

# HW06\_Diffusion

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2022-05-05

## Load Libraries

```
library(tidyverse)
library(deSolve)
library(here)
library(cowplot)
```

## Source Diffusion Function

```
source(here("R/diffusion.R"))
```

### Diffusion Model Parameters

- `initialC` = initial concentration (mg/L)
- `dx` = length of each segment (m)
- `nx` = number of discrete segments (m)
- `nt` = number of discrete time intervals (s)
- `dt` = seconds in each time interval (s)
- `area` = area of cross section of container (m<sup>2</sup>)
- `D` = diffusivity (how easily the chemical diffuses (s/m<sup>2</sup>))

## Run the in class difdussion model examples

```
# run our diffusion model (iterative difference equation) with initial concentration of 10, for 8 times
```

```
# using diffusion parameters 0.5 s/m2, 10 m2
```

```
result = diff1(initialC = 10, nx = 10, dx = 1, nt = 8, dt = 1, D = 0.5, area = 10)
```

```
# a list is returned with our 3 data frames for concentration (conc), qin and qout
result
```

```
## $conc
##      [,1]      [,2]      [,3]      [,4]      [,5]      [,6]      [,7]
## [1,] 10.000000 0.000000 0.000000 0.000000 0.000000 0.000000000 0.000000000
## [2,]  7.500000 2.500000 0.000000 0.000000 0.000000 0.000000000 0.000000000
## [3,]  6.250000 3.125000 0.625000 0.000000 0.000000 0.000000000 0.000000000
## [4,]  5.468750 3.281250 1.093750 0.1562500 0.0000000 0.000000000 0.000000000
## [5,]  4.921875 3.281250 1.406250 0.3515625 0.0390625 0.000000000 0.000000000
## [6,]  4.511719 3.222656 1.611328 0.5371094 0.1074219 0.009765625 0.000000000
## [7,]  4.189453 3.142090 1.745605 0.6982422 0.1904297 0.031738281 0.002441406
## [8,]  3.927612 3.054810 1.832886 0.8331299 0.2777100 0.064086914 0.009155273
```

```

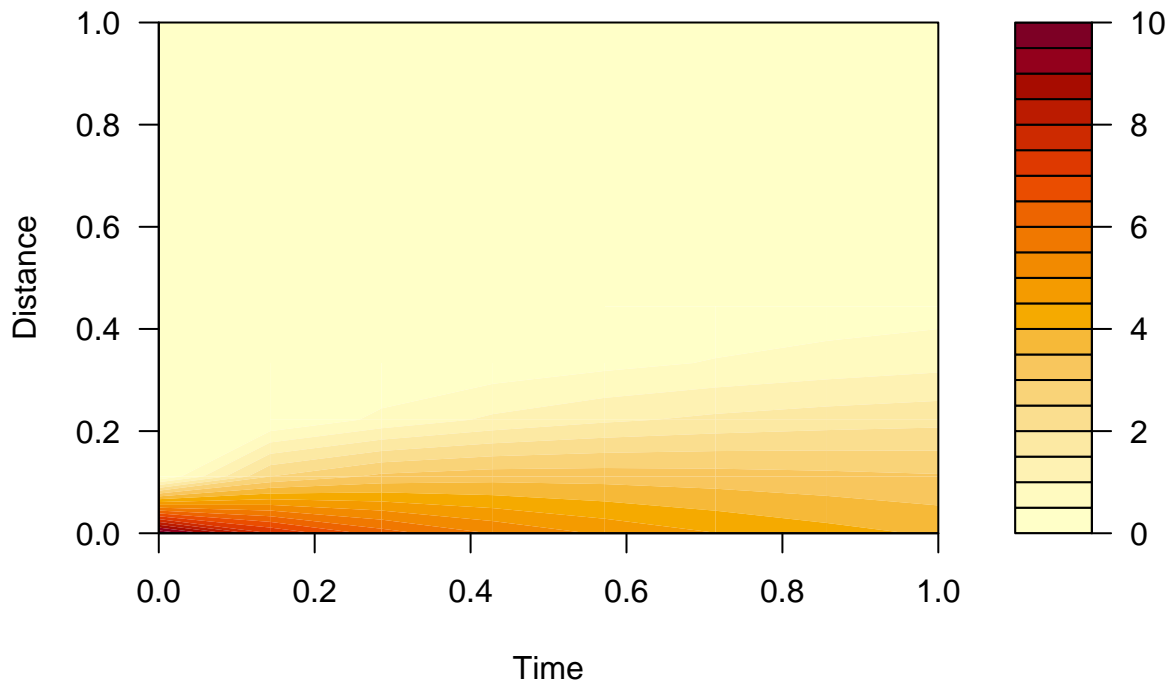
##           [,8] [,9] [,10]
## [1,] 0.0000000000 0 0
## [2,] 0.0000000000 0 0
## [3,] 0.0000000000 0 0
## [4,] 0.0000000000 0 0
## [5,] 0.0000000000 0 0
## [6,] 0.0000000000 0 0
## [7,] 0.0000000000 0 0
## [8,] 0.0006103516 0 0
##
## $qout
##           [,1] [,2] [,3] [,4] [,5] [,6] [,7]
## [1,] 25.000000 0.000000 0.000000 0.000000 0.000000000 0.000000000 0.000000000
## [2,] 12.500000 6.250000 0.000000 0.000000 0.000000000 0.000000000 