, 20)*1e5/12/365)
O2forcdat <- data.frame(time = c(0, 100, 101, 200, 201, 365),
                        conc = c(200, 200, 10, 10, 200, 200))
DIA <- FESDIAdyna (CfluxForc = list(data = fluxforcdat),
                   O2bwForc = list(data = O2forcdat), spinup = 0:365)
image2D(DIA,  which = 3:8, mfrow = c(3,3))
matplot.0D(DIA, which = c("OrgCflux", "O2flux"), mfrow = NULL, lty = 1, lwd = 2, main = "Fluxes")
plot(DIA, which = c("bwO2","NH3flux"), mfrow = NULL, lwd = 2)
```

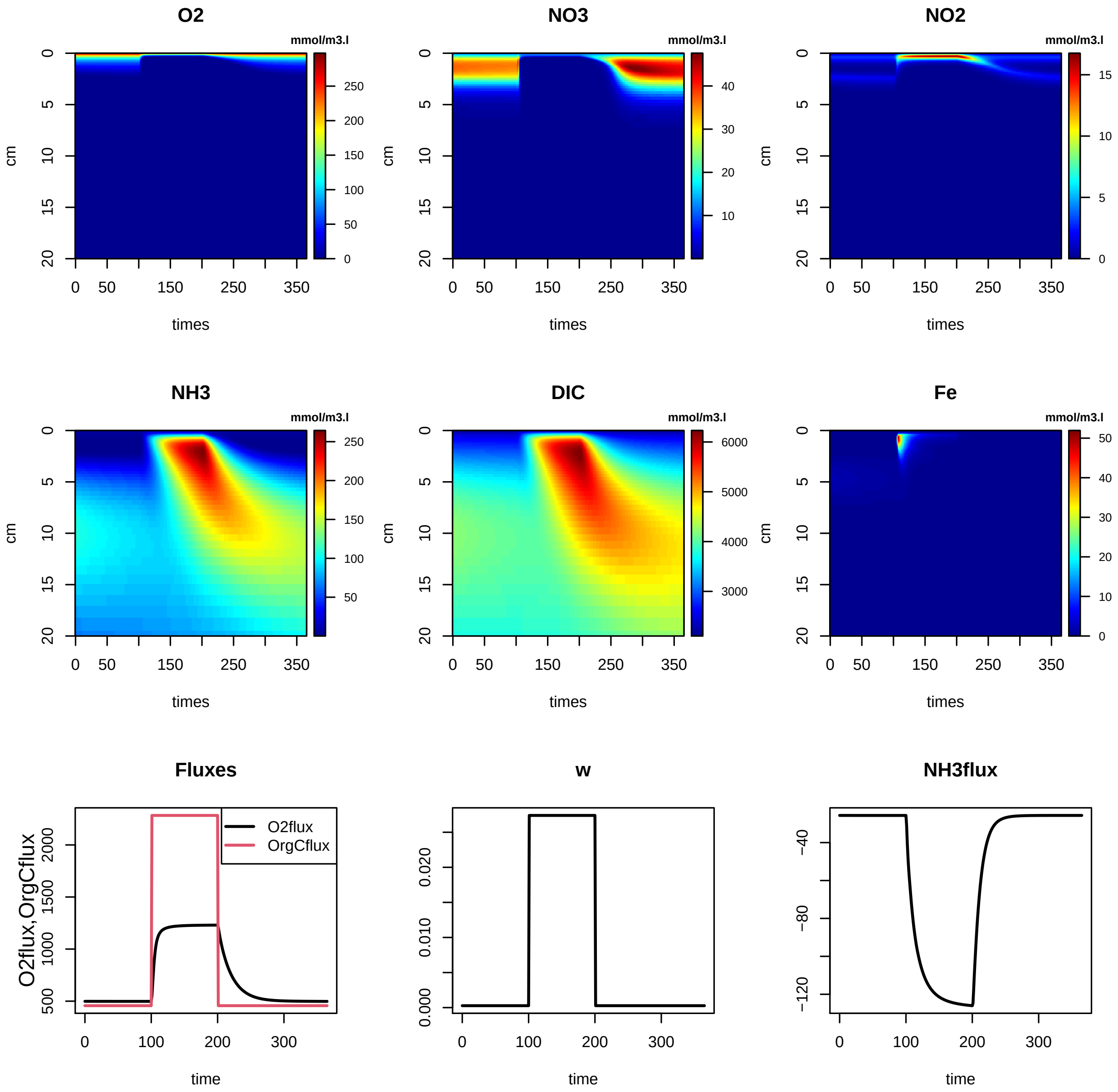


## Flux and sedimentation rates

Other variables that can be forced are *w*, *biot*, *irr* for the sedimentation rate, bioturbation rate and irrigation rates respectively, microphytobenthos production, . . .

```
fluxforcdat <- data.frame(time = c(0, 100, 101, 200, 201, 365),
                          flux = c(20, 20, 100, 100, 20, 20)*1e5/12/365)
seddat <- data.frame(time = c(0, 100, 101, 200, 201, 365),
                     w = c(0.1, 0.1, 10, 10, 0.1, 0.1)/365)  #cm/d
DIA <- FESDIAdyna (CfluxForc = list(data = fluxforcdat),
                   wForc = list(data = seddat),
                   spinup = 0:365)
image2D(DIA, ylim = c(20, 0), which = 3:8, mfrow = c(3,3))
```

