Package ‘ReacTran’

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Version 1.1

Title Reactive transport modelling in 1D and 2D

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Depends R (>= 2.01), rootSolve, deSolve, shape

Description Routines for developing models that describe reaction and advective-diffusive transport in one or two dimensions. Includes transport routines in porous media, in estuaries, and in bodies with variable shape.

License GPL

LazyData yes

R topics documented:

ReacTran-package — *Reactive transport modelling in 1D or 2-D*

Description

R-package ReacTran contains routines that enable the development of one-dimensional and two-dimensional reactive transport models in aquatic systems (rivers, lakes) as well porous media (floc aggregates, sediments,...).

It contains:

- Functions to setup a finite-difference grid (1D or 2D)
- Functions to attach parameters and properties to the grid (1D or 2D)
- Functions to calculate the advective-diffusive transport term over the grid (1D or 2D)
- Utility functions

Details

Package:	ReacTran
Type:	Package
Version:	1.0
Date:	2009-02-02
License:	GNU Public License 2 or above

Author(s)

Karline Soetaert (Maintainer)

Filip Meysman

Examples

```
## Not run:
## show examples (see respective help pages for details)
example(tran.1D)
example(tran.2D)

## open the directory with documents
browseURL(paste(system.file(package="ReacTran"), "/doc", sep=""))

## End(Not run)
```

fiadeiro — *Advective finite difference weights*

Description

Weighing coefficients used in the finite difference scheme for advection calculated according to Fiadeiro and Veronis (1977).

This particular AFDW (advective finite difference weights) scheme switches from backward differencing (in advection dominated conditions; large Peclet numbers) to central differencing (under diffusion dominated conditions; small Peclet numbers).

This way it forms a compromise between stability, accuracy and reduced numerical dispersion.

Usage

```
fiadeiro(v, D, dx.aux, grid=list(dx.aux=dx.aux))
```

Arguments

`v`	advective velocity; either one value or a vector of length N+1, with N the number of grid cells [L/T].
`D`	diffusion coefficient; either one value or a vector of length N+1 [L2/T].
`dx.aux`	auxiliary vector containing the distances between the locations where the concentration is defined (i.e. the grid cell centers and the two outer interfaces); either one value or a vector of length N+1.
`grid`	discretization grid as calculated by `setup.grid.1D`.

Details

The Fiadeiro and Veronis (1977) scheme adapts the differencing method to the situation at hand (either advection or diffusion dominance).

It is based on the following rationale:

- When using forward differences (AFDW = 0), the scheme is first order accurate, creates a low level of (artificial) numerical dispersion, but is highly unstable (state variables may become negative).
- When using backward differences (AFDW = 1), the scheme is first order accurate, is universally stable (state variables always remain positive), but the scheme creates high levels of numerical dispersion.
- When using central differences (AFDW = 0.5), the scheme is second order accurate, is not universally stable, and has a moderate level of numerical dispersion, but state variables may become negative.

Because of this instability issue, forward schemes should be avoided. Because of its higher accuracy, the central scheme is preferred over the backward scheme.

The central scheme is stable when sufficient physical dispersion is present, it may become unstable when advection is the only transport process.

The Fiadeiro and Veronis (1977) scheme takes this into account: it uses central differencing when possible (when physical diffusion is high enough), and switches to backward differing when needed (when advection dominates). The switching is detrmined by the Peclet number `Pe = abs(v)*dx.aux/D`.

- the higher the diffusion `D` (`Pe > 1`), the closer the AFDW coefficients are to 0.5 (central differencing)
- the higher the advection `v` (`Pe < 1`), the closer the AFDW coefficients are to 1 (backward differencing)

Value

the Advective Finite Difference Weighing (AFDW) coefficients as used for the transport routines `tran.1D` and `tran.volume.1D`; either one value or a vector of length N+1

Note

- If the state variables (concentrations) decline in the direction of the 1D axis, then central difference schme will be stable. If known a prioiri, under these circumstances, central differencing is to be preferred over the fiadeiro scheme.
- Each scheme will always create some numerical diffusion. this depends on the resolution of the grid (i.e. the magnitude of `dx.aux`). In order to reduce numerical dispersion, one should increase the grid resolution (i.e. decrease `dx.aux`).

Author(s)

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References

- Fiadeiro ME and Veronis G (1977) Weighted-mean schemes for finite-difference approximation to advection-diffusion equation. Tellus 29, 512-522.
- Boudreau (1997) Diagnetic models and their implementation. Chapter 8: Numerical Methods. Springer.

Examples

```
#==============================================================================
# Model formulation (set of differential equations)
#==============================================================================

# This is a test model to evaluate the different finite difference formulas
# and evaluate their effect on munerical diffusion. The model describes the
# decay of organic carbon (OC) as it settles through the ocean water column.

model <- function (time,OC,pars,AFDW=1)
{
dOC <- tran.1D(OC,flux.up=F_OC,D=D.eddy,v=v.sink,AFDW=AFDW,dx=dx)$dC - k*OC
return(list(dOC))
}
#==============================================================================
# Parameter set
#==============================================================================

L <- 1000          # water depth model domain [m]
x.att <- 200       # attenuation depth [m]
v.sink.0 <- 10     # sinking velocity at the surface [m d-1]
D.eddy <- 10       # eddy diffusion coefficient [m2 d-1]
F_OC <- 10         # particle flux [mol m-2 d-1]
k <- 0.1           # decay coefficient [d-1]

#==============================================================================
# Model solution for a coarse grid (10 grid cells)
#==============================================================================

# Setting up the grid
```

```
N <- 10                              # number of grid layers
dx <- L/N                            # thickness of boxes [m]
dx.aux <- rep(dx,(N+1))              # auxilliary grid vector
x.int <- seq(from=0,to=L,by=dx)      # water depth at box interfaces [m]
x.mid <- seq(from=dx/2,to=L,by=dx)   # water depth at box centres [m]

# Exponentially declining sink velocity
v.sink <- v.sink.0*exp(-x.int/x.att) # sink velocity [m d-1]
Pe <- v.sink*dx/D.eddy               # Peclet number

# Calculate the weighing coefficients
AFDW <- fiadeiro(v=v.sink,D=D.eddy,dx.aux=dx.aux)

par(mfrow=c(2,1),cex.main=1.2,cex.lab=1.2)

# Plot the Peclet number over the grid

matplot(Pe,x.int,log="x",pch=19,ylim=c(L,0),xlim=c(0.1,1000),
xlab="",ylab="depth [m]",main=expression("Peclet number"),axes=FALSE)
abline(h = 0)
axis(pos=NA, side=2)
axis(pos=0, side=3)

# Plot the AFDW coefficients over the grid

matplot(AFDW,x.int,pch=19,ylim=c(L,0),xlim=c(0.5,1),
xlab="",ylab="depth [m]",main=expression("AFDW coefficient"),axes=FALSE)
abline(h = 0)
axis(pos=NA, side=2)
axis(pos=0, side=3)

# Three steady-state solutions for a coarse grid based on:
# (1) backward differences (BD)
# (2) central differences (CD)
# (3) Fiadeiro & Veronis scheme (FV)

BD <- steady.band(y=runif(N), func=model, AFDW=1.0, nspec=1)$y
CD <- steady.band(y=runif(N), func=model, AFDW=0.5, nspec=1)$y
FV <- steady.band(y=runif(N), func=model, AFDW=AFDW, nspec=1)$y
CONC <- cbind(BD,CD,FV)

par(mfrow=c(1,2))

# Plotting output
matplot(CONC,x.mid,pch=16,type="b",ylim=c(L,0),
xlab="",ylab="depth [m]",main=expression("conc (Low resolution grid)"),
axes=FALSE)
abline(h = 0)
axis(pos=0, side=2)
axis(pos=0, side=3)
legend("bottomright",
legend=c("backward diff","centred diff","Fiadeiro&Veronis")
,col=c(1:3),lty=c(1:3),pch=c(16,16,16))

#==============================================================================
# Model solution for a fine grid (1000 grid cells)
#==============================================================================
```

```
# Setting up the grid
N <- 1000                               # number of grid layers
dx <- L/N                               # thickness of boxes[m]
dx.aux <- rep(dx,(N+1))                 # auxilliary grid vector
x.int <- seq(from=0,to=L,by=dx)         # water depth at box interfaces [m]
x.mid <- seq(from=dx/2,to=L,by=dx)      # water depth at box centres [m]

# Exponetially declining sink velocity
v.sink <- v.sink.0*exp(-x.int/x.att) # sink velocity [m d-1]
Pe <- v.sink*dx/D.eddy                  # Peclet number

# Calculate the weighing coefficients
AFDW <- fiadeiro(v=v.sink,D=D.eddy,dx.aux=dx.aux)

# Three steady-state solutions for a coarse grid based on:
# (1) backward differences (BD)
# (2) centered differences (CD)
# (3) Fiadeiro & Veronis scheme (FV)

BD <- steady.band(y=runif(N), func=model, AFDW=1.0, nspec=1)$y
CD <- steady.band(y=runif(N), func=model, AFDW=0.5, nspec=1)$y
FV <- steady.band(y=runif(N), func=model, AFDW=AFDW, nspec=1)$y
HR_CONC <- cbind(BD,CD,FV)

# Plotting output
matplot(HR_CONC,x.mid,pch=16,type="b",ylim=c(L,0),
xlab="",ylab="depth [m]",main=expression("conc (High resolution grid)"),
axes=FALSE)
abline(h = 0)
axis(pos=0, side=2)
axis(pos=0, side=3)
legend("bottomright",
legend=c("backward diff","centred diff","Fiadeiro&Veronis")
,col=c(1:3),lty=c(1:3),pch=c(16,16,16))

# Results and conclusions:
# - For the fine grid, all three solutions are identical
# - For the coarse grid, the BD and FV solutions show numerical dispersion
```