0.000000000
## [3,] 7.812500 6.250000 1.562500 0.000000 0.000000000 0.000000000 0.000000000
## [4,] 5.468750 5.468750 2.343750 0.390625 0.000000000 0.000000000 0.000000000
## [5,] 4.101562 4.687500 2.636719 0.781250 0.09765625 0.000000000 0.000000000
## [6,] 3.222656 4.028320 2.685547 1.074219 0.24414062 0.02441406 0.000000000
## [7,] 2.618408 3.491211 2.618408 1.269531 0.39672852 0.07324219 0.006103516
## [8,] 0.000000 0.000000 0.000000 0.000000 0.000000000 0.000000000 0.000000000
##           [,8] [,9] [,10]
## [1,] 0 0 0
## [2,] 0 0 0
## [3,] 0 0 0
## [4,] 0 0 0
## [5,] 0 0 0
## [6,] 0 0 0
## [7,] 0 0 0
## [8,] 0 0 0
##
## $qin
##           [,1] [,2] [,3] [,4] [,5] [,6] [,7]
## [1,] 0 25.000000 0.000000 0.000000 0.000000 0.000000000 0.000000000
## [2,] 0 12.500000 6.250000 0.000000 0.000000 0.000000000 0.000000000
## [3,] 0 7.812500 6.250000 1.562500 0.000000 0.000000000 0.000000000
## [4,] 0 5.468750 5.468750 2.343750 0.390625 0.000000000 0.000000000
## [5,] 0 4.101562 4.687500 2.636719 0.781250 0.09765625 0.000000000
## [6,] 0 3.222656 4.028320 2.685547 1.074219 0.24414062 0.02441406
## [7,] 0 2.618408 3.491211 2.618408 1.269531 0.39672852 0.07324219
## [8,] 0 0.000000 0.000000 0.000000 0.000000 0.000000000 0.000000000
##           [,8] [,9] [,10]
## [1,] 0.000000000 0 0
## [2,] 0.000000000 0 0
## [3,] 0.000000000 0 0
## [4,] 0.000000000 0 0
## [5,] 0.000000000 0 0
## [6,] 0.000000000 0 0
## [7,] 0.006103516 0 0
## [8,] 0.000000000 0 0
##
# used filled contour to plot results
head(result$conc)

##           [,1] [,2] [,3] [,4] [,5] [,6] [,7] [,8] [,9]
## [1,] 10.000000 0.000000 0.000000 0.0000000 0.0000000 0.000000000 0 0 0

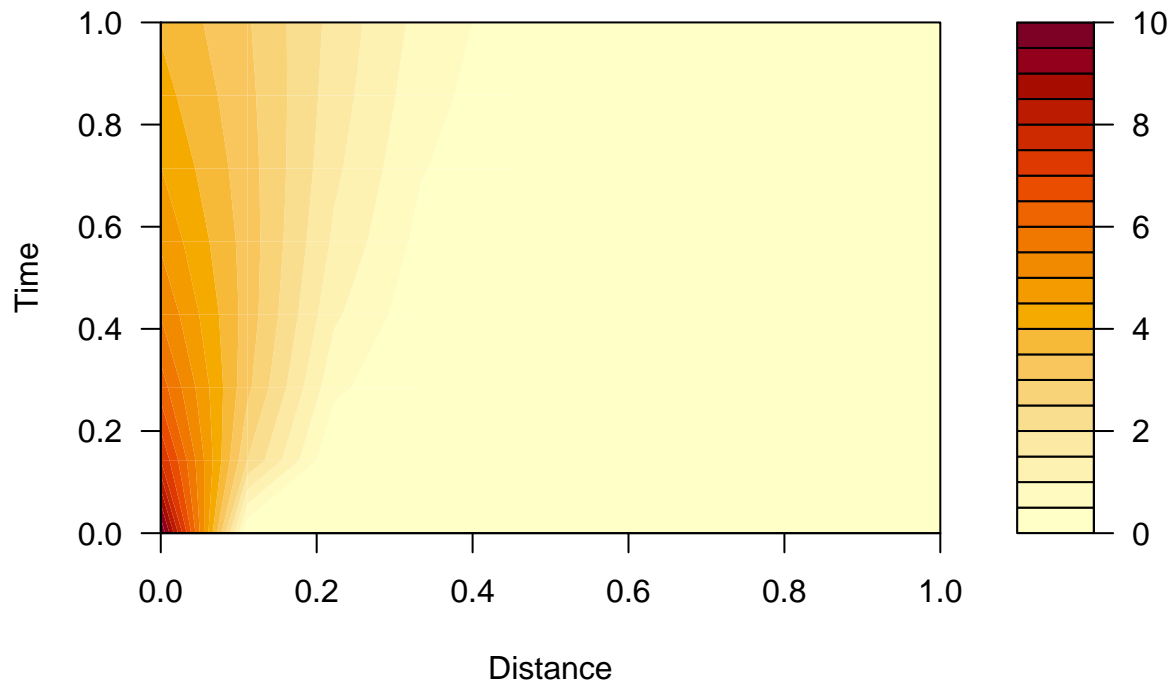
```

```
## [2,] 7.500000 2.500000 0.000000 0.000000 0.000000 0.000000000 0 0 0
## [3,] 6.250000 3.125000 0.625000 0.000000 0.000000 0.000000000 0 0 0
## [4,] 5.468750 3.281250 1.093750 0.156250 0.000000 0.000000000 0 0 0
## [5,] 4.921875 3.281250 1.406250 0.3515625 0.0390625 0.000000000 0 0 0
## [6,] 4.511719 3.222656 1.611328 0.5371094 0.1074219 0.009765625 0 0 0
##      [,10]
## [1,]      0
## [2,]      0
## [3,]      0
## [4,]      0
## [5,]      0
## [6,]      0
```

```
filled.contour(result$conc, xlab="Time", ylab="Distance")
```