```
matplot.0D(DIA, which = c("OrgCflux", "O2flux"), mfrow = NULL, lty = 1, lwd = 2, main = "Fluxes")
plot(DIA, which = c("w", "NH3flux"), mfrow = NULL, lwd = 2)
```



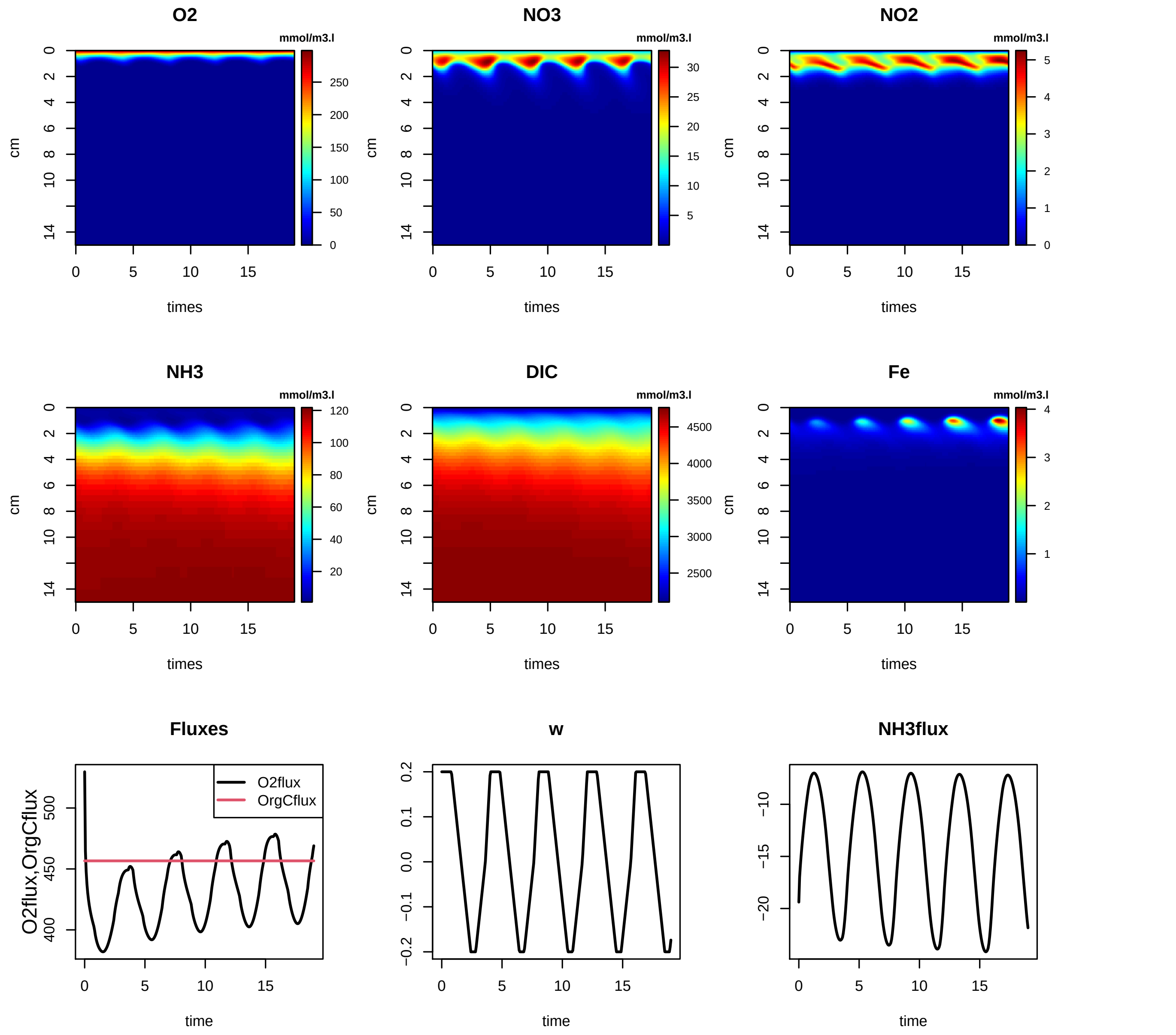
## Deposition-erosion rates.

Particles often go through a repeated deposition-erosion cycle. In the first case, sedimation rates, w is positive, and there is solid deposition; in the latter case, *w* is negative and there is no carbon deposition, *Cdepo*.

```
FF <- c(20, 30, 20, 10, 0, 0, 0, 0, 0, 0)*1e5/12/365
SS <- c(0.2, 0.2, 0.2, 0.1, 0.0,-0.1,-0.2,-0.2,-0.1, 0)  #cm/d
FF <- rep(FF, times = 10)
Fluxforcdat <- data.frame(time = seq(0, to = 39.8, length.out = length(FF)),
                          flux = FF)
```

```
SS <- rep(SS, times = 10)
Seddat <- data.frame(time = seq(0, to = 39.8, length.out = length(SS)),
                     w = SS)

times <- seq(0, 19, length.out = 300)

P <- list(Cflux = FF[1], w = SS[1])
std <- FESDIAsolve(parms = P)
DIA <- FESDIAdyna (wForc = list(data = Seddat), times = times, spinup = times,
                    yini = std$y)
```

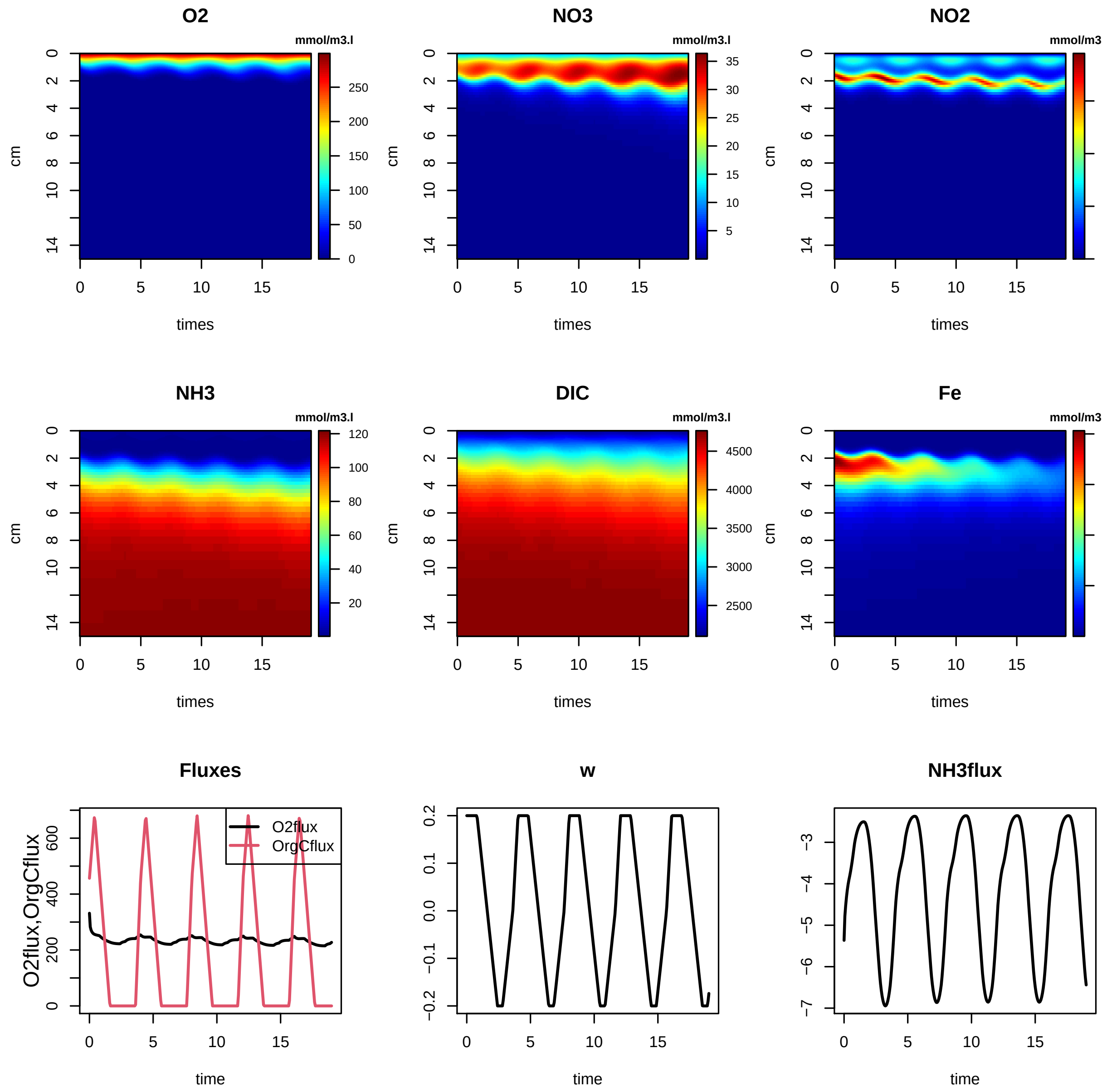
```
image2D(DIA, ylim = c(15, 0), which = 3:8, mfrow = c(3,3))
matplot.0D(DIA, which = c("OrgCflux", "O2flux"), mfrow = NULL, lty = 1, lwd = 2, main = "Fluxes")
plot(DIA, which = c("w","NH3flux"), mfrow = NULL, lwd = 2)
```



In the second run both the sedimentation rate and the carbon flux fluctuate.