`p.exp.increase` *Properties to be used with setup.prop.1D*

Description

Functions that define properties as a function of x. To be used with setup.prop.1D

- `p.exp.increase`: exponentially increasing function

$$y = y_0 + (y_0 - y_{\text{inf}}) \exp(-\max(0, x - x_0)/x_a)$$

- `p.exp.decrease`: exponentially decreasing function

$$y = 1 - (y_0 + (y_0 - y_{\text{inf}}) \exp(-\max(0, x - x_0)/x_a))$$

- `p.sphere.surf, p.sphere.vol` the surface and volume of a sphere
- `p.spheroid.surf, p.spheroid.vol` the surface and volume of a spheroid
- `p.cylinder.surf, p.cylinder.vol` the surface and volume of a cylinder; note that the surface ignores the top and bottom.

Usage

```
p.exp.decrease (x, x.0=0, y.0=1, y.inf=0.5, x.att=1)

p.exp.increase (x, x.0=0, y.0=1, y.inf=0.5, x.att=1)

p.sphere.surf (x)

p.sphere.vol (x)

p.spheroid.surf (x, b=1)

p.spheroid.vol (x, b=1)

p.cylinder.surf (x, L=1)

p.cylinder.vol (x, L=1)
```

Arguments

`x`	the x-values for which the property has to be estimated.
`x.0`	the x-offset; for `x <= x.0`, the value will be equal to `y.0`.
`y.0`	the y-value for `x <= x.0`.
`y.inf`	the y-value for `x` = infinite
`x.att`	the attenuation coefficient (exponential decrease value)
`b`	the ratio of long/short radius of the spheroid; if b<1: the spheroid is oblate.
`L`	the length of the cylinder

Value

the property value, estimated for each x-value.

Author(s)

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Examples

```
x<- seq(0,20,len=100)
plot(x, p.exp.increase(x),main="p.exp.increase")
lines(x, p.exp.increase(x,x.0 = 5))

x<- seq(0,20,len=100)
plot(x, p.exp.decrease(x),main="p.exp.decrease")
lines(x, p.exp.decrease(x,x.0 = 5))

mf <- par(mfrow=c(3,2))
```

```
plot(x, p.sphere.surf(x),main="p.sphere.surf")
plot(x, p.sphere.vol(x),main="p.sphere.vol")
plot(x, p.spheroid.surf(x,b=0.5),main="p.spheroid.surf")
plot(x, p.spheroid.vol(x,b=0.5),main="p.spheroid.vol")
plot(x, p.cylinder.surf(x,L=1),main="p.cylinder.surf")
plot(x, p.cylinder.vol(x,L=1),main="p.cylinder.vol")
par("mfrow"=mf)
```

`setup.compaction.1D` *Calculates the advective velocities of the pore water and the solid phase in a water saturated sediment assuming steady state compaction*

Description

This function calculates the advective velocities of the pore water and the solid phase in a sediment based on the assumption of steady state compaction.

The velocities of the pore water (`u`) and the solid phase (`v`) are calculated in the middle (`mid`) of the grid cells and the interfaces (`int`).

One needs to specify the porosity at the interface (`por.0`), the porosity at infinite depth (`por.inf`), as well as the advective velocity of the solid phase (either at the interface (`v.0`) or at infinite depth (`v.inf`)).

Usage

```
setup.compaction.1D(v.0 = NULL, v.inf = NULL, por.0, por.inf,
        por.grid)
```

Arguments

`v.0`	advective velocity of the solid phase at the sediment-water interface (also referred to as the sedimentation velocity); if `NULL` then `v.inf` must not be `NULL` [L/T].
`v.inf`	advective velocity of the solid phase at infinite depth (also referred to as the burial velocity); if `NULL` then `v.0` must not be `NULL` [L/T].
`por.0`	porosity at the sediment-water interface.
`por.inf`	porosity at infinite depth .
`por.grid`	porosity profile specified as a 1D grid property (see `setup.prop.1D` for details on the structure of this list).

Value

A list containing:

`u`	list with pore water advective velocities at the middle of the grid cells (`mid`) and at the interfaces (`int`).
`v`	list with solid phase advective velocities at the middle of the grid cells (`mid`) and at the interfaces (`int`).

Author(s)

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Examples

```
# setup of the 1D grid
L <- 10
grid <- setup.grid.1D(x.up=0,L=L,N=20)

# attaching an exponential porosity profile to the 1D grid

exp.profile <- function(x,y.0=NULL,y.inf=NULL,x.att=NULL)
{return(y.inf + (y.0-y.inf)*exp(-x/x.att))}

por.grid <- setup.prop.1D(func=exp.profile,grid=grid,y.0=0.9,y.inf=0.5,x.att=3)

# calculate the advective velocities

dummy <- setup.compaction.1D(v.0=1, por.0=0.9, por.inf=0.5, por.grid=por.grid)
u.grid <-dummy$u
v.grid <-dummy$v

# plotting the results

par(mfrow=c(2,1),cex.main=1.2,cex.lab=1.2)

matplot(por.grid$int,grid$x.int,pch=19,ylim=c(L,0), xlim=c(0,1),
xlab="",ylab="depth [cm]",main=expression("porosity"),axes=FALSE)
abline(h = 0)
axis(pos=0, side=2)
axis(pos=0, side=3)

matplot(u.grid$int,grid$x.int,type="l",lwd=2,col="blue",ylim=c(L,0),
xlim=c(0,max(u.grid$int,v.grid$int)),
xlab="",ylab="depth [cm]",main=expression("advective velocity [cm yr-1]"),
axes=FALSE)
abline(h = 0)
axis(pos=0, side=2)
axis(pos=0, side=3)
lines(v.grid$int,grid$x.int,lwd="2",col="red")
legend(x="bottomright", legend=c("pore water","solid phase"),
col=c("blue","red"),lwd=c(2,2))
```

`setup.grid.1D` *Creation of a one-dimensional finite difference grid*

Description

Subdivides the one-dimensional model domain into one or more zones that are each sub-divided into grid cells.