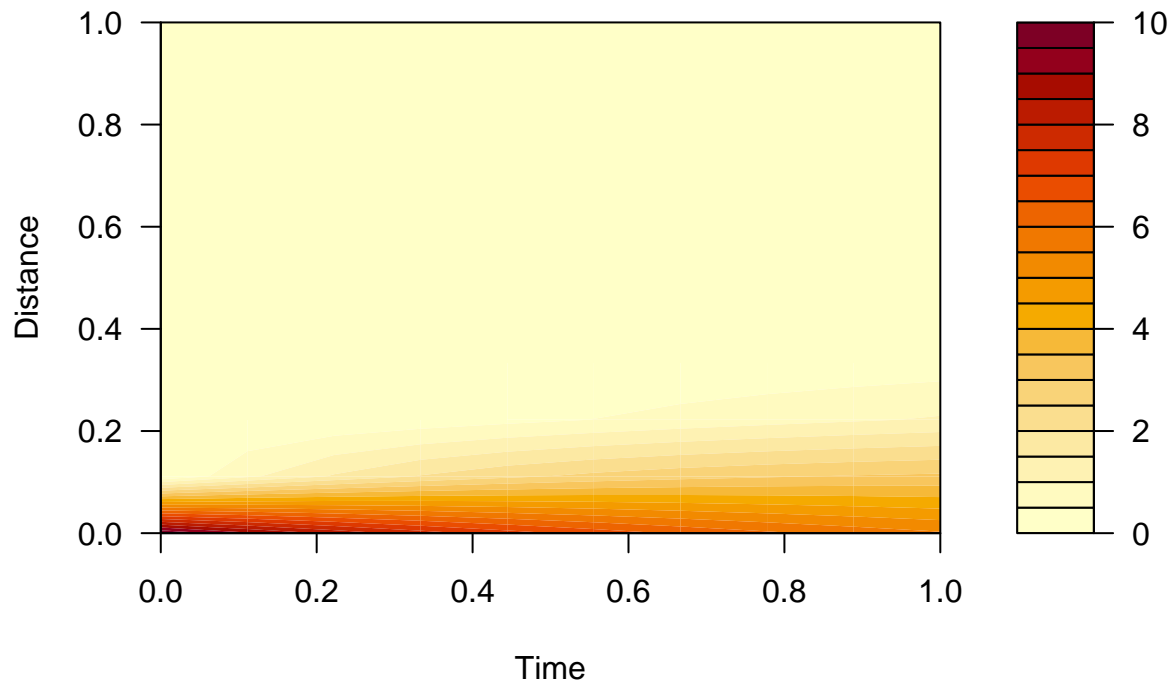


```
# or if you prefer this orientation (Distance on x axis)
filled.contour(t(result$conc), ylab="Time", xlab="Distance")
```