```
DIA2 <- FESDIAdyna (CfluxForc = list(data = Fluxforcdat), wForc = list(data = Seddat),
                    times = times, spinup = times, yini = std$y)
```

```
image2D(DIA2, ylim = c(15, 0), which = 3:8, mfrow = c(3,3))
matplot.0D(DIA2, which = c("OrgCflux", "O2flux"), mfrow = NULL, lty = 1, lwd = 2, main = "Fluxes")
plot(DIA2, which = c("w", "NH3flux"), mfrow = NULL, lwd = 2)
```



```r
print(FESDIAbudgetC(DIA, DIA2))
```

```
## $Fluxes
##                      [,1]          [,2]
## FDETsurf        4.109589e+02  1.695465e+02
## FDETdeep        3.866335e-10  3.866340e-10
## FDETperturb     0.000000e+00  0.000000e+00
## FDETnet         4.109589e+02  1.695465e+02
## SDETsurf        4.566210e+01  1.883850e+01
## SDETdeep        2.481954e+00  2.481954e+00
## SDETperturb     0.000000e+00  0.000000e+00
## SDETnet         4.318015e+01  1.635655e+01
## DICsurf        -4.208532e+02 -2.343151e+02
## DICdeep         2.777929e+01  2.777929e+01
## DICperturb      0.000000e+00   0.000000e+00
## DICnet         -4.486325e+02  -2.620944e+02
## CH4surf        -4.226833e-08  -1.478797e-08
## CH4deep         5.289282e-06   5.289282e-06
## CH4perturb      0.000000e+00   0.000000e+00
## CH4net         -5.331551e-06  -5.304070e-06
## CinCaPsurf      0.000000e+00   0.000000e+00
## CinCaPdeep     2.034832e-147  2.034821e-147
## CinCaPperturb   0.000000e+00   0.000000e+00
## CinCaPnet     -2.034832e-147 -2.034821e-147
## CaCO3surf       0.000000e+00   0.000000e+00
## CaCO3deep       0.000000e+00   0.000000e+00
## CaCO3perturb    0.000000e+00   0.000000e+00
## CaCO3net        0.000000e+00   0.000000e+00
## ARAGsurf        0.000000e+00   0.000000e+00
## ARAGdeep        0.000000e+00   0.000000e+00
## ARAGperturb     0.000000e+00   0.000000e+00
## ARAGnet         0.000000e+00   0.000000e+00
## Totalsurf       3.576783e+01  -4.593009e+01
## Totaldeep       3.026125e+01   3.026125e+01
## Totalperturb    0.000000e+00   0.000000e+00
## Totalnet        5.506581e+00  -7.619134e+01
##
## $Rates
##                             [,1]         [,2]
## OxicMineralisation  339.5186294 167.56756043
## Denitrification      21.6856140  11.60068692
## IronReduction         0.1810795   0.02651364
## SulphateReduction    51.1190771  30.42095945
## Methanogenesis        1.6269094   0.96142924
## TotalMineralisation 414.1313094 210.57714968
## CH4oxidation          0.1286936   0.03331605
## CH4oxid.dist          0.0000000   0.00000000
## CH4oxidAOM            0.7173748   0.48567490
## MPBDICuptake          0.0000000   0.00000000
## MPBFDETproduction     0.0000000   0.00000000
## MPBResp               0.0000000   0.00000000
## CaPprecipitation      0.0000000   0.00000000
## CaPdissolution        0.0000000   0.00000000
## CaCO3dissolution      0.0000000   0.00000000
## ARAGdissolution       0.0000000   0.00000000
## CaCO3production       0.0000000   0.00000000
##
## $Losses
##          [,1]     [,2]
## [1,] 30.26125 30.26125
##
## $dC
##               [,1]           [,2]
## DET   4.000770e+01  -2.465786e+01
## DIC  -3.455713e+01  -5.158481e+01
## CaP -7.091259e-147 -7.091128e-147
## CH4  -3.261982e-02  -3.828955e-02
## sum   5.417957e+00  -7.628096e+01
```

```
##
## $Delta
##          [,1]      [,2]
## [1,] 5.506581 -76.19134
```

# Dynamic runs with explicitly modeled bottom water conditions

## Incubation experiments

The simulation is initiated with the steady-state conditions, while keeping the bottom water conditions constant.