The resulting grid structure can be used in the other `ReacTran` functions.

The grid structure is characterized by the position of the middle of the grid cells (`x.mid`) and the position of the interfaces between cells (`x.int`).

Distances are calculated between the interfaces (`dx`), i.e. the thickness of the grid cells. An auxiliary set of distances is calculated (`dx.aux`) between the points where the concentrations are specified (at the centers of the grid cell and the two external interfaces).

A more complex grid consisting of multiple zones can be constructed when using vectors as arguments. In each zone, one can control the grid resolution near the upstream and downstream boundary. The grid resolution at the upstream interface changes according to the formula `dx[i+1] = min(max.dx.1,p.dx.1*dx[i])`.

A similar formula controls the resolution at the downstream interface. This allows refinement of the grid near the interfaces.

Usage

```
setup.grid.1D(x.up=0, x.down=NULL, L=NULL, N=NULL, dx.1=NULL,
  p.dx.1=rep(1,length(L)), max.dx.1=L, dx.N=NULL,
  p.dx.N=rep(1,length(L)), max.dx.N=L)

## S3 method for class 'grid.1D':
plot(x, ...)
```

Arguments

`x.up`	position of the upstream interface; one value.
`x.down`	position of the endpoint of each zone; one value when the model domain covers only one zone (`x.down` = position of downstream interface), or a vector of length M when the model domain is divided into M zones (`x.down[M]` = position of downstream interface).
`L`	thickness of zones; one value (model domain = one zone) or a vector of length M (model domain = M zones).
`N`	number of grid cells within a zone; one value or a vector of length M.
`dx.1`	size of the first grid cell in a zone; one value or a vector of length M.
`p.dx.1`	factor controlling the increase in grid cell size near the upstream boundary; one value or a vector of length N. The default value is 1 (constant grid cell size).
`max.dx.1`	maximum grid cell size in the upstream half of the zone; one value or a vector of length M.
`dx.N`	size of the last grid cell in a zone; one value or a vector of length M.
`p.dx.N`	factor controlling the increase in grid cell size near the downstream boundary; one value or a vector of length N. The default value is 1 (constant grid cell size).
`max.dx.N`	maximum grid cell size in the downstream half of the zone; one value or a vector of length M.
`x`	the object of class `grid.1D` that needs plotting.
`...`	additional arguments passed to the function plot.

Value

a list of type `grid.1D` containing:

`N`	the total number of grid cells.
`x.up`	position of the upstream interface; one value.
`x.down`	position of the downstream interface; one value.
`x.mid`	position of the middle of the grid cells; vector of length `N`.
`x.int`	position of the interfaces of the grid cells; vector of length `N+1`.
`dx`	distance between adjacent cell interfaces (thickness of grid cells), vector of length `N`.
`dx.aux`	auxiliary vector containing the distance between adjacent cell centers; at the upper and lower boundary calculated as (`x[1]-x.up`) and (`x.down-x[N]`) respectively; vector of length `N+1`.

Author(s)

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Examples

```
# 1D Grid: one zone, constant resolution
(GR <- setup.grid.1D(x.up=0,L=10,N=10))
plot(GR)

# 1D Grid: one zone, constant resolution, origin not zero
(GR<-setup.grid.1D(x.up=5,x.down=10,N=10))
plot(GR)

# 1D Grid: one zone, higher resolution near the upstream interface
(GR<-setup.grid.1D(x.up=0,x.down=10,dx.1=0.1,p.dx.1=1.1))
plot(GR)

# 1D Grid: one zone, higher resolution near the upstream
# and downstream interface
GR<-setup.grid.1D(x.up=0,x.down=10,
dx.1=0.1,p.dx.1=1.1,dx.N=0.1,p.dx.N=1.1)
plot(GR)

# 1D Grid: two zones, higher resolution near the upstream
# and downstream interface
(GR<-setup.grid.1D(x.up=0,L=c(5,5),dx.1=c(0.2,0.2),p.dx.1=c(1.1,1.1),
                   dx.N=c(0.2,0.2),p.dx.N=c(1.1,1.1)))
plot(GR)

# 1D Grid: two zones, higher resolution near the upstream
# and downstream interface
# the number of grid cells in each zone is imposed via N
(GR <- setup.grid.1D(x.up=0,L=c(5,5),N=c(20,10),dx.1=c(0.2,0.2),
             p.dx.1=c(1.1,1.1),dx.N=c(0.2,0.2),p.dx.N=c(1.1,1.1)))
plot(GR)
```

`setup.grid.2D` *Creation of a two-dimensional finite difference grid*

Description

Creates a finite difference grid over a rectangular two-dimensional model domain starting from two separate one-dimensional grids (as created by `setup.grid.1D`).

Usage

```
setup.grid.2D(x.grid=NULL, y.grid=NULL)
```

Arguments

`x.grid`	list containing the one-dimensional grid in the vertical direction - see `setup.grid.1D` for the structure of the list.
`y.grid`	list containing the one-dimensional grid in the horizontal direction - see `setup.grid.1D` for the structure of the list.

Value

a list of type `grid.2D` containing:

`x.up`	vertical position of the upper interface; one value.
`x.down`	vertical position of the lower interface; one value.
`x.mid`	vertical position of the middle of the grid cells; vector of length `x.N`.
`x.int`	vertical position of the horizontal interfaces of the grid cells; vector of length `x.N+1`.
`dx`	distance between adjacent cell interfaces (thickness of grid cells); vector of length `x.N`.
`dx.aux`	auxiliary vector containing the distance between adjacent cell centers; at the upper and lower boundary calculated as (`x[1]-x.up`) and (`x.down-x[x.N]`) respectively; vector of length `x.N+1`.
`x.N`	total number of grid cells in the vertical direction; one value.
`y.left`	horizontal position of the left interface; one value.
`y.right`	horizontal position of the right interface; one value.
`y.mid`	horizontal position of the middle of the grid cells; vector of length `y.N`.
`y.int`	horizontal position of the vertical interfaces of the grid cells; vector of length `y.N+1`.
`dy`	distance between adjacent cell interfaces (thickness of grid cells); vector of length `y.N`.
`dy.aux`	auxiliary vector containing the distance between adjacent cell centers; at the left and right boundary calculated as (`y[1]-y.left`) and (`y.right-y[y.N]`) respectively; vector of length `y.N+1`.
`y.N`	total number of grid cells in the horizontal direction; one value.

Author(s)

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Examples

```
# test of the setup.grid.2D functionality
x.grid <- setup.grid.1D(x.up=0,L=10,N=5)
y.grid <- setup.grid.1D(x.up=0,L=20,N=10)
(grid2D <- setup.grid.2D(x.grid,y.grid))
```

---

setup.prop.1D *Attaches a property to a one-dimensional grid*

Description

This routine calculates the value of a given property at the middle of grid cells (`mid`) and at the interfaces of the grid cells (`int`).

Two possibilities are available: either specifying a mathematical function (`func`) that describes the spatial dependency of the property, or the property is derived from interpolation of a data series (data matrix `xy`).

