Partial Differential Model of the Diffusion-Reaction Equation

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## 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:

with the concentration,  
 the time,  
 the distance from the origin,  
 the comsumption rate,  
and the following boundery conditions:   
  
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)