```
std <- FESDIAsolve(dynamicbottomwater = FALSE, parms = list(Cflux = 20*1e5/12/365))
FESDIAbudgetO2(std, which = "Fluxes")
```

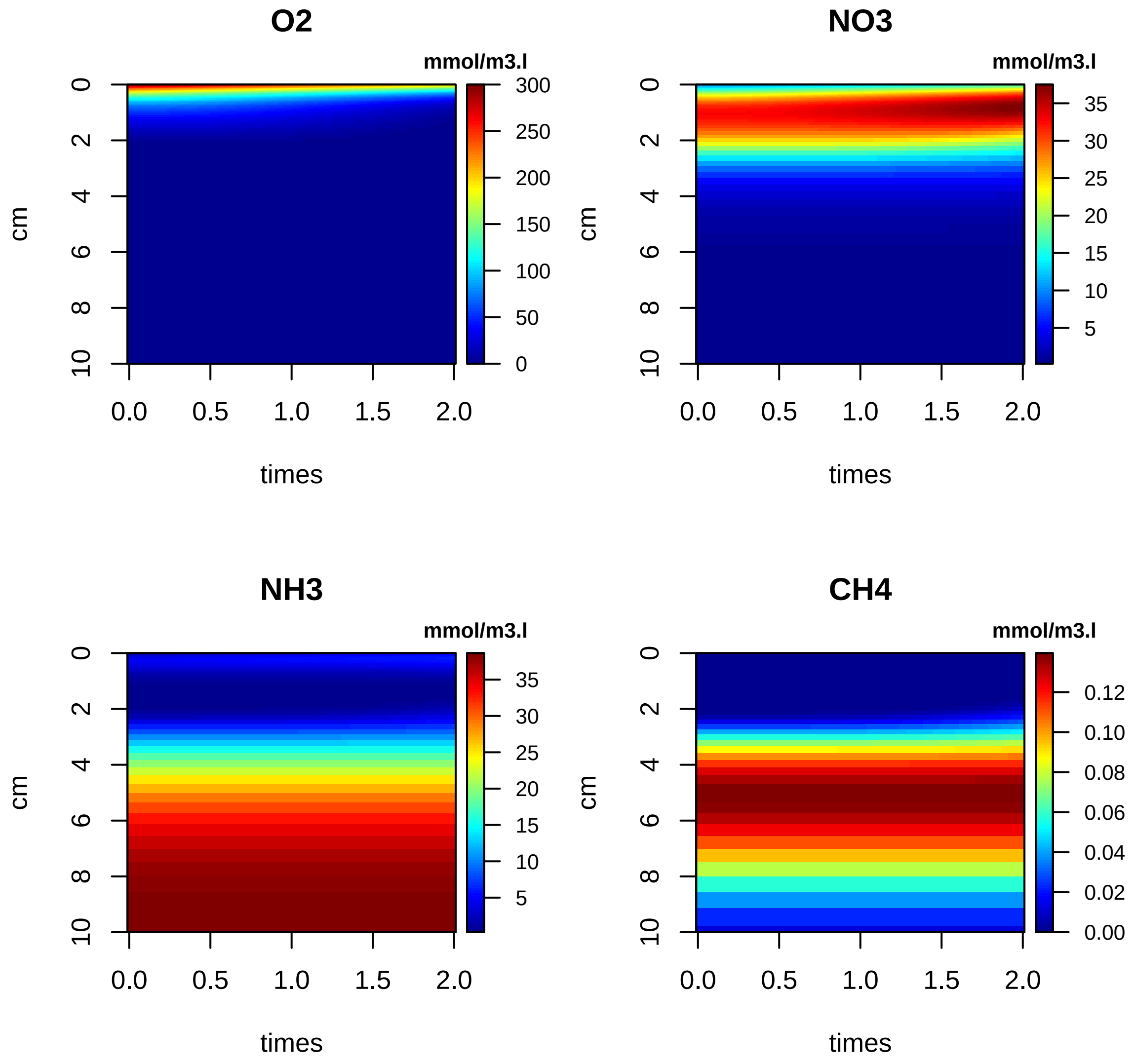
```
##                    O2
## surface  5.067625e+02
## bottom  4.709912e-135
## perturb  0.000000e+00
## netin    5.067625e+02
```

The initial conditions for the dynamic bottom water concentration run needs to have the bottom water concentrations as the first row.

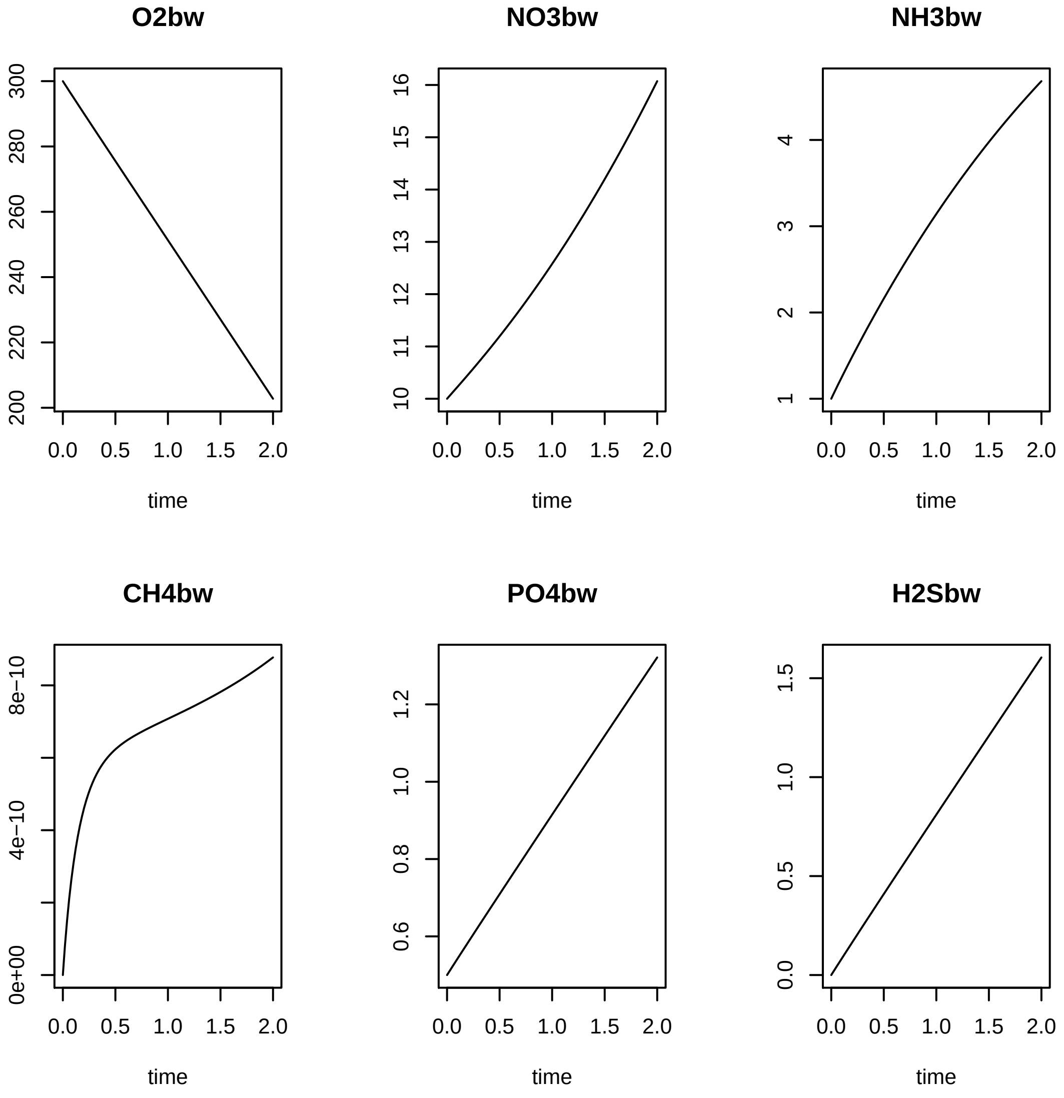
The model is run for two days.

```
P <- FESDIAparms(std, as.vector = TRUE)[c("O2bw", "NO3bw", "NO2bw", "NH3bw", "DICbw", "Febw", "H2Sbw", 

