DRAFT ! Advection, Diffusion & Reaction Modeling

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The movement of compounds in the environment is driven by two processes, advection and diffusion. Of course, these processes occur in three dimensions, but for this class we'll begin with one dimensional processes before getting to more complicated examples.

Introduction

The Problem

The movement of compounds in the environment is driven by three processes: advection , diffusion, and reaction. Of course, these processes occur in three dimensions. The implications of these processes is profound – they determine the fate and transport of pollutants in the environment, the movement of nutrients in the soil, and the movement of solutes in the human body. Our understanding of these processes is critical to understanding issues of environmental quality and justice for human and non-humans alike. We use our undestanding to develop of environmental policy, the management of agricultural systems, and to mitigate the impacts of pollution on human health.

However, these processes are complex and are often difficult to measure. As a result, we often rely on models to help us understand the movement of solutes in the environment. These models are based on the fundamental processes of advection, diffusion, and reaction.

The Processes

Advection and diffusion are two fundamental processes that govern the transport of solutes in the environment. Advection is the process of transport of a solute by the bulk motion of the fluid. Diffusion is the process of transport of a solute by random molecular motion.

In a simple example, if we have a dose of a solute, like a dye in the center of some media, we'll see it spread out by diffusion (Figure 2). If the media is moving, we'll see the dye move with the bulk motion of the media. If the dye reacts with the media, we'll see the dye disappear.

Besides examples we often see with respect to air pollution sources (Figure 1), we might think about solutes as pollutants or nutrients. For example, the movement of a nutrient in a river is driven by the

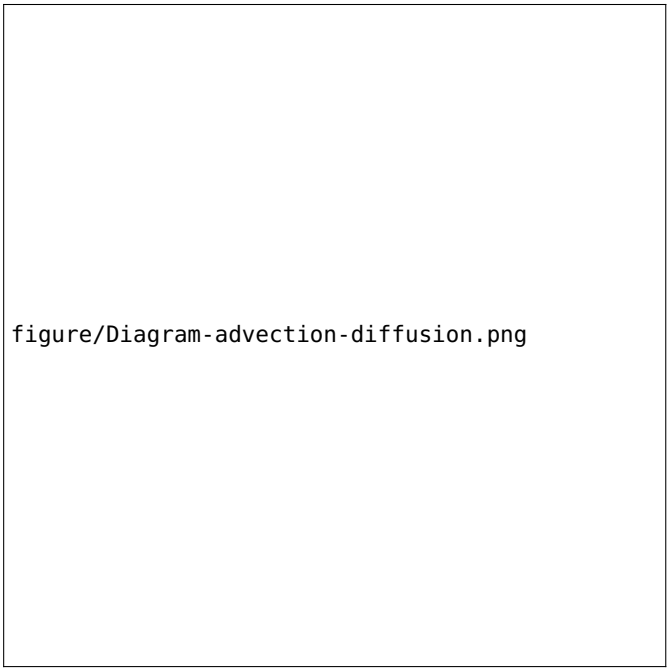


Figure 1: A simple diagram of advection and diffusion that inclues how "solutes" might be deposited downwind of a stationary source if air pollution.

bulk motion of the water (advection) and the random motion of the molecules (diffusion) and the reactions that might occur in the water column and sediments (Figure**??**).

Session Goals

We will not become experts in advection-diffusion-reaction modeling, but we will become familiar with the processes and the equations that describe them. Moreover, we'll see a bit more about how R can be used to model these processes. After this session, I hope you can do the following:

1. Describe the physical processes of advection and diffusion and solute reaction
2. Describe the equations used to model A-D-R.
3. Analyze 1-dimensional movement using advection equations in R.
4. Describe diffusion mathematically
5. Analyze 1-dimensional adveecton-diffusion using R.
6. Appreciate how two-dimensional analysis of advection-diffusion can be modeled in R.

In this session, we'll want to think about the movement of solutes in the porous media, i.e. a soil with air space, sediments with water

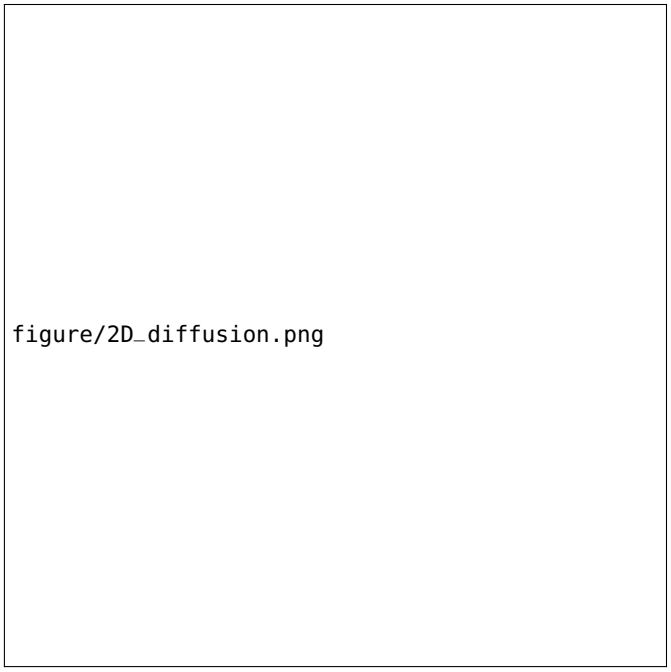


Figure 2: A simple diagram of 2D diffusion.

between the particles. We will refer to the porousity as ξ, which is a proportion between 0 and 1.