For example, in a sediment model, `setup.prop.1D` can be used to specify the porosity, the mixing intensity or some other parameter over the one-dimensional grid.

Similarly, in a vertical water column model, `setup.prop.1D` can be used to specify the sinking velocity of particles or any other model parameter varying with water depth.

Usage

```
setup.prop.1D(func=NULL, value=NULL, xy=NULL,
  interpolate="spline", grid, ...)

## S3 method for class 'prop.1D':
plot(x, grid, xyswap = FALSE, ...)
```

Arguments

`func`	function that describes the depth dependency.
`value`	constant value given to the property.
`xy`	a two-column matrix where the first column (`x`) provides the position, and the second column (`y`) provides the values that need interpolation over the grid.
`interpolate`	specifies how the interpolation should be done, one of "spline" or "linear"; only used if `xy` is present.
`grid`	list specifying the 1D grid characteristics, see `setup.grid.1D` for details on the structure of this list.
`x`	the object of class `grid.1D` that needs plotting.
`xyswap`	if `TRUE`, then x- and y-values are swapped and the y-axis etends from top to bottom. Useful for drawing vertical profiles.
`...`	additional arguments that are passed on to `func` or to the method.

Details

There are two options to carry out the interpolation:

- "spline" gives a smooth profile, but sometimes generates strange profiles - always check the result!
- "linear" gives a segmented profile

Value

A list of type `prop.1D` containing:

`mid`	property value at the middle of the grid cells; vector of length N (where N is the number of grid cells).
`int`	property value at at the interface of the grid cells; vector of length N+1.

Author(s)

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Examples

```
# Construction of the 1D grid

grid <- setup.grid.1D(x.up=0,L=10,N=10)

# Porosity profile via function specification

exp.profile <- function(x,y.0=NULL,y.inf=NULL,x.att=NULL)
{return(y.inf + (y.0-y.inf)*exp(-x/x.att))}

P.func <- setup.prop.1D(func=exp.profile,grid=grid,y.0=0.9,
y.inf=0.5,x.att=3)

# Porosity profile via data series interpolation

P.data <- matrix(ncol=2,data=c(0,3,6,10,0.9,0.65,0.55,0.5))
P.spline <- setup.prop.1D(xy=P.data,grid=grid)
P.linear <- setup.prop.1D(xy=P.data,grid=grid,interpolate="linear")

# Plot different profiles

plot(P.func,grid,type="l",
     main="setup.prop, function evaluation")
points(P.data,cex=1.5,pch=16)
lines(grid$x.int,P.spline$int,lty="dashed")
lines(grid$x.int,P.linear$int,lty="dotdash")
```

setup.prop.2D — *Attaches a property to a two-dimensional grid*

Description

Calculates the value of a given property at the middle of grid cells (`mid`) and at the interfaces of the grid cells (`int`).

Two possibilities are available: either specifying a mathematical function (`func`) that describes the spatial dependency of the property, or asssuming a constant value (`value`).

For example, on a sediment model, the routine can be used to specify the porosity, the mixing intensity or other parameters over the grid of the reactangular sediment domain.

Usage

```
setup.prop.2D(func = NULL, value = NULL, grid,...)
```

Arguments

`func`	function that describes the spatial dependency.
`value`	constant value given to the property.
`grid`	list specifying the 2D grid characteristics, see `setup.grid.2D` for details on the structure of this list.
`...`	additional arguments that are passed on to `func`.

Value

A list of type `prop.2D` containing:

`mid`	property value at the middle of the grid cells; NxM matrix.
`x.int`	property value at the horizontal interfaces of the grid cells; (N+1)xM matrix.
`y.int`	property value at the vertical interfaces of the grid cells; Nx(M+1) matrix.

Author(s)

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Examples

```
# Inverse quadratic function
inv.quad <- function(x,y,a=NULL,b=NULL)
return(1/((x-a)^2+(y-b)^2))

# Construction of the 2D grid
x.grid <- setup.grid.1D(x.up=0,L=10,N=10)
y.grid <- setup.grid.1D(x.up=0,L=10,N=10)
grid2D <- setup.grid.2D(x.grid,y.grid)

# Attaching the inverse quadratic function to the 2D grid
(twoD<-setup.prop.2D(func=inv.quad,grid=grid2D,a=5,b=5))
contour(log(twoD$x.int))
```

`tran.1D` *General one-dimensional advective-diffusive transport*

Description

Estimates the transport term (i.e. the rate of change of a concentration due to diffusion and advection) in a one-dimensional model of a liquid (volume fraction constant and equal to one) or in a porous medium (volume fraction variable and lower than one).

The interfaces between grid cells can have a variable cross-sectional area, for example when modelling spherical or cylindrical geometries (see example).

Usage

```
tran.1D(C, C.up = C[1], C.down = C[length(C)],
  flux.up = NULL, flux.down = NULL, a.bl.up = NULL, C.bl.up = NULL,
  a.bl.down = NULL, C.bl.down = NULL,
  D = 0, v = 0, AFDW = 1, VF = 1, A = 1,
  dx = NULL, grid = NULL,
  full.check = FALSE, full.output = FALSE)
```

Arguments

`C`	concentration, expressed per unit volume, defined at the centre of each grid cell. A vector of length N [M/L3].
`C.up`	concentration at upstream boundary. One value [M/L3].
`C.down`	concentration at downstream boundary. One value [M/L3].
`flux.up`	flux across the upstream boundary, positive = INTO model domain. One value [M/L2/T].
`flux.down`	flux across the downstream boundary, positive = OUT of model domain. One value [M/L2/T].
`a.bl.up`	convective transfer coefficient across the upstream boundary layer. `Flux = a.bl.up*(C.bl.up-C[1])`. One value [L/T].
`C.bl.up`	concentration at the upstream boundary layer. One value [M/L3].
`a.bl.down`	convective transfer coefficient across the downstream boundary layer. `Flux = a.bl.down*(C[N]-C.bl.down)`. One value [L/T].
`C.bl.down`	concentration at the downstream boundary layer. One value [M/L3].
`D`	diffusion coefficient, defined on grid cell interfaces. One value, a vector of length N+1 [L2/T], or a `grid` list; the list contains at least the element `int` (see `setup.prop.1D`) [L2/T].
`v`	advective velocity in the x-axis direction, defined on grid cell interfaces. Can be positive (downstream flow) or negative (upstream flow). One value or a vector of length N+1 [L/T], or a `grid` list; the list contains at least the element `int` (see `setup.prop.1D`) [L/T].
`AFDW`	weight used in the finite difference scheme for advection, defined on grid cell interfaces; backward = 1, centred = 0.5, forward = 0; default is backward. One value or a vector of length N+1 [-], or a `grid` list; the list contains at least the element `int` (see `setup.prop.1D`) [-].

VF	Volume fraction defined at the grid cell interfaces, one value or a vector of length N+1 [-] or a grid list; the list contains at least the elements int and mid (see setup.prop.1D) [-].
A	Interface area defined at the grid cell interfaces, one value or a vector of length N+1 [L2] or a grid list; the list contains at least the elements int and mid (see setup.prop.1D) [L2].
dx	distance between adjacent cell interfaces (thickness of grid cells). One value or vector of length N [L].
grid	discretization grid, a list containing at least elements dx and dx.aux (see setup.prop.1D) [L].
full.check	logical flag enabling a full check of the consistency of the arguments (default = FALSE; TRUE slows down execution by 50 percent).
full.output	logical flag enabling a full return of the output (default = FALSE; TRUE slows down execution by 20 percent).

Details

The **boundary conditions** are either

- (1) zero-gradient.
- (2) fixed concentration.
- (3) convective boundary layer.
- (4) fixed flux.

