AKADEMIA GÓRNICZO-HUTNICZA
IM. STANISŁAWA STASZICA W KRAKOWIE
AGH UNIVERSITY OF SCIENCE
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Biblioteka Programu R:

ReacTran

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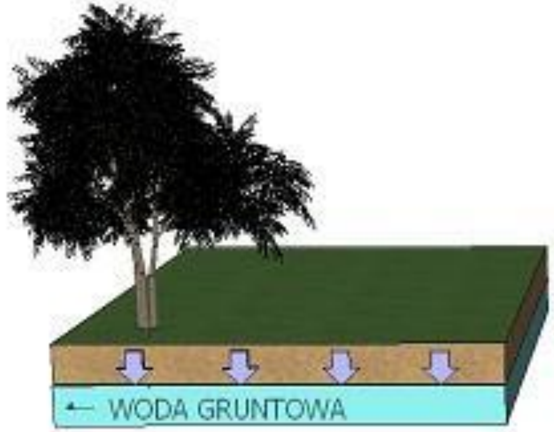
ReacTran

- Wersja: 1.4.3.1
- Tytuł: Reaktywne modelowanie transportu w 1d, 2d i 3d
- Autorzy: Karline Soetaert, Filip Meysman
- Data aktualizacji: 15.08.2017r.

Procedury opracowywania modeli opisujących reakcję i transport adwekcyjno-dyfuzyjny w jednym, dwóch lub trzech wymiarach. Obejmuje układy transportowe w mediach porowatych, ujściach rzek bądź ciałach o zmiennym kształcie.



- Rozkład zanieczyszczeń w rzekach, estuariach, jeziorach, środowiskach morskich
- Analiza składników odżywczych w rzekach, estuariach, jeziorach, środowiskach morskich
- Biogeochemiczne modele dla wód gruntowych
- Biogeochemiczne modele dla osadów, np. ściekowych
- Biogeochemiczne modele biofilmów
- Reakcje i transport w płaskich, cylindrycznych lub sferycznych ciałach, np. organizmy,
- Rozproszenie osobników na powierzchniach płaskich

Główne funkcje pakietu ReacTran

Function	R-package	Description
advection.1D	ReacTran	One-dimensional advection equation, includes TVD slope limiters
advection.volume.1D	ReacTran	One-dimensional advection equation, volumetric transport, includes TVD slope limiters
setup.grid.1D, setup.grid.2D	ReacTran	Creates a finite difference grid
setup.prop.1D, setup.prop.2D	ReacTran	Attaches a property to a grid
tran.1D, tran.2D, tran.3D	ReacTran	General advective-diffusive transport in 1D, 2D, 3D
tran.cylindrical, tran.polar, tran.spherical	ReacTran	Diffusive Transport in polar (*r*, theta), cylindrical (*r*, theta, z) and spherical (*r*, theta, phi) coordinates
tran.volume.1D	ReacTran	1-D Volumetric Advective-Diffusive Transport
ode.1D, ode.2D, ode.3D	deSolve	Integration of reactive transport models in 1D, 2D, 3D
steady.1D, steady.2D, steady.3D	rootSolve	Steady-state solution of reactive transport models in 1D, 2D, 3D

$$\frac{\partial \varphi C}{\partial t} = -\frac{1}{A_x}\cdot\frac{\partial(A_x \cdot J_x)}{\partial x} - \frac{1}{A_y}\cdot\frac{\partial\left(A_y \cdot J_y\right)}{\partial y} - \frac{1}{A_z}\cdot\frac{\partial(A_z \cdot J_z)}{\partial z} + \varphi \cdot R$$

Ogólne równanie bilansu masy

$$J_x = \varphi_x \cdot u_x \cdot C - \varphi_x \cdot \left(D_x \cdot \frac{\partial C}{\partial x}\right)$$

Strumień masy wzdłuż kierunku x

dC	the rate of change of the concentration C due to advective transport, defined in the centre of each grid cell. The rate of change is expressed per unit of (phase) volume [M/L^3/T].
adv.flux	advective flux across at the interface of each grid cell. A vector of length N+1 [M/L2/T] - only for advection.1D.
flux.up	flux across the upstream boundary, positive = INTO model domain. One value [M/L2/T] - only for advection.1D.
flux.down	flux across the downstream boundary, positive = OUT of model domain. One value [M/L2/T] - only for advection.1D.
adv.F	advective mass flow across at the interface of each grid cell. A vector of length N+1 [M/T] - only for advection.volume.1D.
F.up	mass flow across the upstream boundary, positive = INTO model domain. One value [M/T] - only for advection.volume.1D.
F.down	flux across the downstream boundary, positive = OUT of model domain. One value [M/T] - only for advection.volume.1D.
it	number of split time iterations that were necessary.