Advection and Convection: Material and Heat

Advection is the transport of a substance by bulk motion. Convection is the transfer of heat by the actual movement of the warmed matter. The equation that are used to describe advection and convection are similar, but the physical processes are different.

The Processes and the Equations to Describe Them

$$-\frac{1}{A_x \xi_x} \cdot \left(\frac{\partial}{\partial x} A_x \cdot \left(-D \cdot \frac{\partial \xi_x C}{\partial x} \right) - \frac{\partial}{\partial x} \left(A_x \cdot v \cdot \xi_x C \right) \right) \tag{1}$$

Here D is the "diffusion coefficient", v is the "advection rate", and A_x and ξ are the surface area and volume fraction, respectively.

Assuming that A, ξ, D and v are constant along x, we can rewrite this in a more general form:

$$D \frac{\partial^2 C}{\partial x^2} - \mu \frac{\partial C}{\partial x} \tag{2}$$

where $u = v / A_x \xi_x$ is the "velocity" of the fluid.

The movement of compounds in the environment is driven by two processes, advection and diffusion. Of course, these processes occur in three dimensions, but for this class we'll begin with one dimensional processes before getting to more complicated examples.

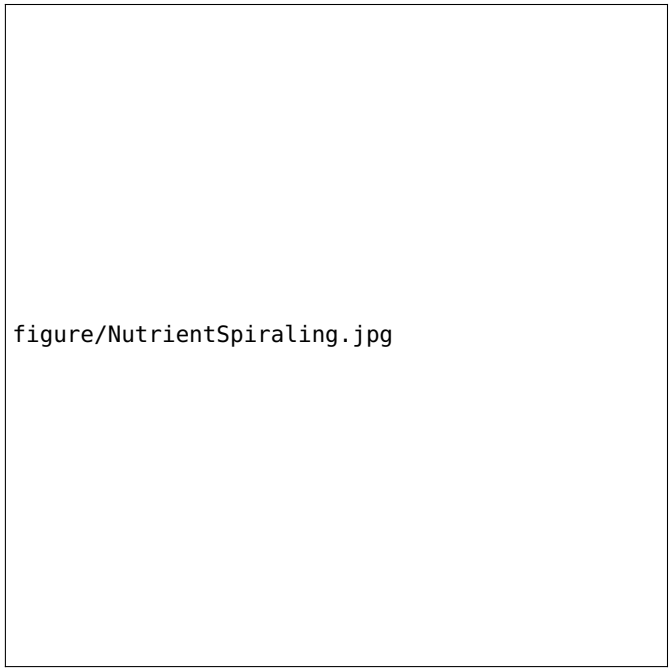


Figure 3: A simple diagram of advection and nutrient reactions (organic substances and inorganic substances) in a river. Although not shown, you might also think about how diffusion might influence the movement of nutrients in the river and in the sediments. The zone where water moves into the sediment bed is called the hyperreic zone. The porosity of the sediments will allow more advective flow that might influence the reaction capacity of solutes in the sediments.

Nevertheless, let's look at the 3-D advection-diffusion-reacton equation in three dimensions:

$$\frac{\partial C}{\partial t} = \nabla \cdot (D\nabla C - \mu C) + R \tag{3}$$

where C is the concentration of the solute, t is time, μ is the velocity of the fluid, D is the diffusion coefficient, and R is the reaction term.

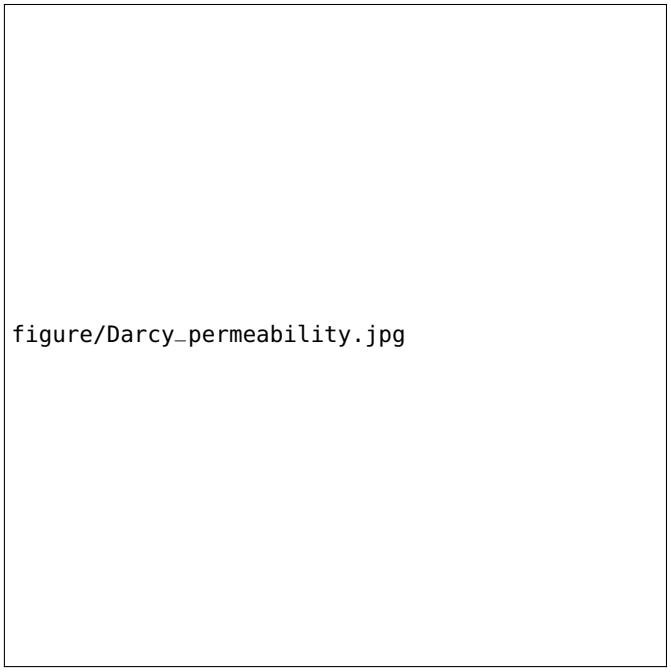
Ok, what what is ∇? It's the gradient operator, which is a vector operator that operates on a scalar function to produce a vector whose magnitude is the maximum rate of change of the function at the point of the gradient and that points in the direction of that maximum rate of change. $\nabla\cdot$ represents divergence. In this equation, ∇C represents concentration gradient.

