A Numerical 3-D Phytoplankton Transport - Reaction Model

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VT Ecosystem Dynamics

Domain and Currency

- The model characterizes a cube of dimensions 10m x 10m x 10m
- Each cube is 1m x 1m x 1m
- There are a total of 1000 spatial cells in the model
- The model currency is gC/m3
- The time step used = 1 day
- The duration of simulations = 30 to 400 days

Model Parameters

Table of Parameter Values and Units

Parameter Values	*Units*
vp = .1	m/d
phyto_flux_top = 0	gC/m2/d
degRate = .15	m3/d/gC
maxUptake =2	gC/d
ksPAR =140	uEinst/m2/sec
light_extinction = 0.7	/gC/m
D_coeff = 0.2	m2/d
del_X = 1	m
del_Y = 1	m
del_Z =1	m
Norm_H = 1	unitless vector
Norm_L = -1	unitless vector
TopDownDiff = 0	gC/m2/d
SideInDiff1 = 0	gC/m2/d
SideInDiff2 = 0	gC/m2/d
SideInDiff3 = 0	gC/m2/d
SideInDiff4 = 0	gC/m2/d
BottomDownDiff =0	gC/m2/d
xz_area = del_X*del_Z = 1	m2
yz_area = del_Y*del_Z = 1	m2
xy_area = del_X*del_Y = 1	m2
volume = (del_X*del_Y*del_Z) = 1	m3
X_extent = 10/del_X = 10	boxes
Y_extent = 10/del_Y = 10	boxes
Z_extent = 10/del_Z = 10	boxes

Scientific Question Tested

- The objective was to examine the relationship between advection, diffusion, and light limited growth in space and through time
- Specifically I tested how varying the sinking rate affected the spatial distribution of phytoplankton over time
- Spoiler; there was a notable difference between 0.1 and 10 m/s sinking rates

Peperzak et al., 2002

Discretizing The A-D-R Equation

recall; $$Flux|_{dispersion} = -D\,\frac{\partial C}{\partial x} \qquad Flux|_{advection} = u \cdot C$$

and generally; $$\frac{\partial C}{\partial t} = -\frac{1}{A} \cdot \frac{\partial A \cdot Flux}{\partial x} + g \cdot C \tag{6.16}$$

This formula is now discretized to represent the rate of change of the concentrations in each box i, C_i, as follows:

$$\frac{dC_i}{dt} = -\frac{1}{A_i}\frac{\Delta_i(A \cdot Flux)}{\Delta x_i} + g \cdot C_i \tag{6.17}$$

Where C_i is concentration in box i, Δx_i is the thickness of box i, A_i is the surface area in the middle of box i, and Δ_i denotes that the flux gradient is to be taken around box i.