Główne dane wejściowe

N	the total number of grid cells [-]
x.up	position of the upstream interface; one value [L]
x.down	position of the downstream interface; one value [L]
x.mid	position of the middle of the grid cells; vector of length N [L]
x.int	position of the interfaces of the grid cells; vector of length N+1 [L]
dx	distance between adjacent cell interfaces (thickness of grid cells); vector of length N [L]

surf	the surface area
vol	the volume

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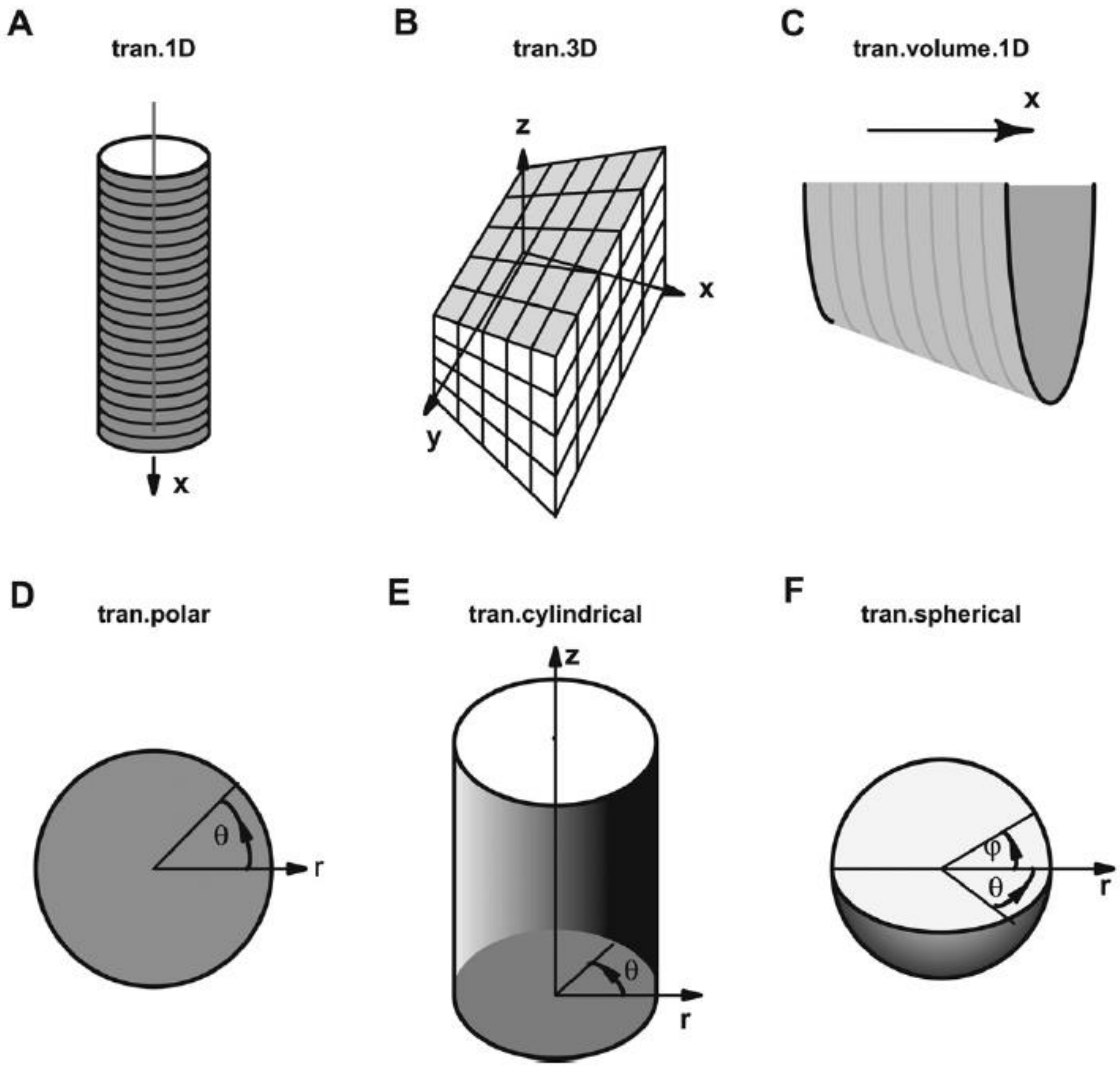
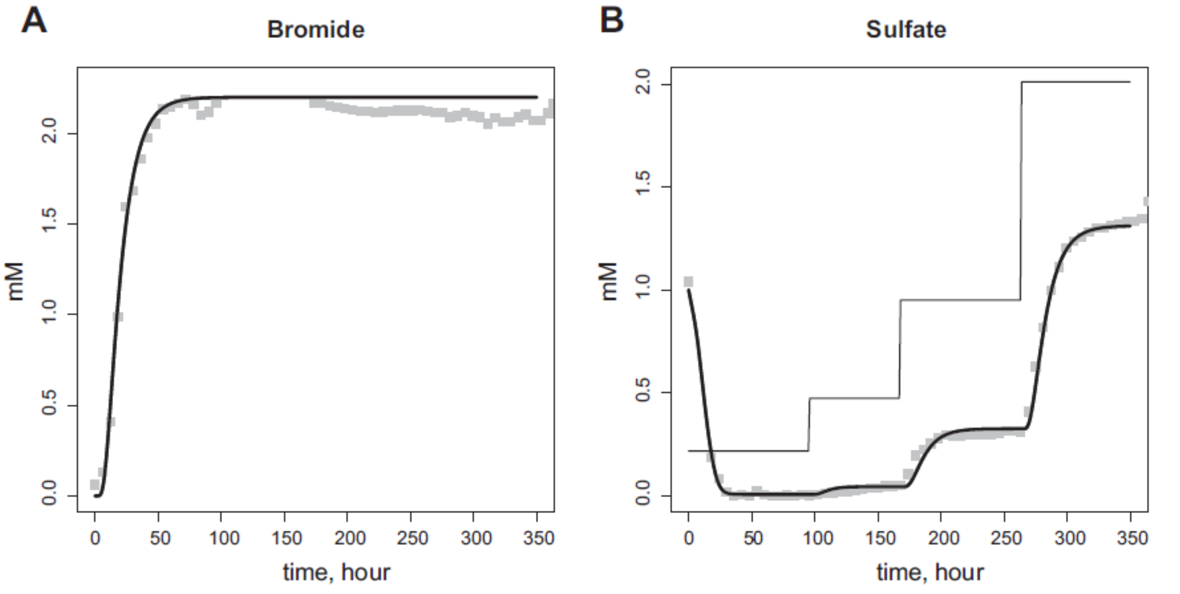
Niektóre kształty geometryczne obsługiwane przez pakiet ReacTran