# order of state variables, FDET,SDET,O2,NO3,NO2,NH3,DIC,Fe,FeOH3,H2S,SO4,CH4,PO4,FeP,CaP,Pads,ALK
BW <- c(0, 0, P[c("O2bw","NO3bw","NO2bw","NH3bw","DICbw","Febw")], 0, P[c("H2Sbw","SO4bw","CH4bw","PO4b
dyn <- FESDIAdyna(dynamicbottomwater = TRUE, yini = rbind(BW, std$y),
      parms = list(Cflux = 20*1e5/12/365), times = seq(0, 2, length.out = 100))
```

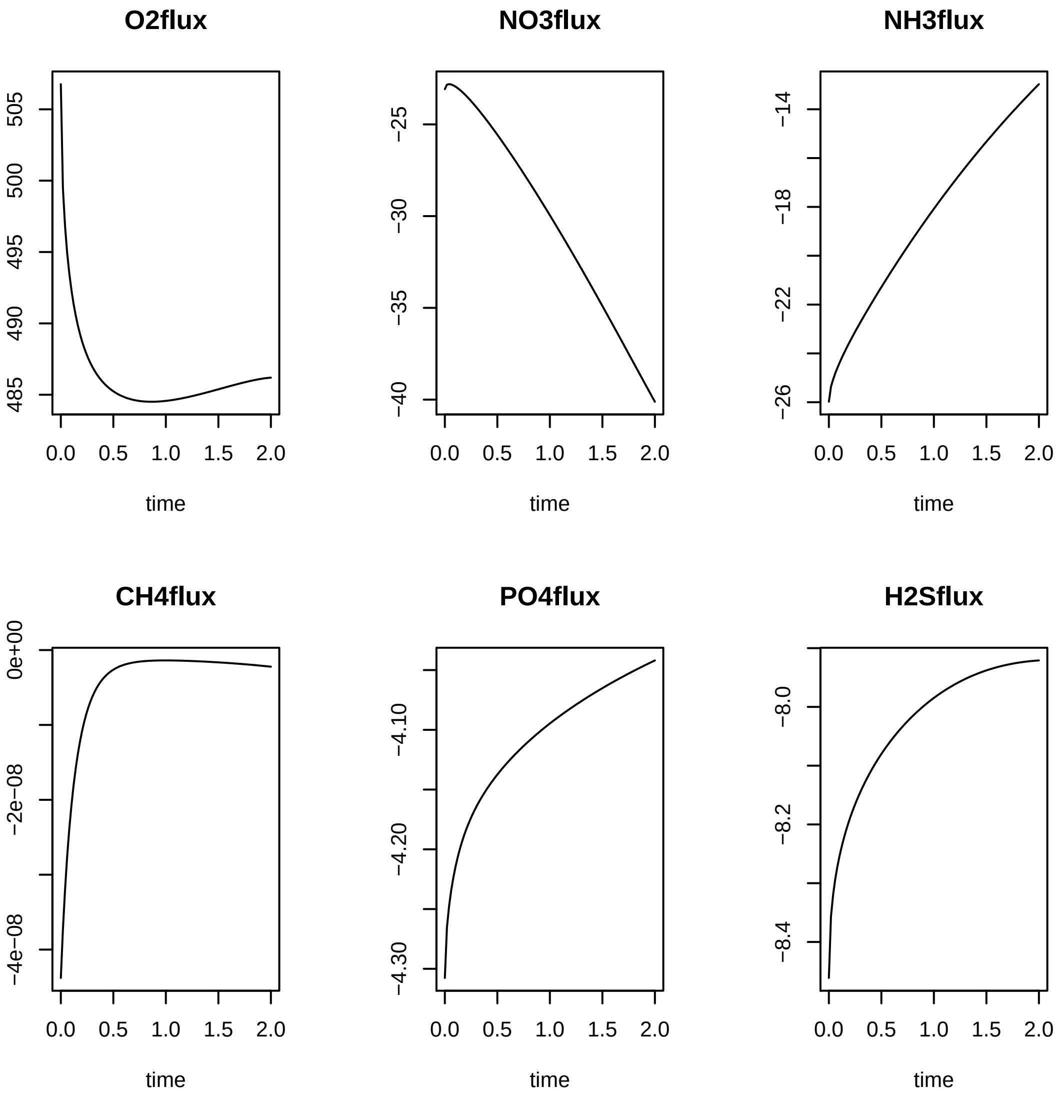
```
image2D(dyn, which = c("O2", "NO3", "NH3","CH4"), ylim = c(10,0))
```



```r
plot(dyn, which = c("O2bw","NO3bw","NH3bw","CH4bw","PO4bw","H2Sbw"))
```



```r
plot(dyn, which = c("O2flux","NO3flux","NH3flux","CH4flux","PO4flux","H2Sflux"))
```



# Perturbation runs

See vignette (“FESDIAperturb”)

# References

Soetaert K, PMJ Herman and JJ Middelburg, 1996a. A model of early diagenetic processes from the shelf to abyssal depths. Geochimica Cosmochimica Acta, 60(6):1019-1040.

Soetaert K, PMJ Herman and JJ Middelburg, 1996b. Dynamic response of deep-sea sediments to seasonal variation: a model. Limnol. Oceanogr. 41(8): 1651-1668.

# APPENDIX

## Parameters and default values.