Advection

Advection is the process of transport of a solute by the bulk motion of the fluid. The rate of advection is proportional to the velocity of the fluid and the concentration of the solute. The rate of advection is given by the equation:

$$\frac{\partial C}{\partial t} + \nabla \cdot (uC) = 0 \tag{4}$$

where C is the concentration of the solute, t is time, and u is the velocity of the fluid.



For one dimensional systems, the equation can be written as:

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = 0 \tag{5}$$

or

$$\frac{\partial C}{\partial t} + \mu_x\frac{\partial C}{\partial x} \tag{6}$$

where C is the concentration of the solute, t is time, u is the velocity of the fluid, and x is the spatial coordinate.

The advection equation is not simple to solve numerically: the system is a hyperbolic partial differential equation, and interest typically centers on discontinuous "shock" solutions (which are notoriously difficult for numerical schemes to handle).

Diffusion

Diffusion is the process of transport of a solute by random molecular motion. The rate of diffusion is proportional to the concentration gradient of the solute. The rate of diffusion is given by the equation:

$$\frac{\partial C}{\partial t} = D\nabla^2 C \tag{7}$$

where D is the diffusion coefficient.

Advection-Diffusion Equation

The advection-diffusion equation is a combination of the advection and diffusion equations. The advection-diffusion equation is given by

the equation:

$$\frac{\partial C}{\partial t} + \nabla \cdot (uC) = D\nabla^2 C \tag{8}$$

or

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = D\frac{\partial^2 C}{\partial x^2} \tag{9}$$

where C is the concentration of the solute, t is time, u is the velocity of the fluid, and D is the diffusion coefficient.

Advection-Difffusion-Reaction Equation

The advection-diffusion-reaction equation is a combination the advection, diffusion, and reaction equations. The advection-diffusion-reaction equation is given by the equation:

$$\frac{\partial C}{\partial t} + \nabla \cdot (uC) = D\nabla^2 C + R \tag{10}$$

where C is the concentration of the solute, t is time, u is the velocity of the fluid, D is the diffusion coefficient, and R is the reaction term.

or in one-dimension:

$$\frac{\partial C}{\partial t} = \mu\frac{\partial C}{\partial x} = D\frac{\partial^2 C}{\partial x^2} + R \tag{11}$$

where C is the concentration of the solute, t is time, u is the velocity of the fluid, D is the diffusion coefficient, and R is the reaction term.

Advenction-Difffusion-Reaction in multi-phase systems and for shapes with variable geometry

The advection-diffusion-reaction equation can be extended to multi-phase systems and to shapes with variable geometry. The advection-diffusion-reaction equation for multi-phase systems and for shapes with variable geometry is given by the equation:

$$\frac{\partial C}{\partial t} + \nabla \cdot (uC) = D\nabla^2 C + R \tag{12}$$

where C is the concentration of the solute, t is time, u is the velocity of the fluid, D is the diffusion coefficient, and R is the reaction term.

ReacTran Package

Soetaert et al. (2017) have developed a nice library in R that solves these equations using finite-difference solutions.

The ReacTran package is a collection of functions for modeling solute transport in 1D, 2D, and 3D. The package includes functions

for solving the advection-diffusion equation, the advection-diffusion-reaction equation, and the advection-diffusion-reaction equation for multi-phase systems and for shapes with variable geometry. The package also includes functions for solving the advection-diffusion equation in 1D, 2D, and 3D. The package also includes functions for solving the advection-diffusion-reaction equation in 1D, 2D, and 3D. The package also includes functions for solving the advection-diffusion-reaction equation for multi-phase systems and for shapes with variable geometry in 1D, 2D, and 3D. The package also includes functions for solving the advection-diffusion equation in 1D, 2D, and 3D. The package also includes functions for solving the advection-diffusion-reaction equation in 1D, 2D, and 3D. The package also includes functions for solving the advection-diffusion-reaction equation for multi-phase systems and for shapes with variable geometry in 1D, 2D, and 3D. The package also includes functions for solving the advection-diffusion equation in 1D, 2D, and 3D. The package also includes functions for solving the advection-diffusion-reaction equation in 1D, 2D, and 3D. The package also includes functions for solving the advection-diffusion-reaction equation for multi-phase systems and for shapes with variable geometry in 1D, 2D, and 3D. The package also includes functions for solving the advection-diffusion equation in 1D, 2D, and 3D. The package also includes functions for solving the advection-diffusion-reaction equation in 1D, 2D, and 3D. The package also includes functions for solving the advection-diffusion-reaction equation for multi-phase systems and for shapes with variable geometry in 1D, 2D, and 3D. The package also includes functions for solving the advection-diffusion equation in 1D, 2D, and 3D.