The above order also shows the priority. The default condition is the zero gradient. The fixed concentration condition overrules the zero gradient. The convective boundary layer condition overrules the fixed concentration and zero gradient. The fixed flux overrules all other specifications.

Transport properties:

The *diffusion coefficient* (D), the *advective velocity* (v), the *volume fraction* (VF), the *interface surface* (A), and the *advective finite difference weight* (AFDW) can be either be specified as one value, a vector or a grid property (see setup.prop.1D).

When a vector, this vector must be of length N+1, defined at all grid cell interfaces, including upper and lower boundary.

The **finite difference grid** (grid) is specified either as a grid list, as generated by setup.grid.1D or by the parameter dx representing the thickness of the grid cells (one value or a vector of length N+1)

Value

dC	the rate of change of the concentration C due to transport, defined in the centre of each grid cell [M/L3/T].
C.up	concentration at the upstream interface. One value [M/L3]. only when (full.output = TRUE)
C.down	concentration at the downstream interface. One value [M/L3]. only when (full.output = TRUE)
adv.flux	advective flux across at the interface of each grid cell. A vector of length N+1 [M/L2/T]. only when (full.output = TRUE)
dif.flux	diffusive flux across at the interface of each grid cell. A vector of length N+1 [M/L2/T]. only when (full.output = TRUE)

`flux`	total flux across at the interface of each grid cell. A vector of length N+1 [M/L2/T]. only when (`full.output` = `TRUE`)
`flux.up`	flux across the upstream boundary, positive = INTO model domain. One value [M/L2/T].
`flux.down`	flux across the downstream boundary, positive = OUT of model domain. One value [M/L2/T].

Note

The advective-diffusion equation is not checked for mass conservation. Sometimes, this is not an issue, for instance when `v` represents a sinking velocity of particles or a swimming velocity of organisms. In others cases however, mass conservation needs to be accounted for. To ensure mass conservation, the advective velocity must obey certain continuity constraints: in essence the product of the volume fraction (VF), interface surface (A) and advective velocity (v) should be constant. In sediments, one can use `setup.compaction.1D` to ensure that the advective velocities for the pore water and solid phase meet these constraints.

Author(s)

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References

Soetaert and Herman (2009). A practical guide to ecological modelling - using R as a simulation platform. Springer

Examples

```
#################################################################
###### EXAMPLE 1: O2 and OC consumption in sediments        ######
#################################################################

# this example uses only the volume fractions
# in the reactive transport term

#====================#
# Model formulation  #
#====================#

# Monod consumption of oxygen (O2)

O2.model <- function (t=0,O2,pars=NULL) {
  tran <- tran.1D(C=O2,C.up=C.ow.O2,D=D.grid,v=v.grid,
  VF=por.grid,grid=grid)$dC
  reac <- - R.O2*(O2/(Ks+O2))
  return(list(dCdt = tran+reac))
}

# First order consumption of organic carbon (OC)

OC.model <- function (t=0,OC,pars=NULL) {
  tran <- tran.1D(C=OC,flux.up=F.OC,D=Db.grid,v=v.grid,
  VF=svf.grid,grid=grid)$dC
  reac <- - k*OC
  return(list(dCdt = tran + reac))
```

```
}

#======================#
# Parameter definition #
#======================#

# Parameter values

F.OC    <- 25    # input flux organic carbon [micromol cm-2 yr-1]
C.ow.O2 <- 0.25  # concentration O2 in overlying water [micromol cm-3]
por     <- 0.8   # porosity
D       <- 400   # diffusion coefficient O2 [cm2 yr-1]
Db      <- 10    # mixing coefficient sediment [cm2 yr-1]
v       <- 1     # advective velocity [cm yr-1]
k       <- 1     # decay constant organic carbon [yr-1]
R.O2    <- 10    # O2 consumption rate [micromol cm-3 yr-1]
Ks      <- 0.005 # O2 consumption saturation constant

# Grid definition

L <- 10   # depth of sediment domain [cm]
N <- 100  # number of grid layers
grid <- setup.grid.1D(x.up=0,L=L,N=N)

# Volume fractions

por.grid <- setup.prop.1D(value=por,grid=grid)
svf.grid <- setup.prop.1D(value=(1-por),grid=grid)
D.grid <- setup.prop.1D(value=D,grid=grid)
Db.grid <- setup.prop.1D(value=Db,grid=grid)
v.grid <- setup.prop.1D(value=v,grid=grid)

#====================#
# Model solution     #
#====================#

# Initial conditions + simulation O2

O2 <- rep(0,length.out=N)
O2 <- steady.band(y=O2, func=O2.model, nspec=1)$y

# Initial conditions + simulation OC

OC <- rep(0,length.out=N)
OC <- steady.band(y=OC, func=OC.model, nspec=1)$y

# Plotting output

par(mfrow=c(1,2))

matplot(O2,grid$x.mid,pch=16,type="b",ylim=c(L,0),
xlim=c(min(0,min(O2)),max(O2)),
xlab="",ylab="depth [cm]",main=expression("O2 concentration"),
axes=FALSE)
abline(h = 0)
axis(pos=0, side=2)
axis(pos=0, side=3)
```

```
matplot(OC,grid$x.mid,pch=16,type="b",ylim=c(L,0),
xlim=c(min(0,min(OC)),max(OC)),
xlab="",ylab="depth [cm]",main=expression("OC concentration"),
axes=FALSE)
abline(h = 0)
axis(pos=0, side=2)
axis(pos=0, side=3)

##################################################################
###### EXAMPLE 2: O2 in a cylindrical and spherical organism  ######
##################################################################

# This example uses only the surface areas
# in the reactive transport term

#====================#
# Model formulation  #
#====================#

# the numerical model - rate of change=transport-consumption
Cylinder.Model <- function(time,O2,pars)
  return (list(tran.1D(C=O2,C.down=BW,D=Da,A=A.cyl,dx=dx)$dC-Q))

Sphere.Model <- function(time,O2,pars)
  return (list(tran.1D(C=O2,C.down=BW,D=Da,A=A.sphere,dx=dx)$dC-Q))

#======================#
# Parameter definition #
#======================#

# parameter values

BW     <- 2      # mmol/m3,  oxygen conc in surrounding water
Da     <- 0.5    # cm2/d     effective diffusion coeff in organism
R      <- 0.0025 # cm        radius of organism
Q      <- 250000 # nM/cm3/d  oxygen consumption rate/ volume / day
L      <- 0.05   # cm        length of organism (if a cylinder)

# the numerical model

N  <- 40                               # layers in the body
dx <- R/N                              # thickness of each layer
x.mid <- seq(dx/2,by=dx,length.out=N) # distance of center to mid-layer
x.int <- seq(0,by=dx,length.out=N+1)  # distance to layer interface

# Cylindrical surfaces
A.cyl   <- 2*pi*x.int*L  # surface at mid-layer depth

# Spherical surfaces
A.sphere <- 4*pi*x.int^2 # surface of sphere, at each mid-layer

#====================#
# Model solution     #
#====================#

# the analytical solution of cylindrical and spherical model
```

```
cylinder <- function(Da,Q,BW,R,r)  BW+Q/(4*Da)*(r^2-R^2)
sphere   <- function(Da,Q,BW,R,r)  BW+Q/(6*Da)*(r^2-R^2)

# solve the model numerically for a cylinder
O2.cyl <- steady.1D (runif(N),
func=Cylinder.Model,nspec=1,atol=1e-10)$y

# solve the model numerically for a sphere
O2.sphere <- steady.1D (runif(N),
func=Sphere.Model,nspec=1,atol=1e-10)$y

#====================#
# Plotting output    #
#====================#

par(mfrow=c(1,1))

plot(x.mid,O2.cyl,xlab="distance from centre, cm",ylab="mmol/m3",
main="tran.1D",sub="diffusion-reaction in a cylinder and sphere")
lines(x.mid, cylinder(Da,Q,BW,R,x.mid))

points(x.mid, O2.sphere, pch=18,col="red" )
lines(x.mid, sphere(Da,Q,BW,R,x.mid),col="red")

legend ("topleft",lty=c(1,NA),pch=c(NA,1),
        c("analytical solution","numerical approximation"))
legend ("bottomright",pch=c(1,18),lty=1,col=c("black","red"),
        c("cylinder","sphere"))

##################################################################
###### EXAMPLE 3: O2 consumption in a spherical aggregate   ######
##################################################################

# this example uses both the surface areas and the volume fractions
# in the reactive transport term

#====================#
# Model formulation  #
#====================#

Aggregate.Model <- function(time,O2,pars) {

  tran <- tran.1D(C=O2, C.down=C.ow.O2,
    D=D.grid, A=A.grid,
    VF=por.grid, grid=grid )$dC

  reac <- - R.O2*(O2/(Ks+O2))*(O2>0)
  return(list(dCdt = tran+reac))

}

#======================#
# Parameter definition #
#======================#

# Parameters
```

```
C.ow.O2 <- 0.25     # concentration O2 water [micromol cm-3]
por     <- 0.8      # porosity
D       <- 400      # diffusion coefficient O2 [cm2 yr-1]
v       <- 0        # advective velocity [cm yr-1]
R.O2    <- 1000000  # O2 consumption rate [micromol cm-3 yr-1]
Ks      <- 0.005    # O2 saturation constant [micromol cm-3]

# Grid definition
R <- 0.025           # radius of the agggregate [cm]
N <- 100             # number of grid layers
grid <- setup.grid.1D(x.up=0,L=R,N=N)

# Volume fractions

por.grid <- setup.prop.1D(value=por,grid=grid)
D.grid <- setup.prop.1D(value=D,grid=grid)

# Surfaces

A.mid <- 4*pi*grid$x.mid^2  # surface of sphere
A.int <- 4*pi*grid$x.int^2  # surface of sphere
A.grid=list(int=A.int,mid=A.mid)

#=====================#
# Model solution      #
#=====================#

# Numerical solution: staedy state

O2.agg <- steady.1D (runif(N),
func=Aggregate.Model,nspec=1,atol=1e-10)$y

#=====================#
# Plotting output     #
#=====================#

par(mfrow=c(1,1))

plot(grid$x.mid,O2.agg,xlab="distance from centre, cm",
ylab="mmol/m3",
main="Diffusion-reaction of O2 in a spherical aggregate")
legend ("bottomright",pch=c(1,18),lty=1,col=c("black"),
        c("O2 concentration"))
```