```r
knitr:::kable(FESDIAparms())
```

| | parms | units | description |
|---|---:|---|---|
| Cflux | 4.566210e+02 | nmolC/cm2/d | total organic C deposition |
| pFast | 9.000000e-01 | - | part FDET in carbon flux |
| FeOH3flux | 1.000000e+00 | nmol/cm2/d | deposition rate of FeOH3 |
| CaPflux | 0.000000e+00 | nmol/cm2/d | deposition rate of CaP |
| rFast | 6.849320e-02 | /d | decay rate FDET |
| rSlow | 1.370000e-04 | /d | decay rate SDET |
| NCrFdet | 1.509434e-01 | molN/molC | NC ratio FDET |
| NCrSdet | 1.509434e-01 | molN/molC | NC ratio SDET |
| PCrFdet | 9.434000e-03 | molP/molC | PC ratio FDET |
| PCrSdet | 9.434000e-03 | molP/molC | PC ratio SDET |
| BCupLiq | 2.000000e+00 | - | upper boundary liq. 1:flux, 2:conc, 3:0-grad |
| BCdownLiq | 3.000000e+00 | - | lower boundary liq. 1:flux, 2:conc, 3:0-grad |
| O2bw | 3.000000e+02 | mmol/m3 | upper boundary O2 -if BC=1: flux, 2:conc |
| NO3bw | 1.000000e+01 | mmol/m3 | upper boundary NO3 -if BC=1: flux, 2:conc |
| NO2bw | 0.000000e+00 | mmol/m3 | upper boundary NO2 -if BC=1: flux, 2:conc |
| NH3bw | 1.000000e+00 | mmol/m3 | upper boundary NH3 -if BC=1: flux, 2:conc |
| CH4bw | 0.000000e+00 | mmol/m3 | upper boundary CH4 -if BC=1: flux, 2:conc |
| PO4bw | 5.000000e-01 | mmol/m3 | upper boundary PO4 -if BC=1: flux, 2:conc |
| DICbw | 2.100000e+03 | mmol/m3 | upper boundary DIC -if BC=1: flux, 2:conc |
| Febw | 0.000000e+00 | mmol/m3 | upper boundary Fe2+ -if BC=1: flux, 2:conc |
| H2Sbw | 0.000000e+00 | mmol/m3 | upper boundary H2S -if BC=1: flux, 2:conc |
| SO4bw | 3.100000e+04 | mmol/m3 | upper boundary SO4 -if BC=1: flux, 2:conc |
| ALKbw | 2.400000e+03 | mmol/m3 | upper boundary alkalinity -if BC=1: flux, 2:conc |
| O2dw | NA | mmol/m3 | lower boundary O2 -if BC=1: flux, 2:conc |
| NO3dw | NA | mmol/m3 | lower boundary NO3 -if BC=1: flux, 2:conc |
| NO2dw | NA | mmol/m3 | lower boundary NO2 -if BC=1: flux, 2:conc |
| NH3dw | NA | mmol/m3 | lower boundary NH3 -if BC=1: flux, 2:conc |
| CH4dw | NA | mmol/m3 | lower boundary CH3 -if BC=1: flux, 2:conc |
| PO4dw | NA | mmol/m3 | lower boundary PO4 -if BC=1: flux, 2:conc |
| DICdw | NA | mmol/m3 | lower boundary DIC -if BC=1: flux, 2:conc |
| Fedw | NA | mmol/m3 | lower boundary Fe2+ -if BC=1: flux, 2:conc |
| H2Sdw | NA | mmol/m3 | lower boundary H2S -if BC=1: flux, 2:conc |
| SO4dw | NA | mmol/m3 | lower boundary SO4 -if BC=1: flux, 2:conc |
| ALKdw | NA | mmol/m3 | lower boundary alkalinity -if BC=1: flux, 2:conc |
| w | 2.700000e-06 | cm/d | advection rate |
| biot | 2.739700e-03 | cm2/d | bioturbation coefficient |
| biotdepth | 5.000000e+00 | cm | depth of mixed layer |
| biotatt | 1.000000e+00 | /cm | attenuation coeff below biotdepth |
| irr | 0.000000e+00 | /d | bio-irrigation rate |
| irrdepth | 5.000000e+00 | cm | depth of irrigated layer |
| irratt | 1.000000e+00 | cm | attenuation coeff below irrdepth |
| gasflux | 0.000000e+00 | cm/d | piston velocity for dry flats |
| NH3Ads | 1.300000e+00 | - | Adsorption coeff ammonium |
| rnitri1 | 2.000000e+01 | /d | Max nitrification rate step1 (NH3ox) |
| rnitri2 | 2.000000e+01 | /d | Max nitrification rate step2 (NO2ox) |

| | parms | units | description |
|---|---|---|---|
| ranammox | 1.000000e-01 | /(mmol/m3)/d | Anammox rate |
| ksO2nitri | 1.000000e+00 | mmolO2/m3 | half-sat O2 in nitrification |
| ksO2oxic | 3.000000e+00 | mmolO2/m3 | half-sat O2 in oxic mineralisation |
| ksNO3denit | 3.000000e+01 | mmolNO3/m3 | half-sat NO3 in denitrification |
| kinO2denit | 1.000000e+00 | mmolO2/m3 | half-sat O2 inhib denitrification |
| kinNO3anox | 1.000000e+00 | mmolNO3/m3 | half-sat NO3 inhib anoxic degr |
| kinO2anox | 1.000000e-03 | mmolO2/m3 | half-sat O2 inhib anoxic min |
| temperature | 1.000000e+01 | dgC | temperature |
| salinity | 3.500000e+01 | psu | salinity |
| TOC0 | 5.000000e-01 | % | refractory Carbon conc |
| rFePadsorp | 1.000000e-06 | /d | rate FeP adsorption |
| rCaPprod | 0.000000e+00 | /d | rate CaP production |
| rCaPdiss | 0.000000e+00 | /d | rate CaP dissolution |
| CPrCaP | 2.869565e-01 | mol/mol | C:Pratio in CaP |
| rPads | 0.000000e+00 | /d | adsorption rate PO4 |
| rPdes | 0.000000e+00 | /d | desorption rate of adsorbed P |
| maxPads | 1.000000e+03 | mmolP/m3solid | Max adsorbed P concentration |
| ksFeOH3 | 1.250000e+04 | mmolFeOH3/m3 | half-sat FeOH3 conc in iron reduction |
| kinFeOH3 | 1.250000e+04 | mmolFeOH3/m3 | half-sat FeOH3 inhibition S reduction |
| ksSO4BSR | 1.600000e+03 | mmolS/m3 | half-sat SO4 conc in sulphate reduction |
| kinSO4Met | 1.000000e+03 | mmolS/m3 | half-sat SO4 inhibition methanogenesis |
| rFeox | 3.000000e-01 | /(mmol/m3)/d | Max rate Fe oxidation |
| rH2Sox | 5.000000e-04 | /(mmol/m3)/d | Max rate H2S oxidation |
| rFeS | 1.000000e-03 | /(mmol/m3)/d | maximum rate FeS production |
| rCH4ox | 2.700000e+01 | /(mmol/m3)/d | Max rate CH4 oxidation with O2 |
| rAOM | 3.000000e-05 | /(mmol/m3)/d | Max rate anaerobic oxidation Methane |
| rSurfH2Sox | 0.000000e+00 | /d | Max rate H2S oxidation with BW O2 |
| rSurfCH4ox | 0.000000e+00 | /d | Max rate CH4 oxidation with BW O2 |
| ksSurfALK | 3.000000e+03 | mmol/m3 | half-sat Alkalinity in oxidation of H2S/CH4 with bwO2 |
| ksO2reox | 1.000000e+00 | mmolO2/m3 | half-sat Oxygen in oxidation of H2S/CH4 with bwO2 |
| ODUoxdepth | 5.000000e+00 | cm | Max depth H2S/CH4 oxidation with BW O2 |
| ODUoxatt | 1.000000e+00 | /cm | depth attenuation ODU oxidation |
| por0 | 9.000000e-01 | - | surface porosity |
| pordeep | 5.000000e-01 | - | deep porosity |
| porcoeff | 3.000000e-01 | cm | porosity decay coefficient |
| formationtype | 1.000000e+00 | - | formationfactor, 1=sand,2=fine sand,3=general |
| dilution | 0.000000e+00 | /d | relaxation towards background conc |
| Hwater | 1.000000e+01 | cm | height of water over core |
| Cfall | 1.000000e+02 | cm/d | fall speed of organic C (FDET, SDET) |
| FePfall | 1.000000e+02 | cm/d | fall speed of FeP |
| FeOH3fall | 1.000000e+02 | cm/d | fall speed of FeOH3 |
| CaPfall | 1.000000e+02 | cm/d | fall speed of CaP |
| addalk | 1.000000e+00 | - | solve for alkalinity |
| MPBprod | 0.000000e+00 | mmol/m3/d | maximal MPB production rate |
| kMPB | 4.000000e+00 | /cm | sedimentary light extinction coefficient |
| kDINupt | 1.000000e-02 | mmol/m3 | DIN limitation constant MPB |
| kPO4upt | 1.000000e-03 | mmol/m3 | P limitation constant MPB |
| kDICupt | 1.000000e+00 | mmol/m3 | C limitation constant MPB |

## State variables