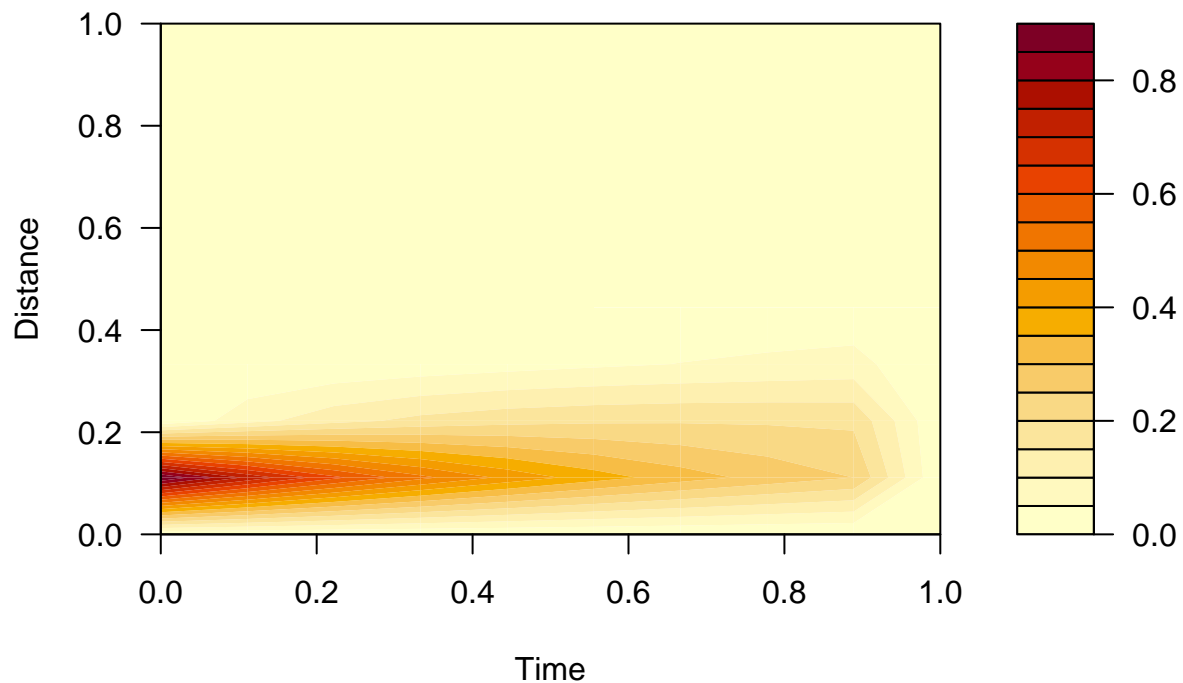


In class example of changing parameters (diffusivity  $D$ , and space and time steps ( $dx$ ,  $dt$ ))

```
# changes diffusivity and other parameters particularly  
# diffusivity, dx and dt  
  
res = diff1(initialC = 10, nx = 10, dx = 1, nt = 10, dt = 30, D = 0.006, area = 1)  
  
filled.contour(res$conc, xlab="Time", ylab="Distance")
```



```
# we can also see how much material moved from place to place each time step
filled.contour(res$qin, xlab="Time", ylab="Distance")
```