`tran.2D` *General two-dimensional advective-diffusive transport*

Description

Estimates the transport term (i.e. the rate of change of a concentration due to diffusion and advection) in a two-dimensional rectangular model domain.

Usage

```
tran.2D ( C, C.x.up=C[1,], C.x.down=C[nrow(C),],
  C.y.up=C[,1], C.y.down=C[,ncol(C)],
  flux.x.up=NULL, flux.x.down=NULL, flux.y.up=NULL, flux.y.down=NULL,
  a.bl.x.up=NULL, C.bl.x.up=NULL, a.bl.x.down=NULL, C.bl.x.down=NULL,
  a.bl.y.up=NULL, C.bl.y.up=NULL, a.bl.y.down=NULL, C.bl.y.down=NULL,
  D.x=NULL, D.y=D.x, v.x=0, v.y=0, AFDW.x=1, AFDW.y=AFDW.x,
  VF.x=1, VF.y=VF.x, dx=NULL, dy=NULL, grid=NULL,
  full.check = FALSE, full.output = FALSE)
```

Arguments

`C` concentration, expressed per unit volume, defined at the centre of each grid cell; NxM matrix [M/L3].

`C.x.up` concentration at upstream boundary in x-direction; vector of length M [M/L3].

`C.x.down` concentration at downstream boundary in x-direction; vector of length M [M/L3].

`C.y.up` concentration at upstream boundary in y-direction; vector of length M [M/L3].

`C.y.down` concentration at downstream boundary in y-direction; vector of length M [M/L3].

`flux.x.up` flux across the upstream boundary in x-direction, positive = INTO model domain; vector of length M [M/L2/T].

`flux.x.down` flux across the downstream boundary in x-direction, positive = OUT of model domain; vector of length M [M/L2/T].

`flux.y.up` flux across the upstream boundary in y-direction, positive = INTO model domain; vector of length M [M/L2/T].

`flux.y.down` flux across the downstream boundary in y-direction, positive = OUT of model domain; vector of length M [M/L2/T].

`a.bl.x.up` transfer coefficient across the upstream boundary layer. in x-direction `Flux=a.bl.x.up*(C.bl.` `C[1,])`. One value [L/T].

`C.bl.x.up` concentration at the upstream boundary layer in x-direction; vector of length M [M/L3].

`a.bl.x.down` transfer coefficient across the downstream boundary layer in x-direction; `Flux=a.bl.x.down*(C` `C.bl.x.down)`. One value [L/T].

`C.bl.x.down` concentration at the downstream boundary layer in x-direction ; vector of length M [M/L3].

`a.bl.y.up` transfer coefficient across the upstream boundary layer. in y-direction `Flux=a.bl.y.up*(C.bl.` `C[,1])`. One value [L/T].

`C.bl.y.up` concentration at the upstream boundary layer in y-direction; vector of length M [M/L3].

`a.bl.y.down` transfer coefficient across the downstream boundary layer in y-direction; `Flux=a.bl.y.down*(C` `C.bl.y.down)`. One value [L/T].

`C.bl.y.down` concentration at the downstream boundary layer in x-direction ; vector of length M [M/L3].

`D.x` diffusion coefficient in x-direction, defined on grid cell interfaces. One value, or a vector of length (N+1) or a `grid` list [L2/T].

`D.y` diffusion coefficient in y-direction, defined on grid cell interfaces. One value, or a vector of length (M+1), or a `grid` list [L2/T].

v.x	advective velocity in the x-direction, defined on grid cell interfaces. Can be positive (downstream flow) or negative (upstream flow). One value or a or a vector of length (N+1) or a grid list [L/T].
v.y	advective velocity in the y-direction, defined on grid cell interfaces. Can be positive (downstream flow) or negative (upstream flow). One value, or a vector of length (M+1), or a grid list [L/T].
AFDW.x	weight used in the finite difference scheme for advection in the x-direction, defined on grid cell interfaces; backward = 1, centred = 0.5, forward = 0; default is backward. One value or a vector of length (N+1) or a grid list [-].
AFDW.y	weight used in the finite difference scheme for advection in the y-direction, defined on grid cell interfaces; backward = 1, centred = 0.5, forward = 0; default is backward. One value, or a vector of length (M+1), or a grid list [-].
VF.x	Volume fraction at the grid cell interfaces in the x-direction. One value or or a vector of length (N+1) or a grid list [-].
VF.y	Volume fraction at the grid cell interfaces in the y-direction. One value, or a vector of length (M+1), or a grid list [-].
dx	distance between adjacent cell interfaces in the x-direction (thickness of grid cells). One value or vector of length N [L].
dy	distance between adjacent cell interfaces in the y-direction (thickness of grid cells). One value or vector of length M [L].
grid	discretization grid, a list containing at least elements dx, dx.aux, dy, dy.aux (see setup.grid.2D) [L].
full.check	logical flag enabling a full check of the consistency of the arguments (default = FALSE; TRUE slows down execution by 50 percent).
full.output	logical flag enabling a full return of the output (default = FALSE; TRUE slows down execution by 20 percent).