```r
knitr:::kable(FESDIAsvar())
```

| names | units | description |
|---|---|---|
| FDET | mmolC/m3 solid | Fast decaying Detritus (solid) |
| SDET | mmolC/m3 solid | Slow decaying Detritus (solid) |
| O2 | mmolO/m3 liquid | Oxygen (liquid) |
| NO3 | mmolN/m3 liquid | Nitrate (liquid) |
| NO2 | mmolN/m3 liquid | Nitrite (liquid) |
| NH3 | mmolN/m3 liquid | Ammonium/ammonia (liquid) |
| DIC | mmolC/m3 liquid | Dissolved Inorganic Carbon (liquid) |
| Fe | mmolFe/m3 liquid | Fe2+ (liquid) |
| FeOH3 | mmolFe/m3 solid | Fe-oxide (solid) |
| H2S | mmolS/m3 liquid | Sulphide (liquid) |
| SO4 | mmolS/m3 liquid | Sulphate (liquid) |
| CH4 | mmolC/m3 liquid | Methane (liquid) |
| PO4 | mmolP/m3 liquid | Phosphate (liquid) |
| FeP | mmolP/m3 solid | Iron-bound P (solid) |
| CaP | mmolP/m3 solid | Ca-bound P (solid) |
| Pads | mmolP/m3 solid | Adsorbed P (solid) |
| ALK | mmol/m3 liquid | Alpkalinity (liquid) |

## Zero-D ordinary variables

```r
knitr:::kable(FESDIA0D())
```

| names | values | units | description |
|---|---|---|---|
| O2flux | NA | nmolO2/cm2/d | O2 influx sediment-water |
| O2deepflux | NA | nmolO2/cm2/d | O2 efflux lower boundary |
| NO3flux | NA | nmolN/cm2/d | NO3 influx sediment-water |
| NO3deepflux | NA | nmolN/cm2/d | NO3 efflux lower boundary |
| NO2flux | NA | nmolN/cm2/d | NO2 influx sediment-water |
| NO2deepflux | NA | nmolN/cm2/d | NO2 efflux lower boundary |
| NH3flux | NA | nmolN/cm2/d | NH3 influx sediment-water |
| NH3deepflux | NA | nmolN/cm2/d | NH3 efflux lower boundary |
| PO4flux | NA | nmolP/cm2/d | PO4 influx sediment-water |
| PO4deepflux | NA | nmolP/cm2/d | PO4 efflux lower boundary |
| DICflux | NA | nmolC/cm2/d | DIC influx sediment-water |
| DICdeepflux | NA | nmolC/cm2/d | DIC efflux lower boundary |
| Feflux | NA | nmolFe/cm2/d | Fe2+ influx sediment-water |
| Fedeepflux | NA | nmolFe/cm2/d | Fe2+ efflux lower boundary |
| H2Sflux | NA | nmolS/cm2/d | H2S influx sediment-water |
| H2Sdeepflux | NA | nmolS/cm2/d | H2S efflux lower boundary |
| SO4flux | NA | nmolS/cm2/d | SO4 influx sediment-water |
| SO4deepflux | NA | nmolS/cm2/d | SO4 efflux lower boundary |
| CH4flux | NA | nmolC/cm2/d | CH4 influx sediment-water |
| CH4deepflux | NA | nmolC/cm2/d | CH4 efflux lower boundary |
| ALKflux | NA | nmol/cm2/d | Alkalinity influx sediment-water |
| ALKdeepflux | NA | nmol/cm2/d | Alkalinity efflux lower boundary |
| FDETflux | NA | nmolC/cm2/d | FDET flux to sediment |

| names | values | units | description |
|---|---|---|---|
| FDETdeepflux | NA | nmolC/cm2/d | FDET efflux lower boundary |
| SDETflux | NA | nmolC/cm2/d | SDET flux to sediment |
| SDETdeepflux | NA | nmolC/cm2/d | SDET efflux lower boundary |
| FePsurfflux | NA | nmolP/cm2/d | FeP flux upper boundary |
| FePdeepflux | NA | nmolP/cm2/d | FeP efflux lower boundary |
| CaPsurfflux | NA | nmolP/cm2/d | CaP flux upper boundary |
| CaPdeepflux | NA | nmolP/cm2/d | CaP efflux lower boundary |
| FeOH3surfflux | NA | nmolFe/cm2/d | FeOH3 flux upper boundary |
| FeOH3deepflux | NA | nmolFe/cm2/d | FeOH3 efflux lower boundary |
| OrgCflux | NA | nmolC/cm2/d | OrgC influx to sediment |
| OrgNflux | NA | nmolN/cm2/d | OrgN influx to sediment |
| OrgPflux | NA | nmolP/cm2/d | OrgP influx to sediment |
| DINDIPflux | NA | molN/molP | DIN:DIP ratio flux sediment-water |
| DINDIPmean | NA | molN/molP | DIN:DIP mean concentration |
| DINDIPdeep | NA | molN/molP | DIN:DIP deep concentration |
| TotMin | NA | nmolC/cm2/d | Vertically integrated Mineralisation |
| TotOxic | NA | nmolC/cm2/d | Vertically integrated oxic Mineralisation |
| TotDenit | NA | nmolC/cm2/d | Vertically integrated Denitrification |
| TotFered | NA | nmolC/cm2/d | Vertically integrated Iron reduction |
| TotBSR | NA | nmolC/cm2/d | Vertically integrated Sulphate reduction |
| TotMeth | NA | nmolC/cm2/d | Vertically integrated Methanogenesis |
| PartOxic | NA | - | Part of mineralisation by oxic min |
| PartDenit | NA | - | Part of mineralisation by denitrification |
| PartFered | NA | - | Part of mineralisation by iron reduction |
| PartBSR | NA | - | Part of mineralisation by sulphate reduction |
| PartMethano | NA | - | Part of mineralisation by methanogenisis |
| TotNitri1 | NA | nmolN/cm2/d | Vertically integrated nitrification step 1 (NH3 ox) |
| TotNitri2 | NA | nmolN/cm2/d | Vertically integrated nitrification step 2 (NO2 ox) |
| TotAnammox | NA | nmolN/cm2/d | Vertically integrated anammox |
| TotFeoxid | NA | nmolFe/cm2/d | Vertically integrated Fe2+ oxidation |
| TotH2Soxid | NA | nmolS/cm2/d | Vertically integrated H2S oxidation |
| TotCH4oxid | NA | nmolC/cm2/d | Vertically integrated CH4 oxidation |
| TotAOM | NA | nmolS/cm2/d | Vertically integrated Anaerobic oxidation methane |
| TotFeSprod | NA | nmolFe/cm2/d | Vertically integrated FeS production |
| TotFePprod | NA | nmolFe/cm2/d | Vertically integrated FeP production |
| TotCaPprod | NA | nmolP/cm2/d | Vertically integrated CaP production |
| TotFePdesorp | NA | nmolP/cm2/d | Vertically integrated FeP desorption |
| TotCaPdiss | NA | nmolP/cm2/d | Vertically integrated CaP dissolution |
| TotPadsorb | NA | nmolP/cm2/d | Vertically integrated P adsorption |
| TotNH3prod | NA | nmolN/cm2/d | Vertically integrated NH3 production |
| TotPO4prod | NA | nmolP/cm2/d | Vertically integrated PO4 production |
| TotNH3ads | NA | nmolN/cm2/d | Vertically integrated NH3 adsorption |
| TotO2prod | NA | nmolO/cm2/d | Vertically integrated O2 production (?) |
| TotH2Soxsurf | NA | nmolS/cm2/d | Vertically integrated H2S oxidation by surface O2 |
| TotCH4oxsurf | NA | nmolC/cm2/d | Vertically integrated CH4 oxidation by surface O2 |
| TotALkprod | NA | nmol/cm2/d | Total alkalinity production |
| PartPremoved | NA | - | Part P removed |
| PartNremoved | NA | - | Part N removed |
| TotMPBNO3uptake | NA | nmolN/cm2/d | Vertically integrated MPB NO3 uptake |
| TotMPBNH3uptake | NA | nmolN/cm2/d | Vertically integrated MPB NH3 uptake |
| TotMPBPO4uptake | NA | nmolP/cm2/d | Vertically integrated MPB PO4 uptake |
| TotMPBDICuptake | NA | nmolC/cm2/d | Vertically integrated MPB DIC uptake |

| names | values | units | description |
|---|---|---|---|
| TotMPBO2prod | NA | nmolO2/cm2/d | Vertically integrated MPB O2 production |
| TotalFDET | NA | nmolC/cm2 | Vertically integrated Fast decaying Detritus |
| TotalSDET | NA | nmolC/cm2 | Vertically integrated Slow decaying Detritus |
| TotalO2 | NA | nmolO/cm2 | Vertically integrated Oxygen |
| TotalNO3 | NA | nmolN/cm2 | Vertically integrated Nitrate |
| TotalNO2 | NA | nmolN/cm2 | Vertically integrated Nitrite |
| TotalNH3 | NA | nmolN/cm2 | Vertically integrated Ammonium/ammonia |
| TotalDIC | NA | nmolC/cm2 | Vertically integrated Dissolved Inorganic Carbon |
| TotalFe | NA | nmolFe/cm2 | Vertically integrated Fe |
| TotalFeOH3 | NA | nmolFe/cm2 | Vertically integrated FeOH3 |
| TotalH2S | NA | nmolS/cm2 | Vertically integrated H2S |
| TotalSO4 | NA | nmolS/cm2 | Vertically integrated SO4 |
| TotalCH4 | NA | nmolC/cm2 | Vertically integrated CH4 |
| TotalPO4 | NA | nmolP/cm2 | Vertically integrated Phosphate |
| TotalFeP | NA | nmolP/cm2 | Vertically integrated Iron-bound P |
| TotalCaP | NA | nmolP/cm2 | Vertically integrated Ca-bound P |
| TotalPads | NA | nmolP/cm2 | Vertically integrated Adsorbed P |
| Cflux | NA | nmolC/cm2/d | Carbon flux to sediment |
| FeOH3flux | NA | nmolP/cm2/d | FeOH3 flux to sediment |
| CaPflux | NA | nmolP/cm2/d | CaP flux to sediment |
| w | NA | cm/d | Sedimentation rate |
| biotfac | NA | - | Bioturbation multiplication factor |
| irrfac | NA | - | Irrigation multiplication factor |
| rFast | NA | /d | Decay rate FDET |
| rSlow | NA | /d | Decay rate SDET |
| pFast | NA | - | Part FDET in flux |
| MPBprod | NA | mmol/m3/d | MicroPhytoBenthos forcing |
| gasflux | NA | cm/d | Gas exchange flux (piston velocity) |
| bwO2 | NA | mmol/m3 | Bottom water O2 concentration |
| bwNO3 | NA | mmol/m3 | Bottom water NO3 concentration |
| bwNO2 | NA | mmol/m3 | Bottom water NO2 concentration |
| bwNH3 | NA | mmol/m3 | Bottom water NH3 concentration |
| bwCH4 | NA | mmol/m3 | Bottom water CH4 concentration |
| bwFe | NA | mmol/m3 | Bottom water Fe concentration |
| bwH2S | NA | mmol/m3 | Bottom water H2S concentration |
| bwSO4 | NA | mmol/m3 | Bottom water SO4 concentration |
| bwPO4 | NA | mmol/m3 | Bottom water PO4 concentration |
| bwDIC | NA | mmol/m3 | Bottom water DIC concentration |
| bwALK | NA | mmol/m3 | Bottom water alkalinity concentration |
| Hwater | NA | cm | Height of water above the sediment |
| Ratefactor | NA | - | Rate multiplication factor |

## One-D ordinary variables