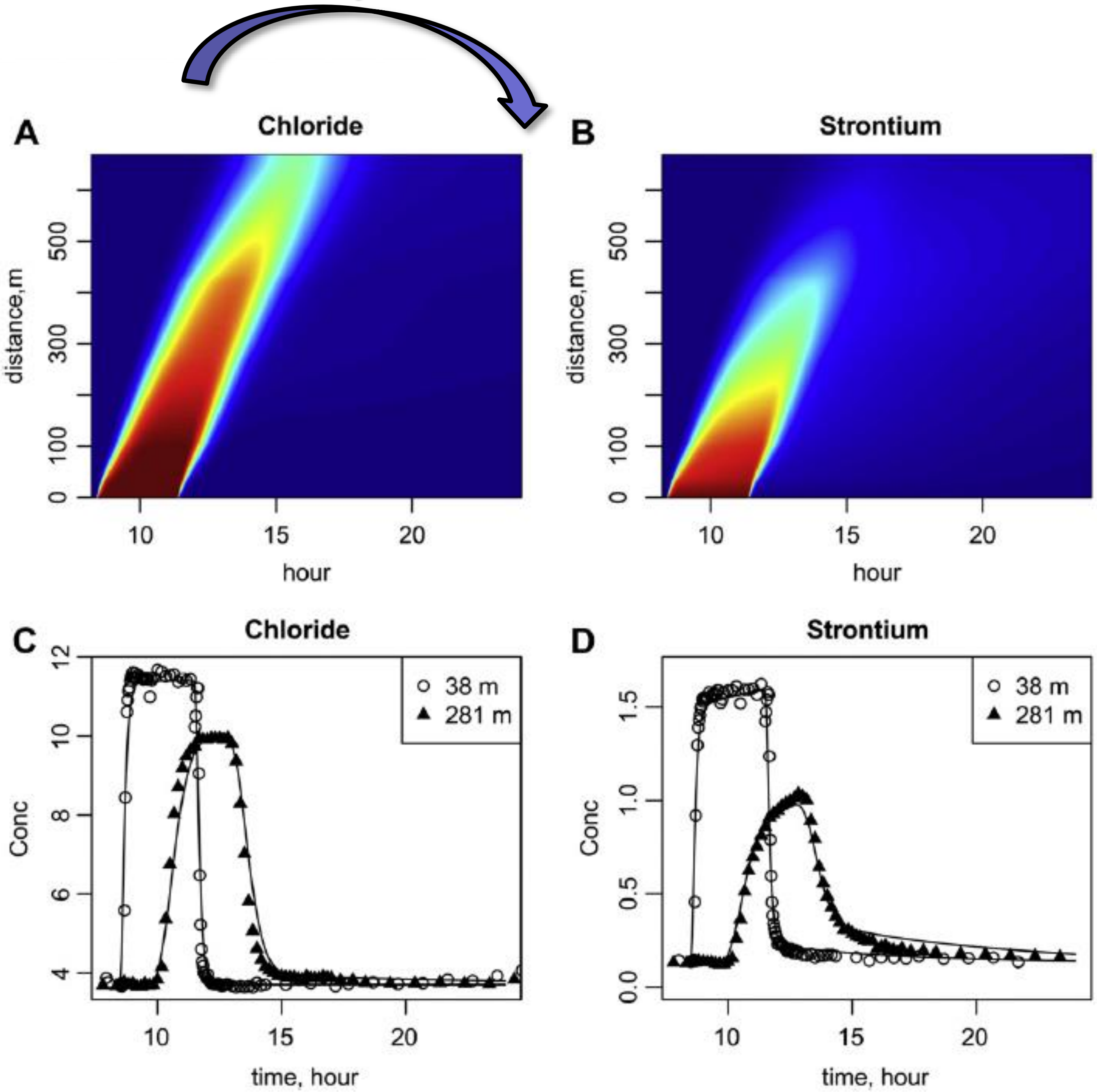
Zastosowanie laboratoryjne: dynamika siarczanu w osadzie w przepływowym bioreaktorze

```
library(ReacTran)

FTR.model = function (time, SO4, pars) {

    transport = tran.1D (C = SO4, flux.up = Flux, v = v, D = D, dx = grid)
    reaction  = r * SO4 / (ks+SO4)

    dSO4 = transport$dC - reaction

    list(dSO4, SO4out = SO4[N.layer])
}

# parameters
Flux = 0.006 ; D = 0.039 ; v = 0.092 ; ks = 0.16 ; r = 0.032

# the model grid
N.layer = 100
grid = setup.grid.1D(L = 2, N = N.layer)

# model solution and plotting
times  = seq (from = 0, to = 100, by = 1
SO4ini = rep(1, length.out = N.layer)
out    = ode.1D(func = FTR.model, y = SC
         nspec = 1)

plot(out, which = "SO4out", xlab = "time
     ylab = "mM", main = "Sulfate")
```