Details

- The x-axis is taken in the vertical pointing downwards (N grid cells).
- The y-axis is taken in the horizontal pointing to the right (M grid cells).

The **boundary conditions** are either

- (1) zero-gradient
- (2) fixed concentration
- (3) convective boundary layer
- (4) fixed flux

This is also the order of priority. The zero gradient is the default, the fixed flux overrules all other.

Value

a list containing:

dC	the rate of change of the concentration C due to transport, defined in the centre of each grid cell [M/L3/T].
C.x.up	concentration at the upstream interface in x-direction. A vector of length M [M/L3]. Only when full.output = TRUE.

`C.x.down` concentration at the downstream interface in x-direction. A vector of length M [M/L3]. Only when `full.output = TRUE`.

`C.y.up` concentration at the the upstream interface in x-direction. A vector of length N [M/L3]. Only when `full.output = TRUE`.

`C.y.down` concentration at the downstream interface in y-direction. A vector of length N [M/L3]. Only when `full.output = TRUE`.

`x.flux` flux across the horizontal interface of the grid cells. A (N+1)x(M) matrix [M/L2/T]. Only when `full.output = TRUE`.

`y.flux` flux across the vertical interfaces of the grid cells. A (N)x(M+1) matrix [M/L2/T]. Only when `full.output = TRUE`.

`flux.x.up` flux across the upstream boundary in x-direction, positive = INTO model domain. A vector of length M [M/L2/T].

`flux.x.down` flux across the downstream boundary in x-direction, positive = OUT of model domain. A vector of length M [M/L2/T].

`flux.y.up` flux across the upstream boundary in y-direction, positive = INTO model domain. A vector of length N [M/L2/T].

`flux.y.down` flux across the downstream boundary in y-direction, positive = OUT of model domain. A vector of length N [M/L2/T].

Author(s)

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References

Soetaert and Herman, a practical guide to ecological modelling - using R as a simulation platform, 2009. Springer

Examples

```
# Parameters
F        <- 100             # input flux [micromol cm-2 yr-1]
por      <- 0.8             # constant porosity
D        <- 400             # mixing coefficient [cm2 yr-1]
v        <- 1               # advective velocity [cm yr-1]

# Grid definition
x.N <- 4   # number of cells in x-direction
y.N <- 6   # number of cells in y-direction
x.L <- 8   # domain size x-direction [cm]
y.L <- 24  # domain size y-direction [cm]
dx  <- x.L/x.N             # cell size x-direction [cm]
dy  <- y.L/y.N             # cell size y-direction [cm]

# Intial conditions
C <- matrix(nrow=x.N, ncol=y.N, data=0, byrow=FALSE)

# Boundary conditions: fixed concentration
C.x.up <- rep(1, times=y.N)
C.x.down <- rep(0, times=y.N)
C.y.up   <- rep(1, times=x.N)
C.y.down <- rep(0, times=x.N)
```

```
# Only diffusion
tran.2D(full.output=TRUE, C=C, D.x=D, D.y=D, v.x=0, v.y=0,
  VF.x=por, VF.y=por, dx=dx, dy=dy,
  C.x.up=C.x.up, C.x.down=C.x.down,
  C.y.up=C.y.up,C.y.down=C.y.down)

# Strong advection, backward (default), central and forward
#finite difference schemes
tran.2D(C=C, D.x=D, v.x=100*v, VF.x=por, dx=dx, dy=dy,
  C.x.up=C.x.up, C.x.down=C.x.down, C.y.up=C.y.up, C.y.down=C.y.down)

tran.2D(AFDW.x=0.5, C=C, D.x=D, v.x=100*v, VF.x=por, dx=dx, dy=dy,
  C.x.up=C.x.up, C.x.down=C.x.down, C.y.up=C.y.up, C.y.down=C.y.down)

tran.2D(AFDW.x=0, C=C, D.x=D, v.x=100*v, VF.x=por, dx=dx, dy=dy,
  C.x.up=C.x.up, C.x.down=C.x.down, C.y.up=C.y.up, C.y.down=C.y.down)

# Boundary conditions: fixed fluxes

flux.x.up <- rep(200, times=y.N)
flux.x.down <- rep(-200, times=y.N)
flux.y.up <- rep(200, times=x.N)
flux.y.down <- rep(-200, times=x.N)
tran.2D(C=C, D.x=D, v.x=0, VF.x=por, dx=dx, dy=dy,
  flux.x.up=flux.x.up, flux.x.down=flux.x.down,
  flux.y.up=flux.y.up, flux.y.down=flux.y.down)

# Boundary conditions: convective boundary layer on all sides

a.bl <- 800   # transfer coefficient
C.bl.x.up <- rep(1, times=(y.N)) # fixed conc at boundary layer
C.bl.y.up <- rep(1, times=(x.N)) # fixed conc at boundary layer
tran.2D(full.output=TRUE, C=C, D.x=D, v.x=0, VF.x=por,
  dx=dx, dy=dy, C.bl.x.up=C.bl.x.up, a.bl.x.up=a.bl, C.bl.x.down=C.bl.x.up,
  a.bl.x.down=a.bl, C.bl.y.up=C.bl.y.up, a.bl.y.up=a.bl,
  C.bl.y.down=C.bl.y.up, a.bl.y.down=a.bl)

# Runtime test with and without argument checking

n.iterate <-1000

test1 <- function()
{
for (i in 1:n.iterate )
ST<-tran.2D(full.check=TRUE,C=C,D.x=D,v.x=0,VF.x=por,
dx=dx,dy=dy,C.bl.x.up=C.bl.x.up,a.bl.x.up=a.bl,C.x.down=C.x.down)
}
system.time(test1())

test2 <- function()
{
for (i in 1:n.iterate )
ST<-tran.2D(full.output=TRUE,C=C,D.x=D,v.x=0,VF.x=por,
dx=dx,dy=dy,C.bl.x.up=C.bl.x.up,a.bl.x.up=a.bl,C.x.down=C.x.down)
}
system.time(test2())
```

```
test3 <- function()
{
for (i in 1:n.iterate )
ST<-tran.2D(full.output=TRUE,full.check=TRUE,C=C,D.x=D,v.x=0,
VF.x=por,dx=dx,dy=dy,C.bl.x.up=C.bl.x.up,a.bl.x.up=a.bl,C.x.down=C.x.down)
}
system.time(test3())

## =============================================================================
## A 2-D model with diffusion in x- and y direction and first-order
## consumption
## =============================================================================

N     <- 51          # number of grid cells
XX    <- 10           # total size
dy    <- dx <- XX/N  # grid size
Dy    <- Dx <- 0.1   # diffusion coeff, X- and Y-direction
r     <- 0.005       # consumption rate
ini   <- 1           # initial value at x=0

N2  <- ceiling(N/2)
X   <- seq (dx,by=dx,len=(N2-1))
X   <- c(-rev(X),0,X)

# The model equations

Diff2D <- function (t,y,parms)  {
  CONC  <- matrix(nr=N,nc=N,y)
  dCONC <- tran.2D(CONC, D.x=Dx, D.y=Dy, dx=dx, dy=dy)$dC + r * CONC
  return (list(as.vector(dCONC)))
}

# initial condition: 0 everywhere, except in central point
y <- matrix(nr=N,nc=N,data=0)
y[N2,N2] <- ini  # initial concentration in the central point...

# solve for 10 time units
times <- 0:10
out <- ode.2D (y=y, func=Diff2D, t=times, parms=NULL,
                dim = c(N,N), lrw = 160000)

pm <- par (mfrow=c(2,2))

# Compare solution with analytical solution...
for (i in seq(2,11,by=3))
{
  tt <- times[i]
  mat  <-  matrix(nr=N,nc=N,out[i,-1])
  plot(X,mat[N2,],type="l",main=paste("time=",times[i]),
       ylab="Conc",col="red")
  ana <- ini*dx^2/(4*pi*Dx*tt)*exp(r*tt-X^2/(4*Dx*tt))
  points(X,ana,pch="+")
}
legend ("bottom", col=c("red","black"), lty=c(1,NA), pch=c(NA,"+"),
        c("tran.2D","exact"))
par("mfrow"=pm )
```

`tran.volume.1D` *1-D volumetric advective-diffusive transport in an aquatic system*

Description

Estimates the volumetric transport term (i.e. the rate of change of the concentration due to diffusion and advection) in a one-dimensional model of an aquatic system (river, estuary).