Applications using R

R as a Calculator and Modeling Environment

We can use R to solve the advection-diffusion equation. The following code uses the 'deSolve' package to solve the advection-diffusion equation for a simple one-dimensional case.

```
# Load the deSolve package
library(deSolve)

# Define the advection-diffusion equation
advection_diffusion <- function(t, C, parms) {
  with(as.list(parms), {
    dC <- D * (diff(C, lag = 2) - 2 * diff(C, lag = 1) + diff(C, lag = 0)) / dx^2
    dC[1] <- 0
```

```
    dC[n] <- 0
    list(dC)
  })
}

# Set the parameters
parms <- list(
  D = 0.1,  # Diffusion coefficient
  dx = 0.1  # Spatial step
)

# Set the initial conditions
C0 <- c(0, rep(0, 98), 1, rep(0, 98), 0)

# Set the times at which to evaluate the solution
times <- seq(0, 100, by = 1)

# Solve the advection-diffusion equation

out <- ode(y = C0, times = times, func = advection_diffusion, parms = parms)

# Plot the solution

plot(out, xlab = "Distance", ylab = "Concentration", type = "l")
```

1D Transportion Model

The 'ReacTran' package provides a function to solve the advection-diffusion-reaction equation for a simple one-dimensional case.

```
# Load the ReacTran package
library(ReacTran)

## Loading required package:  rootSolve
## Loading required package:  deSolve
## Loading required package:  shape
```

```
tran.1D(C = 1, D = 0, flux.up = 1, v = 5, A= 1, dx = 1, full.output = TRUE)

## $dC
## [1] -4
##
## $C.up
## [1] 0.2
```

```
##
## $C.down
## [1] 1
##
## $dif.flux
## [1] 0 0
##
## $adv.flux
## [1] 1 5
##
## $flux
## [1] 1 5
##
## $flux.up
## [1] 1
##
## $flux.down
## [1] 5
```

Solving a 1-D reaction tranport mdodel

```
library(ReacTran)
out <- steady.1D(func = advModel, y = runif(25), params = parms, nspace= 1, positive = TRUE)
```

We can use R to solve the advection-diffusion-reaction equation. The following code uses the 'deSolve' package to solve the advection-diffusion-reaction equation for a simple one-dimensional case.

```
# Load the deSolve package
library(deSolve)

# Define the advection-diffusion-reaction equation
advection_diffusion_reaction <- function(t, C, parms) {
  with(as.list(parms), {
    dC <- D * (diff(C, lag = 2) - 2 * diff(C, lag = 1) + diff(C, lag = 0)) / dx^2 - k * C
    dC[1] <- 0
    dC[n] <- 0
    list(dC)
  })
}

# Set the parameters
parms <- list(
```

```
  D = 0.1,  # Diffusion coefficient
  dx = 0.1,  # Spatial step
  k = 0.01  # Reaction rate
)

# Set the initial conditions
C0 <- c(0, rep(0, 98), 1, rep(0, 98), 0)

# Set the times at which to evaluate the solution
times <- seq(0, 100, by = 1)

# Solve the advection-diffusion-reaction equation
out <- ode(y = C0, times = times, func = advection_diffusion_reaction, parms = parms)

# Plot the solution
plot(out, xlab = "Distance", ylab = "Concentration", type = "l")
```