## Homework Responses

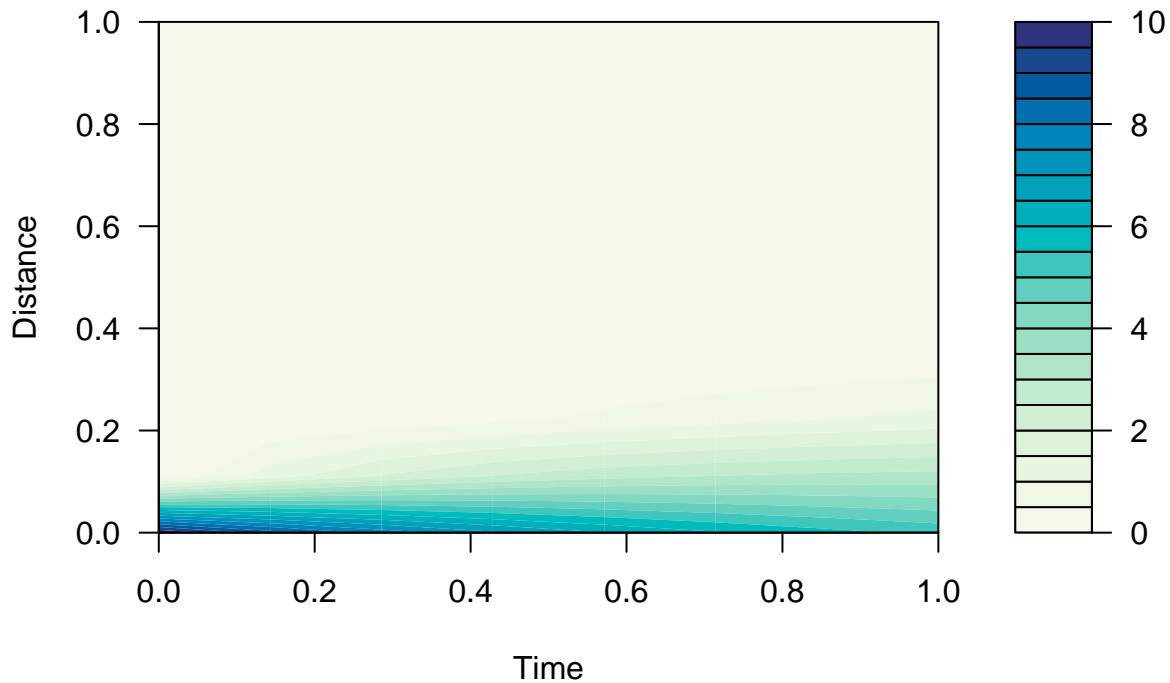
### Change diffusivity and length of segment

```
# changes diffusivity (D) and length of segment (dx)
# original params: initialC = 10, nx = 10, dx = 1, nt = 8, dt = 1, D = 0.5, area = 10
```

```
resultA = diff1(initialC = 10, nx = 10, dx = 4, nt = 8, dt = 1, D = 1, area = 10)

resultA_plot1 <- filled.contour(resultA$conc,
                                color.palette = function(n) hcl.colors(n, "GnBu", rev = TRUE),
                                plot.title = title(main = "Diffusion - Change in Diffusivity and Segment Length", xlab="Time"))
```

## Diffusion – Change in Diffusivity and Segment Length

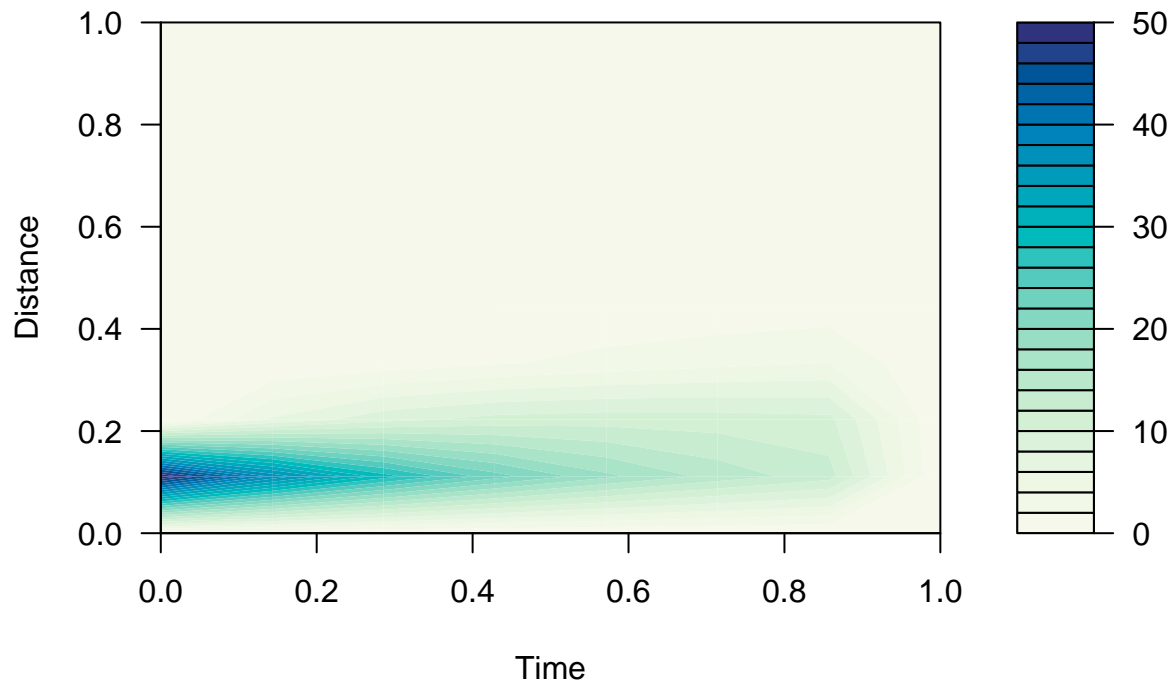


```
resultA_plot1
```

```
## NULL
```

```
# how much material moved from place to place each time step
resultA_plot2 <-filled.contour(resultA$qin,
                                color.palette = function(n) hcl.colors(n, "GnBu", rev = TRUE),
                                plot.title = title(main = "Diffusion Movement", xlab="Time", ylab="Distance"))
```