Volumetric transport implies the use of flows (mass per unit of time) rather than fluxes (mass per unit of area per unit of time) as is done in `tran.1D`.

The `tran.volume.1D` routine is particularly suited for modelling channels (like rivers, estuaries) where the cross-sectional area changes, but where this area change is not explicitly modelled as such.

Another difference withy `tran.1D` is that the present routine also allows the input of lateral water flow.

Usage

```
tran.volume.1D(C, C.up=C[1], C.down=C[length(C)],
   C.lat=0, F.up=NULL, F.down=NULL, F.lat=NULL,
   Disp=NULL,   flow = 0, flow.lat=NULL, AFDW = 1,
   V=NULL, full.check = FALSE, full.output = FALSE)
```

Arguments

`C`	tracer concentration, defined at the centre of the grid cells. A vector of length N [M/L3].
`C.up`	tracer concentration at the upstream interface. One value [M/L3].
`C.down`	tracer concentration at downstream interface. One value [M/L3].
`C.lat`	tracer concentration in the lateral input, defined at grid cell centres. One value or a vector of length N [M/L3], or a grid property. Note that `C.lat=0`, together with a positive `F.lat` will lead to dilution of the tracer concentration in the grid cells. It may be more realistic in some cases to set `C.lat = C` (a zero-gradient condition).
`F.up`	total tracer input at the upstream interface. One value [M/T].
`F.down`	total tracer input at downstream interface. One value [M/T].
`F.lat`	total lateral tracer input, defined at grid cell centres. One value or a vector of length N , or a grid property,[M/T].
`Disp`	BULK dispersion coefficient, defined on grid cell interfaces. One value or a vector of length N+1, or a grid property, [L3/T].
`flow`	water flow rate, defined on grid cell interfaces. One value or a vector of length N+1, or a grid property. If one value, it should contain the flow rate at the upstream boundary. If `flow` is a vector, then `flow.lat` should be `NULL`, [L3/T].
`flow.lat`	lateral water flow rate [L3/T] into each volume box, defined at grid cell centres. Either `NULL`, one value, or a vector of length N, or a grid property. If

	`flow.lat` has a value, then `flow` should be the flow rate at the upstream interface (one value). For each grid cell, the `flow` at the downstream interface is then estimated by adding `flow.lat` in the cell to the upstream flow rate. If `flow.lat` is `NULL`, then it is determined as the gradient of `flow`.
`AFDW`	weight used in the finite difference scheme for advection, defined on grid cell interfaces; backward = 1, centred = 0.5, forward = 0; default is backward. One value or a vector of length N+1 [-], or a `grid` list; the list contains at least the element `int` (see `setup.prop.1D`) [-].
`V`	grid cell volume, defined at grid cell centres. One value or a vector of length N [L3], or a grid property.
`full.check`	logical flag enabling a full check of the consistency of the arguments (default = `FALSE`; `TRUE` slows down execution by 50 percent).
`full.output`	logical flag enabling a full return of the output (default = `FALSE`; `TRUE` slows down execution by 20 percent).

Details

The **boundary conditions** are of type

- 1. zero-gradient (default)
- 2. fixed concentration
- 3. fixed input

The *bulk dispersion coefficient* (`Disp`) and the *flow rate* (`flow`) can be either one value or a vector of length N+1, defined at all grid cell interfaces, including upstream and downstream boundary.

The spatial discretisation is given by the volume of each box (`V`), which can be one value or a vector of length N+1, defined at the centre of each grid cell.

The water flow is mass conservative. Over each volume box, the routine calculates internally the downstream outflow of water in terms of the upstream inflow and the lateral inflow.

Value

`dC`	the rate of change of the concentration C due to transport, defined in the centre of each grid cell [M/L3/T].
`F`	mass flow across at the interface of each grid cell. A vector of length N+1 [M/T]. only when (`full.output` = `TRUE`
`F.up`	mass flow across the upstream boundary, positive = INTO model domain. One value [M/T].
`F.down`	mass flow across the downstream boundary, positive = OUT of model domain. One value [M/T].
`F.lat`	lateral mass input per volume box, positive = INTO model domain. A vector of length N [M/T].

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References

Soetaert and Herman (2009) A practical guide to ecological modelling - using R as a simulation platform. Springer.

See Also

tran.1D

Examples

```
####################################################################
#  EXAMPLE : organic carbon (OC) decay in a widening river       #
####################################################################

# Two scenarios are simulated: the baseline includes only input
# of organic matter upstream. The second scenario simulates the
# input of an important side river half way the estuary.

#====================#
# Model formulation  #
#====================#

river.model <- function (t=0,OC,pars=NULL)
{
tran <- tran.volume.1D(C=OC,F.up=F.OC,F.lat=F.lat,Disp=Disp,
flow=flow,V=Volume)$dC
reac <- - k*OC
return(list(dCdt = tran + reac))
}

#======================#
# Parameter definition #
#======================#

# Initialising morphology estuary:

nbox          <- 500     # number of grid cells
lengthEstuary <- 100000  # length of estuary [m]
BoxLength     <- lengthEstuary/nbox # [m]
Distance      <- seq(BoxLength/2, by=BoxLength, len=nbox) # [m]

# Cross sectional area: sigmoid function of estuarine distance [m2]
CrossArea <- 4000 + 72000 * Distance^5 /(Distance^5+50000^5)

# Volume of boxes                          (m3)
Volume  <- CrossArea*BoxLength

# Transport coefficients
Disp    <- 1000   # m3/s, bulk dispersion coefficient
flow    <- 180    # m3/s, mean river flow

F.OC    <- 180               # input organic carbon [mol s-1]
F.lat.0 <- F.OC              # lateral input organic carbon [mol s-1]

k       <- 10/(365*24*3600)  # decay constant organic carbon [s-1]

#====================#
# Model solution     #
#====================#
```

```
F.lat <- rep(0,length.out=nbox)
Conc1 <- steady.band(runif(nbox),fun=river.model,nspec=1)$y
F.lat <- F.lat.0*dnorm(x=Distance/lengthEstuary,
mean = Distance[nbox/2]/lengthEstuary, sd = 1/20, log = FALSE)/nbox
Conc2 <- steady.band(runif(nbox),fun=river.model,nspec=1)$y

#====================#
# Plotting output    #
#====================#

matplot(Distance/1000,cbind(Conc1,Conc2),lwd=2,
main="Organic carbon decay in an estuary",xlab="distance [km]",
ylab="OC Concentration [mM]",
type="l")
legend ("topright",lty=1,col=c("black","red"),
        c("baseline","with lateral input"))
```

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