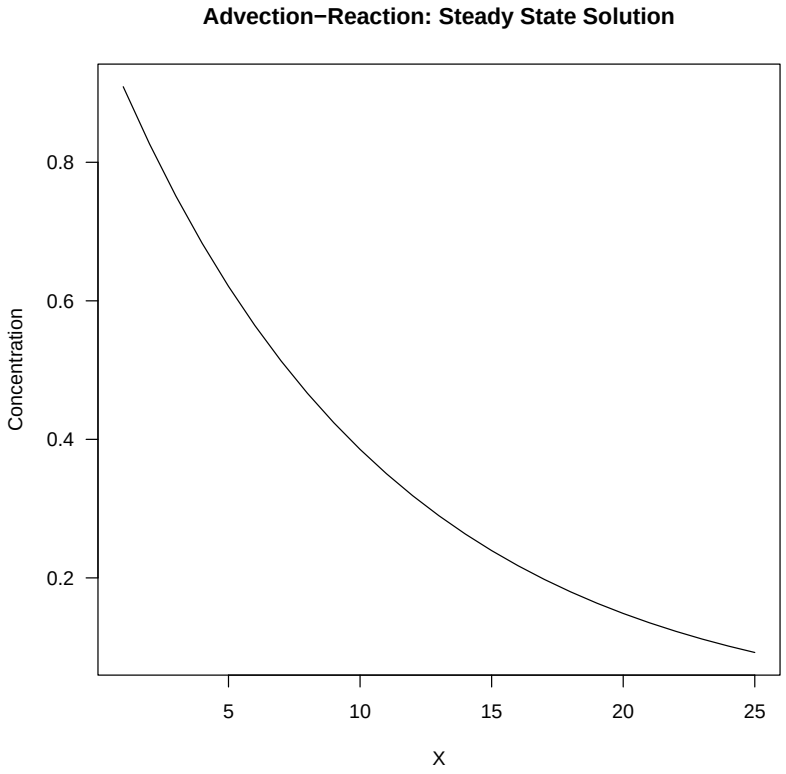
1-D Reaction-Transport Model

```
library(ReacTran)

parms <- c(F0 = 1, v=1, k = 0.1, D = 0, dx = 1)

advModel <- function(t, C, parms) {
  with(as.list(parms), {
    Tran <- tran.1D(C = C, D = D, flux.up = F0, v = v, dx = dx)
    Consumption = k * C
    dC <- Tran$dC - Consumption

    return(list(dC = dC, Consumption = Consumption, flux.up = Tran$flux.up, flux.down = Tran$flux.down))
  })
}

out <- steady.1D(func = advModel, y = runif(25), parms = parms, nspec= 1, positive = TRUE)

parms <- c(F0 = 1, v=1, k = 0.5, D=0, dx = 1)
out2 <- steady.1D(func = advModel, y = runif(25), parms = parms, nspec= 1, positive = TRUE)

parms <- c(F0 = 1, v=1, k = 0.5, D=50, dx = 1)
out3 <- steady.1D(func = advModel, y = runif(25), parms = parms, nspec= 1, positive = TRUE)
```

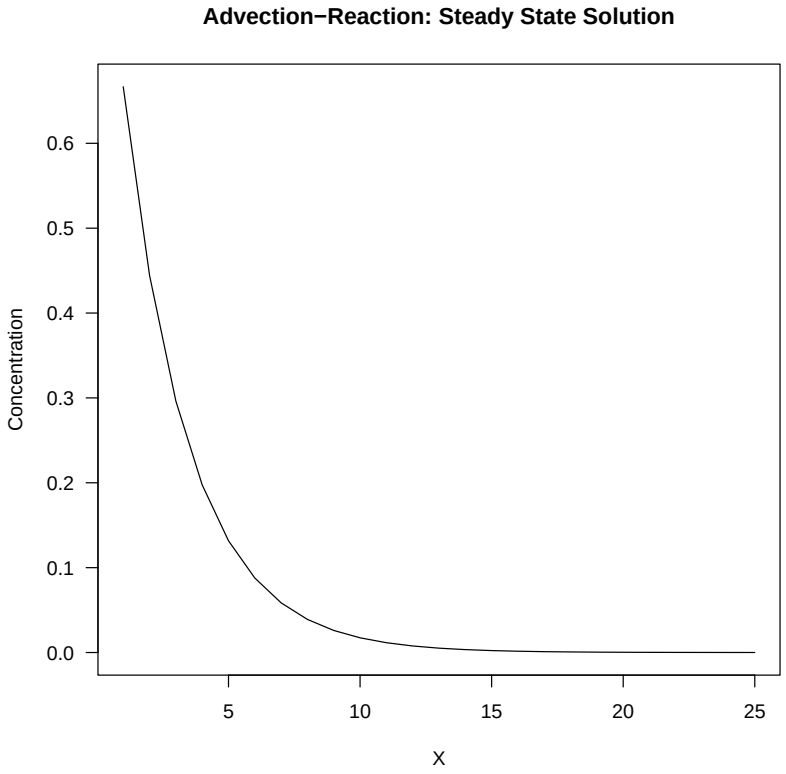
```
out
```

```
## $y
##  [1] 0.9090909 0.8264463 0.7513148 0.6830135 0.6209213 0.5644739 0.5131581
##  [8] 0.4665074 0.4240976 0.3855433 0.3504939 0.3186308 0.2896644 0.2633313
## [15] 0.2393921 0.2176291 0.1978447 0.1798588 0.1635080 0.1486436 0.1351306
## [22] 0.1228460 0.1116782 0.1015256 0.0922960
##
## $Consumption
##  [1] 0.09090909 0.08264463 0.07513148 0.06830135 0.06209213 0.05644739
##  [7] 0.05131581 0.04665074 0.04240976 0.03855433 0.03504939 0.03186308
## [13] 0.02896644 0.02633313 0.02393921 0.02176291 0.01978447 0.01798588
## [19] 0.01635080 0.01486436 0.01351306 0.01228460 0.01116782 0.01015256
## [25] 0.00922960
##
## $flux.up
## [1] 1
##
## $flux.down
## [1] 0.092296
##
## attr(,"precis")
## [1] 4.406130e-01 2.339217e-09
## attr(,"steady")
## [1] TRUE
## attr(,"class")
## [1] "steady1D"  "rootSolve" "list"
## attr(,"dimens")
## [1] 25
## attr(,"nspec")
## [1] 1
```