## Diffusion Movement



```
resultA_plot2
```

```
## NULL
```

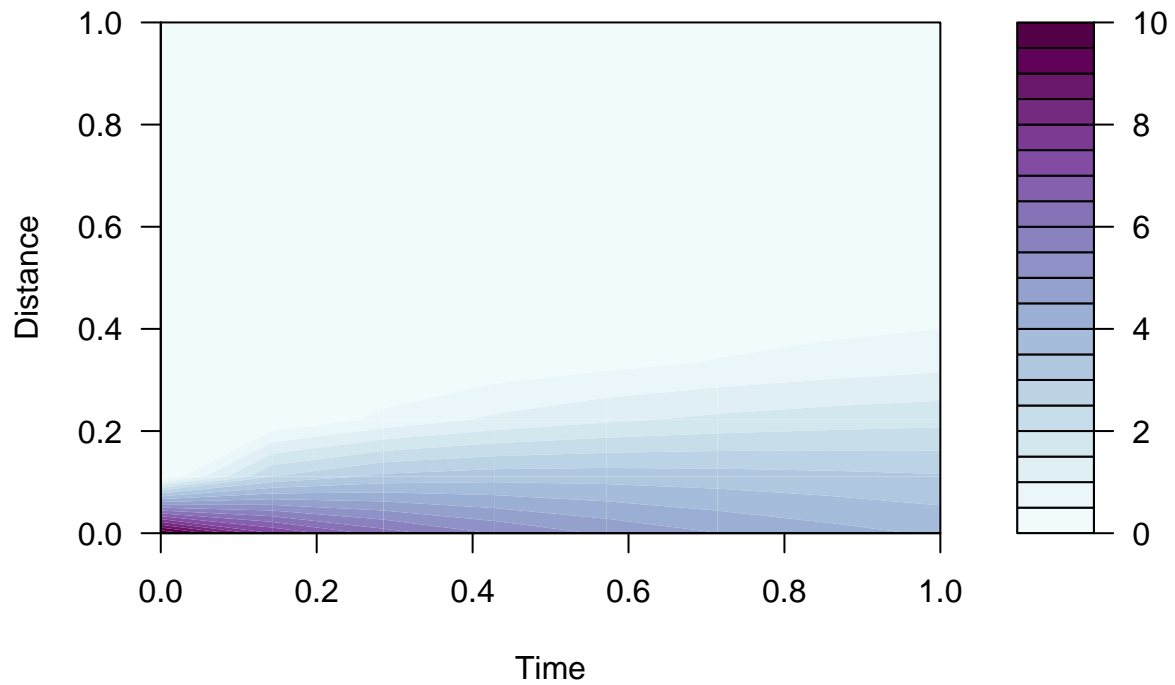
## Change space step (dx), time step (dt)

```
# changes length of segment (dx) and time (dt)
# original params: initialC = 10, nx = 10, dx = 1, nt = 8, dt = 1, D = 0.5, area = 10

resultb = diff1(initialC = 10, nx = 10, dx = .5, nt = 8, dt = .5, D = 0.5, area = 10)

resultB_plot1 <- filled.contour(resultb$conc,
  color.palette = function(n) hcl.colors(n, "BuPu", rev = TRUE),
  plot.title = title(main = "Diffusion - Change in Time & Segment Length", xlab="Time", ylab="Distance"))
```