from A Practical Guide To Ecological Modelling Using R as a Simulation Platform

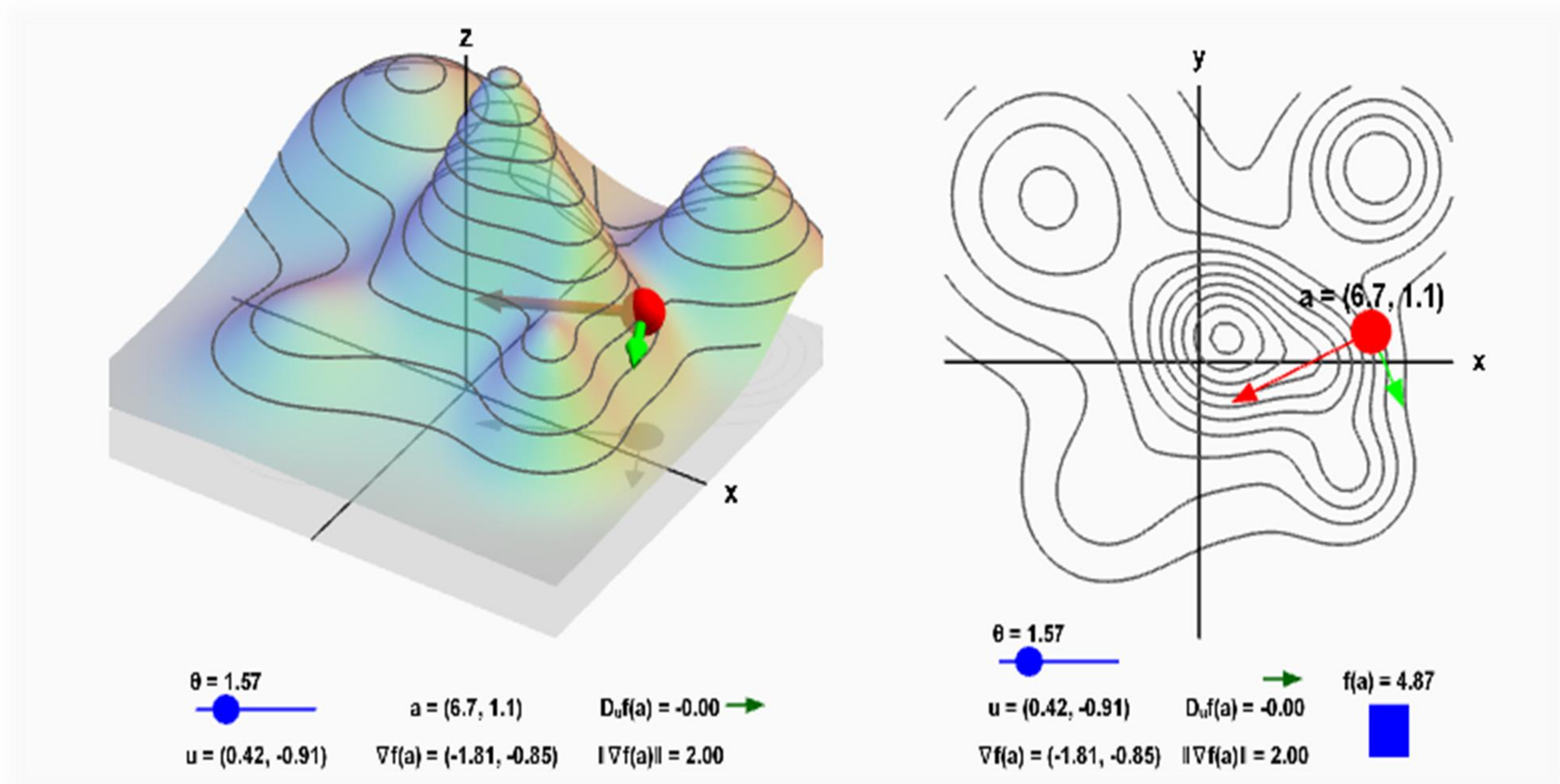
Discretization Continued

Keeping this in mind, the flux gradient for box i is then defined as the difference of the fluxes at the interface with the next box (i,i+1) and with the previous box (i−1, i). Thus we write:

$$\frac{dC_i}{dt} = -\frac{A_{i,i+1} \cdot Flux_{i,i+1} - A_{i-1,i} \cdot Flux_{i-1,i}}{A_i \cdot \Delta x_i} + g \cdot C_i \qquad (6.18)$$