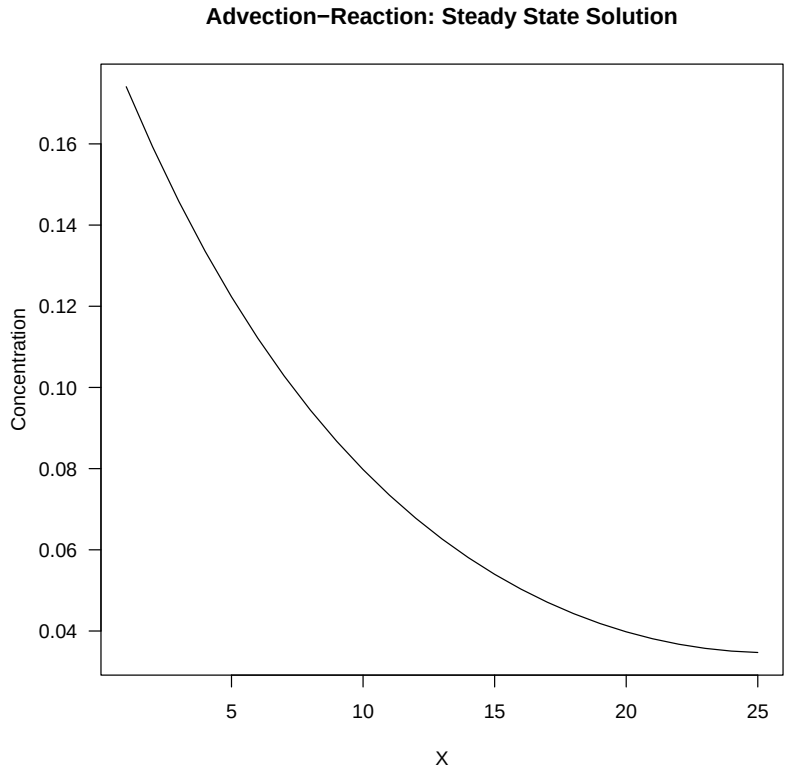
```
par(mfrow=c(1,3))
plot(out, xlab = "X", ylab = "Concentration", las=1, main="Advection-Reaction: Steady State Solution")
```




```
plot(out2, xlab = "X", ylab = "Concentration", las=1, main="Advection-Reaction: Steady State Solution")
```




```
plot(out3, xlab = "X", ylab = "Concentration", las=1, main="Advection-Reaction: Steady State Solution")
```



Oxygen Consumption Porous Spherical Particle

We will be modeling the consumption of oxygen in a "sand-sized" porous spherical particle. The model is based on the following equation:

$$\frac{\partial C}{\partial t} = -v\frac{\partial C}{\partial x} - k(C)$$

where C is the concentration of oxygen, D is the diffusion coefficient, v is the velocity of the fluid, and $k(C)$ is the rate of oxygen consumption.

At this scale the velocity will be zero. Thus, we will rely on diffusion to for the oxygen movement to where it is consumed.

We start with defining the size and porosity of the particle and use R to create a grid to solve the advection-diffusion-reaction equation.

Parameter	Description	Typical Range	Modelled Value
R	Radius of the particle	$0.005 - 0.2$ cm	0.025 cm
Porosity	Proportion of void space	$0.005 - -0.7$	0.7

Table 1: Chararacteristics of the Particle

We will create a grid to model the particle with Radius R and N

(= 100) grid points. We will also define the properties of the particle such as porosity, diffusion coefficient (D = 400), and the rate of oxygen consumption, $R_{02} = 10^6$.

Although we are modeling a one-dimensional system, we will need to create a grid surface as a circle to effectively model the particle surface area changes as O2 diffuses into the particle and is consumed by the reactions in the particle.

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

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

sphere.surf <- function(x) 4*pi*x^2
A.grid <- setup.prop.1D(func=sphere.surf,  grid=grid)
```

Finally, we need to define the O2 concentration at the surface of the particle and the O2 consumption rate of the particle.

Parameter	Description	Typical Range	Modelled Value
C_{ow}	Concentration of O2 in Water	$0.1 - 0.3$	0.25
R_{02}	Rate of oxygen consumption	$10^5 - 10^6$ /year	10^6 /year
K_s	O2 saturation	$0.001 - 0.01$	0.005

Table: Oxygen Consumption in the Particle

Note, we often measure oxygen using ppm (parts per million), but the model uses . The conversion is 1 ppm = 0.0224 , thus, we are modeling *Ks* within a range of 2.24 - 6.72 ppm, using Ks = 0.22 .

Next we create a function to model the oxygen consumption in the, particle that relies on We will use the `tran.1D` function to solve the advection-diffusion equation and the `steady.1D` function to solve the steady state solution of the advection-diffusion-reaction equation.