## Diffusion – Change in Time & Segment Length



```
resultB_plot1
```

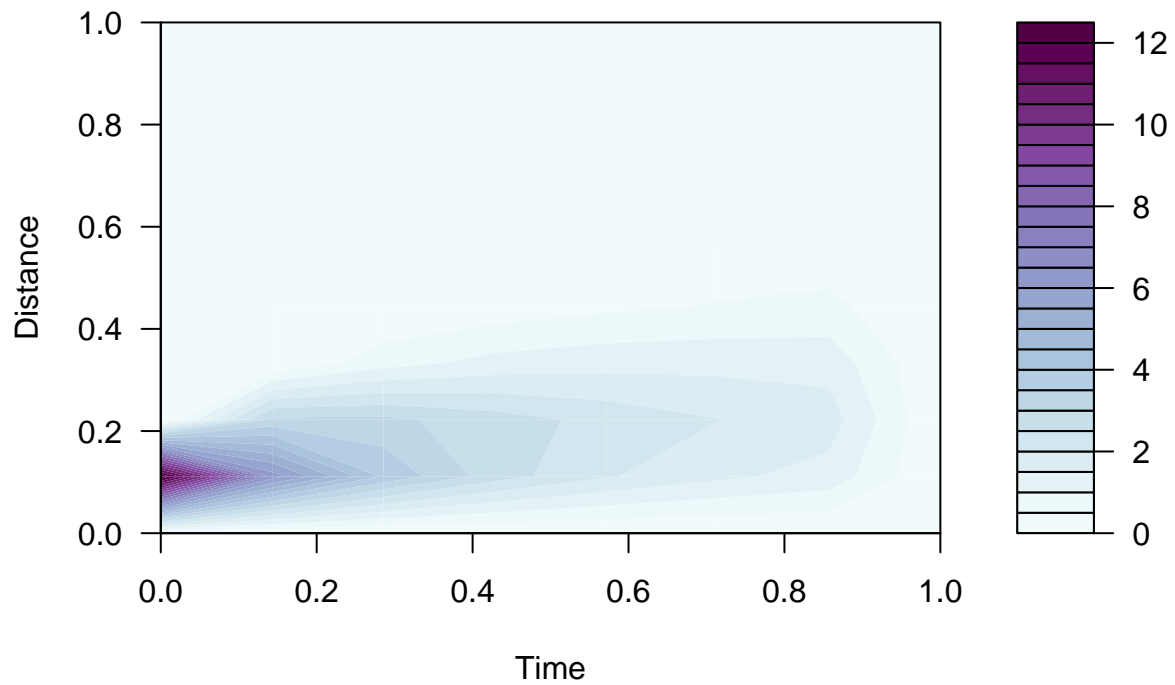
```
## NULL
```

```
# how much material moved from place to place each time step
```

```
resultB_plot2 <-filled.contour(resultb$qin,  
  color.palette = function(n) hcl.colors(n, "BuPu", rev = TRUE),  
  plot.title = title(main = "Diffusion Movement", xlab="Time", ylab="Distance"))
```



## Diffusion Movement



```
resultB_plot2
```

```
## NULL
```

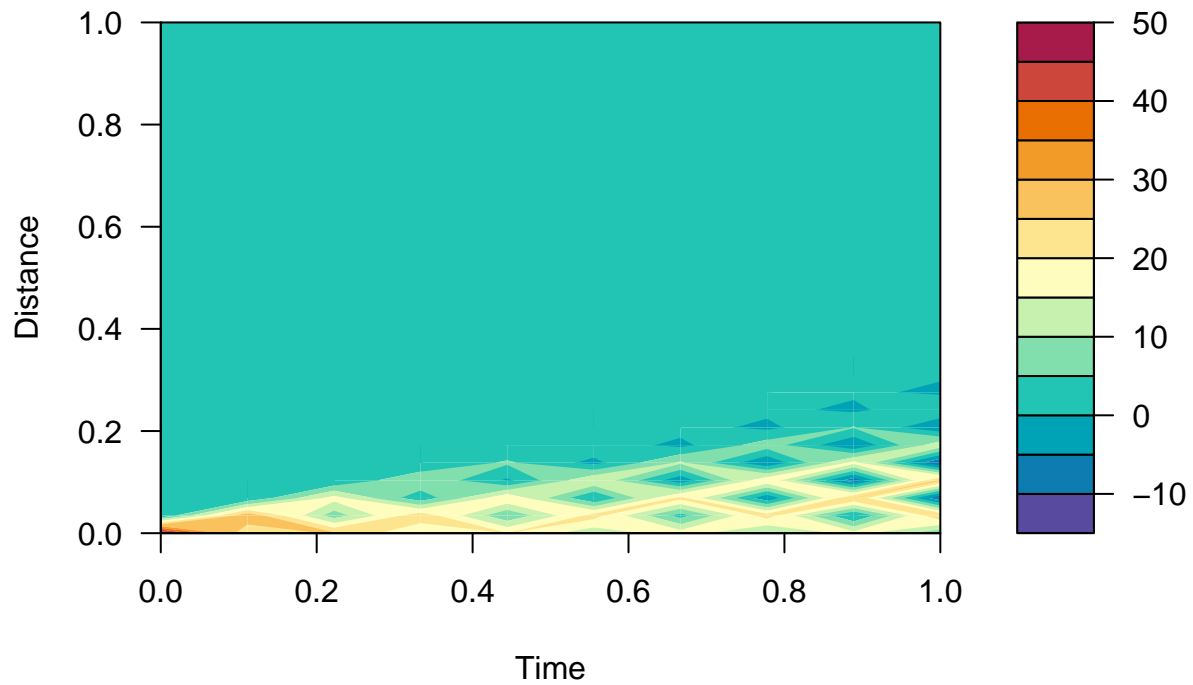
## Change all parameters

```
# original params: initialC = 10, nx = 10, dx = 1, nt = 8, dt = 1, D = 0.5, area = 10
```

```
resultc = diff1(initialC = 50, nx = 30, dx = 6, nt = 10, dt = 10, D = .7, area = 60)
```

```
resultC_plot1 <- filled.contour(resultc$conc,  
  color.palette = function(n) hcl.colors(n, "spectral", rev = TRUE),  
  plot.title = title(main = "Diffusion - Change in All Parameters", xlab="Time", ylab = "Distance"))
```