```
knitr:::kable(FESDIA1D())
```

| names | units | description |
|---|---|---|
| TOC | % | Total Organic Carbon % profile |
| DICprodMin | nmolC/cm3 liquid/d | DIC production profile (mineralisation) |
| DINprodMin | nmolN/cm3 liquid/d | DIN production profile (mineralisation) |

| names | units | description |
|---|---|---|
| DIPprodMin | nmolP/cm3 liquid/d | DIP production profile (mineralisation) |
| O2prod | nmolO/cm3 liquid/d | O2 production profile (microphytobenthos) |
| Oxicmin | nmolC/cm3 liquid/d | Oxic mineralisation profile |
| Denitrific | nmolC/cm3 liquid/d | Denitrification profile |
| Feredmin | nmolC/cm3 liquid/d | Fe reduction mineralisation profile |
| BSRmin | nmolC/cm3 liquid/d | Sulphate reduction mineralisation profile |
| Methmin | nmolC/cm3 liquid/d | Methanogensis mineralisation profile |
| nitri1 | nmolN/cm3 liquid/d | Nitrification step 1 profile (NH3 oxidation) |
| nitri2 | nmolN/cm3 liquid/d | Nitrification step 2 profile (NO2 oxidation) |
| Anammox | nmolN/cm3 liquid/d | Anammox profile |
| Feoxid | nmolFe/cm3 liquid/d | Fe2+ oxidation profile |
| H2Soxid | nmolS/cm3 liquid/d | H2S oxidaton profile |
| CH4oxid | nmolC/cm3 liquid/d | CH4 oxidation profile |
| AOM | nmolS/cm3 liquid/d | Anaerobic oxidation of methane profile |
| FeSprod | nmolFe/cm3 liquid/d | FeS production profile |
| FePadsorp | nmolFe/cm3 liquid/d | FeP adsorption profile |
| FePdesorp | nmolP/cm3 solid/d | FeP desorption profile |
| CaPprod | nmolP/cm3 liquid/d | CaP production profile |
| CaPdiss | nmolP/cm3 solid/d | CaP dissolution profile |
| Padsorb | nmolP/cm3 solid/d | P adsorption profile |
| H2Soxsurf | nmolS/cm3 liquid/d | H2S oxidation with surface O2 profile |
| CH4oxsurf | nmolC/cm3 liquid/d | CH4 oxidation with surface O2 profile |
| O2distConsump | nmolO/cm3 liquid/d | O2 uptake oxidation with surface O2 profile |
| ALKprod | nmol/cm3 liquid/d | Alkalinity production profile |
| DICprodCH4 | nmolC/cm3 liquid/d | DIC production via Methane profile |
| MPBCprod | nmolC/cm3 solid/d | MPB production profile |
| MPBuptakeNO3 | nmolN/cm3 liquid/d | MPB NO3 uptake profile |
| MPBuptakeNH3 | nmolN/cm3 liquid/d | MPB NH3 uptake profile |
| MPBuptakePO4 | nmolP/cm3 liquid/d | MPB PO4 uptake profile |
| MPBuptakeDIC | nmolC/cm3 liquid/d | MPB DIC uptake profile |