```
Aggregate.Model <- function(time, O2, pars) {
  tran <- tran.1D(C = O2, C.down = C.ow.02, D = D.grid,
          A=A.grid, VF = por.grid, dx = grid)
    reac <- - R.02 * (O2 /(Ks + O2))
    return(list(dCdt= tran$dC + reac, reac = reac,
                flux.up=tran$flux.up, flux.down=tran$flux.down))
}


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

The plot shows the oxygen concentration in the particle. The concentration is highest at the surface and decreases as it moves into the

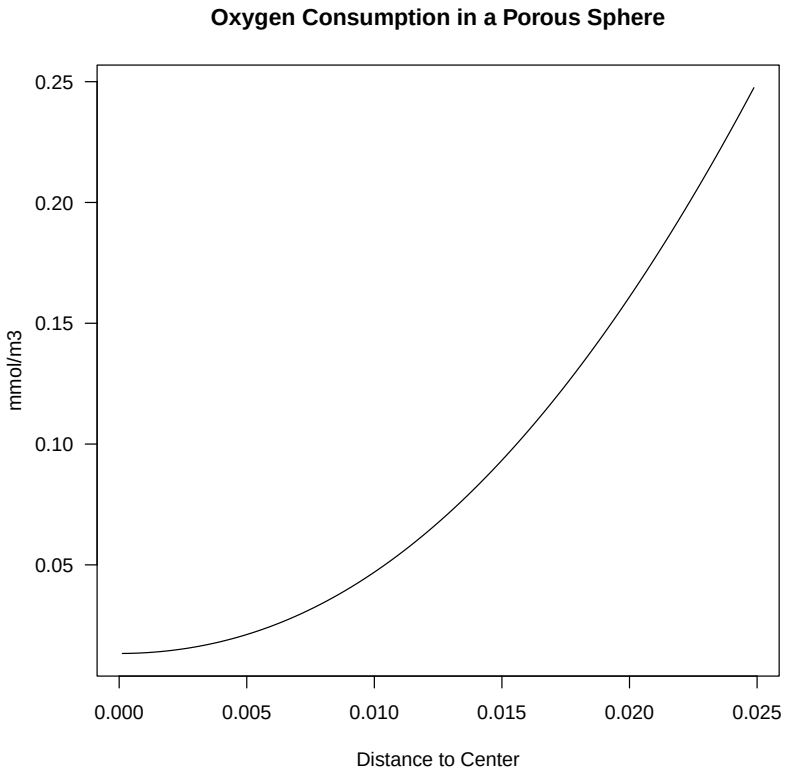
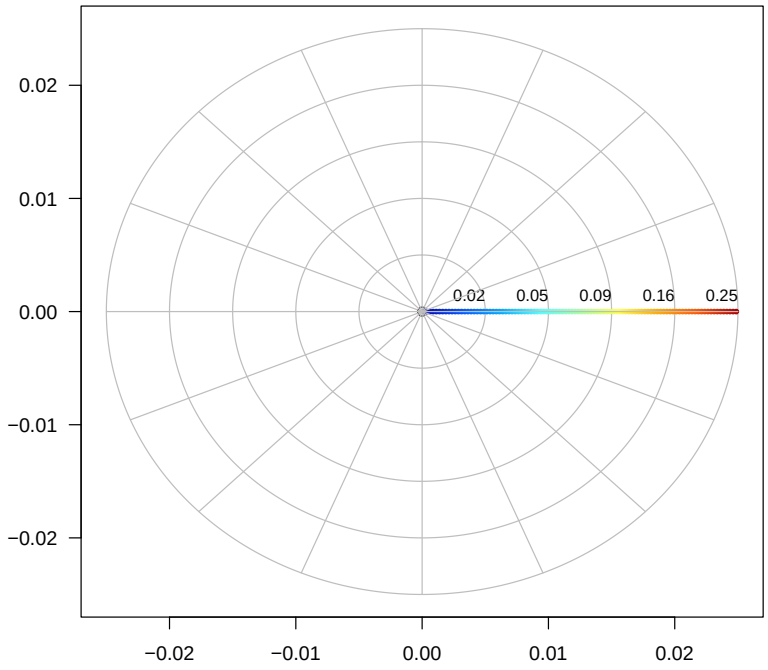


Figure 4: Oxygen Consumption in a Porous Sphere

particle. The concentration is zero at the center of the particle.

```
diffusion2D <- function(t,conc,par){
Conc <- matrix(nr=n,nc=n,data=conc) # vector to 2-D matrix
dConc <- -r*Conc*Conc # consumption
BND <- rep(1,n) # boundary concentration

# constant production in certain cells
dConc[ii]<- dConc[ii]+ p

#diffusion in X-direction; boundaries=imposed concentration

Flux <- -Dx * rbind(rep(0,n),(Conc[2:n,]-Conc[1:(n-1),]),rep(0,n))/dx
dConc <- dConc - (Flux[2:(n+1),]-Flux[1:n,])/dx

#diffusion in Y-direction
Flux <- -Dy * cbind(rep(0,n),(Conc[,2:n]-Conc[,1:(n-1)]),rep(0,n))/dy
dConc <- dConc - (Flux[,2:(n+1)]-Flux[,1:n])/dy
```




```
return(list(as.vector(dConc)))
}
```

After specifying the values of the parameters, 10 cells on the 2-D grid where there will be substance produced are randomly selected (ii).