Zastosowanie praktyczne: eksperyment wstrzyknięcia znacznika w mały strumień

```
library(ReacTran)

Rivermodel = function (time, state, pars)
  C    = state[1         :Nb    ]  # concen
  Cs   = state[(Nb+1)    :(2*Nb)]  # concen
  Csed = state[(2*Nb+1) :(3*Nb)]  # sorbat

  Cup  = Cfun(time)                # upstre

  tranC = tran.volume.1D(C = C, C.up = Cup
                        flow = Q, Disp =

  exchange = alpha * (Cs - C)
  sorption = sorp *(Csed-C)

  dC    = tranC$dC + exchange + sorption *
  dCs   =          - exchange * area/area2
  dCsed =

  list(c(dC, dCs, dCsed))
)

# model grid
dx       = 1
riverlen = 669
Nb       = riverlen/dx                    #
xgrid    = setup.grid.1D(N = Nb, L = river

# parameters
area     = 0.52; area2    = 1.56; ased = 1
Vol      = area*dx
disp     = 0.40
D        = disp*area/dx
Q        = 0.0125
alpha    = 4.5e-5
qlat     = 2.151e-6; Clat     = 0.13
sorp     = 5.6e-5;   sorpS    = 1
kd       = 7e-5               # m3/mass
CsB      = 0.13

# Upstream concentration:  a time series
Time = c(8.25, 8.399, 8.400, 11.399, 11.4,
C_up = c(0.13,  0.13, 1.73,    1.73, 0.13,
Cfun = approxfun(Time, C_up, rule = 2)

# model solution and plotting30
```



Podsumowanie

1. Modele w pakiecie: krótkie, czytelne, sprawnie rozwiązane
2. Szeroki zakres procesów transportowych w środowisku wodnym
3. Model coraz częściej wykorzystywany w podejmowaniu decyzji i zarządzaniu zasobami naturalnymi

Dziękuję za uwagę.