Partial Differential Model of the Diffusion-Reaction Equation

David Ellison, PhD

September 1, 2017

Load Partial Differential Equation Libraries

```
suppressWarnings(suppressMessages(library(deSolve)))
suppressWarnings(suppressMessages(require(ReacTran)))
```

Explained 1D Diffusion-Reaction Equation Initial Values and Boundary Conditions

In this example we consider the 1_D diffusion-reaction model:

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x}\left(D \cdot \frac{\partial C}{\partial x}\right) - Q$$

with C the concentration,
t the time,
x the distance from the origin,
Q the comsumption rate,
and the following boundery conditions: $\frac{\partial C}{\partial x_{x=0}} = 0$

$C_{x=10} = C_{ext}$
and we create `Grid` as 10 cm (**L**) into 1000 boxes (**N**) e.g. 100mm, or 0.1mm per step

Set up Coefficients & 1D function

```
Grid <-setup.grid.1D(N=1000, L=10)
D <- 1 #diffusion constant
Q <- 1 #uptake rate
Cext <- 20
pde1D <-function(t, C, params){
  tran=tran.1D(C=C, D=D, C.down=Cext, dx= Grid)$dC
  list(tran-Q)
}
```

Model the Diffusion-Reaction Equation Over 100 Time Points (Days)

```
times <- seq(0,100,by=1) #time in days
out <- ode.1D(y=rep(1, Grid$N),times=times,func=pde1D,parms=NULL,nspec=1)
tail(out[,1:11],n=5) # the last five time points, for positions 1:10 ~1mm
```

```
##        time         1         2         3         4         5         6
##  [97,]   96 -27.43429 -27.43419 -27.43401 -27.43372 -27.43335 -27.43288
##  [98,]   97 -27.49682 -27.49672 -27.49654 -27.49626 -27.49588 -27.49541
##  [99,]   98 -27.55783 -27.55773 -27.55754 -27.55726 -27.55689 -27.55642
## [100,]   99 -27.61735 -27.61725 -27.61706 -27.61678 -27.61641 -27.61594
```

```
## [101,]  100 -27.67542 -27.67532 -27.67513 -27.67485 -27.67447 -27.67400
##                 7         8         9        10
##  [97,] -27.43232 -27.43166 -27.43091 -27.43007
##  [98,] -27.49485 -27.49419 -27.49344 -27.49260
##  [99,] -27.55585 -27.55520 -27.55444 -27.55360
## [100,] -27.61537 -27.61471 -27.61396 -27.61311
## [101,] -27.67344 -27.67278 -27.67202 -27.67118
```

Visualize the Diffusion Equation over 100 Days, Approximates Steady-State

```
image(out, xlab="Time (days)", ylab="Distance (cm)", main="Diffusion PDE",
add.contour=TRUE)
```