14 Package rootSolve : roots, gradients and steady-states in R 0.0 0.2 0.4 0.6 0.8 1.0 0.0 0.2 0.4 0.6 0.8 1.0 2-D diffusion+production x y
Figure 5: Steady-state solution of the nonlinear 2-Dimensional model

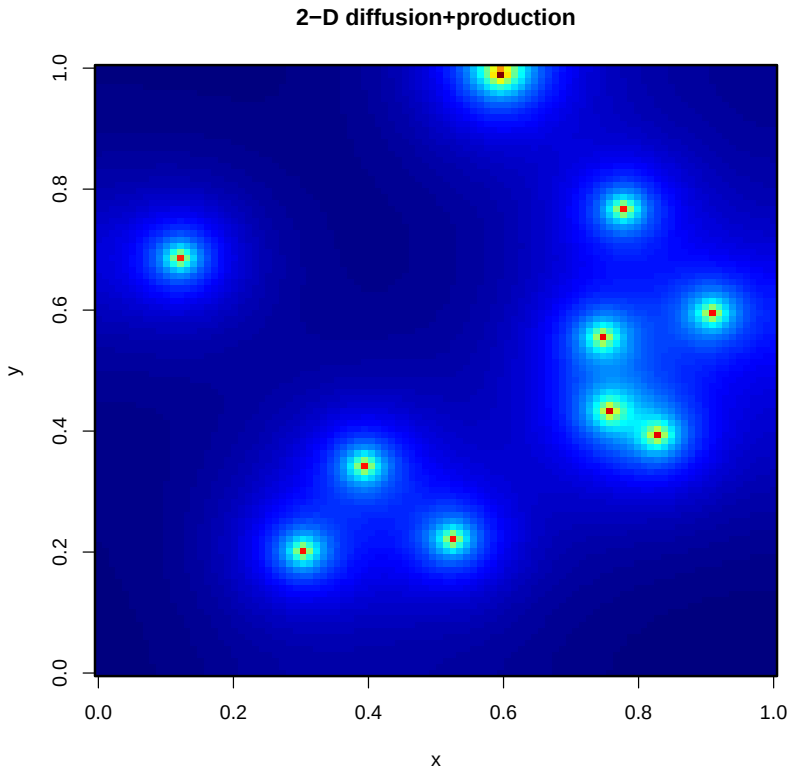
```
# parameters
dy <- dx <- 1 # grid size
Dy <- Dx <- 1.5 # diffusion coeff, X- and Y-direction
r <- 0.01 # 2-nd-order consumption rate (/time)
p <- 20 # 0-th order production rate (CONC/t)
n <- 100
# 10 random cells where substance is produced at rate p
ii <- trunc(cbind(runif(10)*n+1,runif(10)*n+1))
```

The steady-state is found using function steady.2D. It takes as arguments a.o. the dimensionality of the problem (dimens) and lrw=1000000, the length of the work array needed by the solver. If this value is set too small, the solver will return with the size needed. It takes about 0.5 second to solve this 10000 state variable model.

```
Conc0 <- matrix(nr=n,nc=n,10.)
print(system.time(
ST3 <- steady.2D(Conc0,func=diffusion2D,parms=NULL,pos=TRUE,dimens=c(n,n),
lrw=1000000,atol=1e-10,rtol=1e-10,ctol=1e-10)
))

##    user  system elapsed
##   0.225   0.014   0.240
```

user system elapsed 1.044 0.032 1.076 The S3 image method is used to generate the steady-state plot.

```
image(ST3,main="2-D diffusion+production", xlab="x", ylab="y")
```



Considering 2D Models

2.4. Steady-state solution of 2-D PDEs Function steady.2D effciently snds the steady-state of 2-dimensional problems. Karline Soetaert 13 In the following model @C @t = Dx @2C @x2 + Dy @2C @y2 .. r C2 + pxy a substance C is consumed at a quadratic rate (r C2), while dispersing in X- and Y-direction. At certain positions (x,y) the substance is produced (rate p). The model is solved on a square (100*100) grid. There are zero- ux boundary conditions at the 4 boundaries. The term Dx @2C @x2 is in fact shorthand for: .. @Flux @x where Flux = ..Dx @C @x i.e. it is the negative of the ux gradient, where the ux is due to diffusion. In the numerical approximation fo the ux, the concentration gradient is approximated as the subtraction of two matrices, with the columns or rows shifted (e.g. Conc[2:n,]-Conc[1:(n-1),]). The ux gradient is then also approximated by subtracting entire matrices (e.g. Flux[2:(n+1),]-Flux[1:(n),]). This is very fast. The zero-ux at the boundaries is imposed by binding a column or row with 0-s.

Conclusion

References

Soetaert, K., Meysman, F., and Soetaert, M. K. (2017). Package âĂŸreactranâĂŹ.