## Diffusion – Change in All Parameters



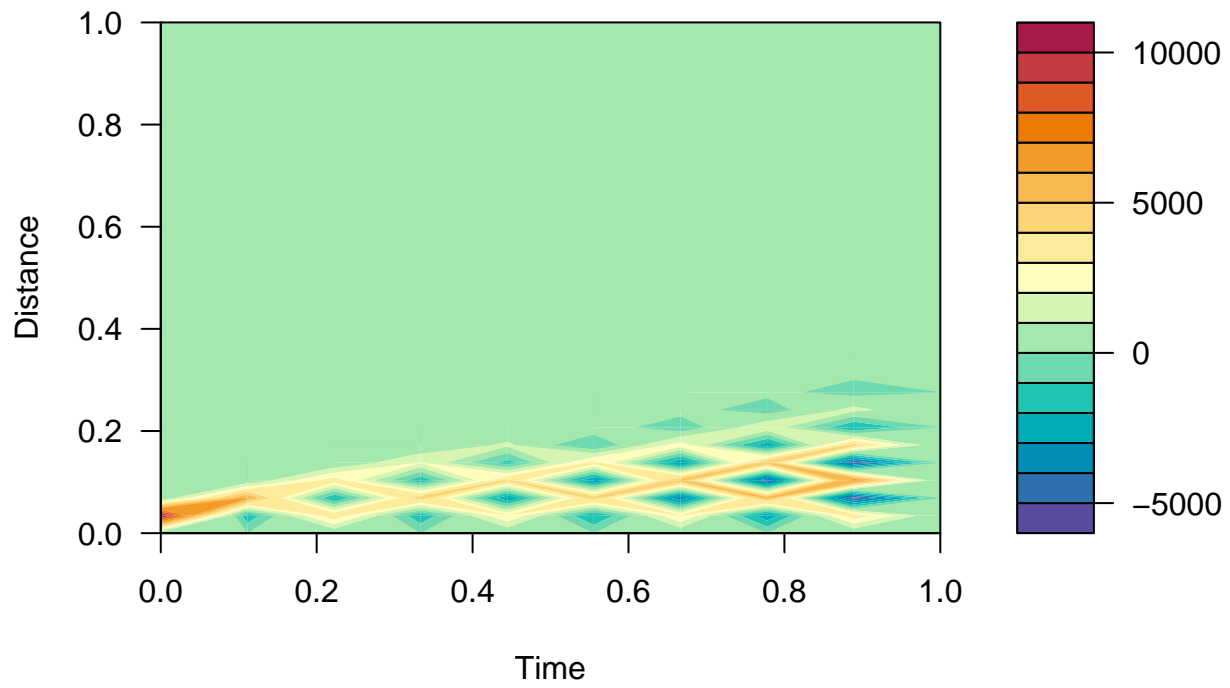
```
resultC_plot1
```

```
## NULL
```

```
# how much material moved from place to place each time step
```

```
resultC_plot2 <-filled.contour(resultc$qin,  
  color.palette = function(n) hcl.colors(n, "spectral", rev = TRUE),  
  plot.title = title(main = "Diffusion Movement", xlab="Time", ylab="Distance"))
```

## Diffusion Movement



```
resultC_plot2
```

```
## NULL
```