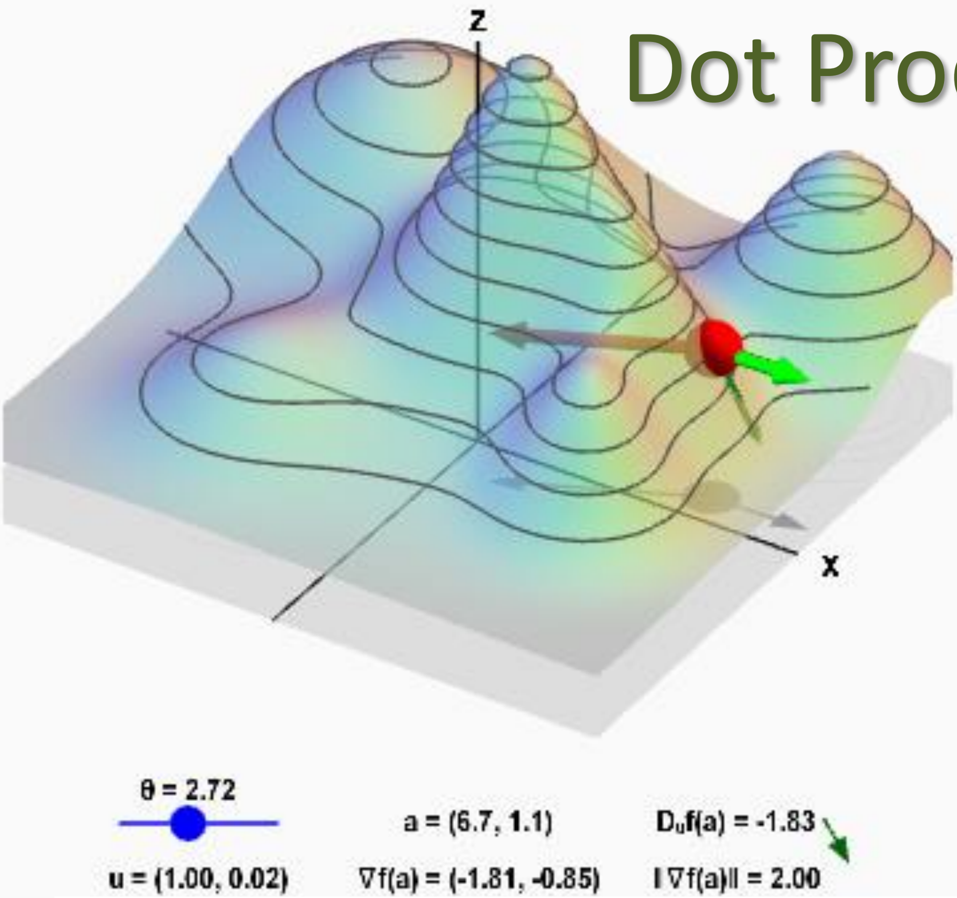
Here $Flux_{i-1,i}$ is the flux on the interface between cell i−1 and i, and $A_{i-1,i}$ is the surface area on this interface.

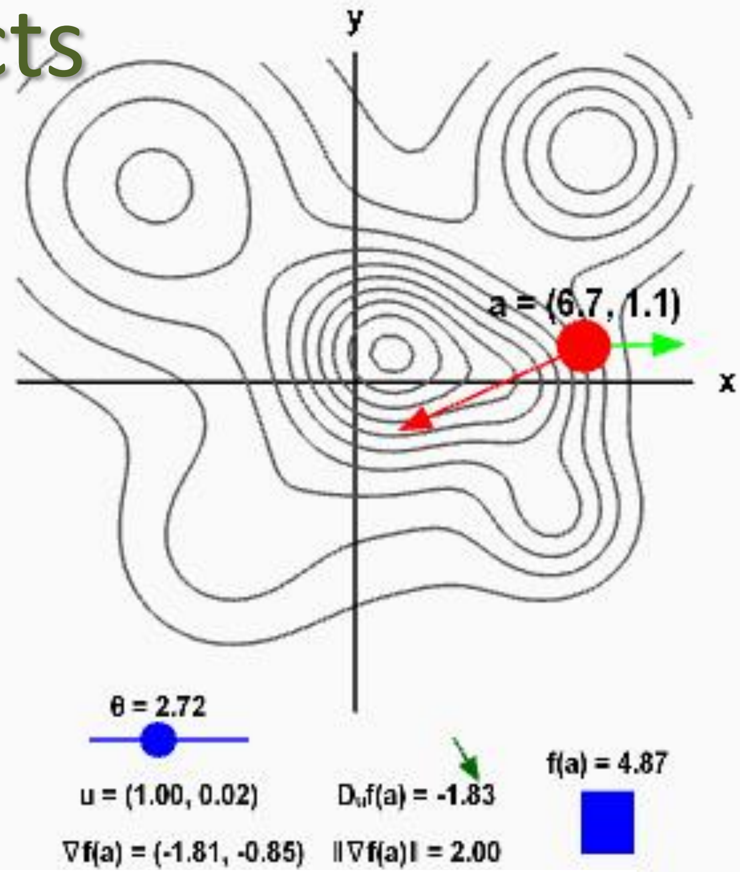
Why We Can Reduce Space to 3 Axes Pt. A: The Gradient Function



Nykamp DQ, "Gradient and directional derivative on a mountain." From *Math Insight*.
http://mathinsight.org/applet/gradient_directional_derivative_mountain

Pt. B: The Directional Derivative and Dot Products





It turns out that the relationship between the gradient and the directional derivative can be summarized by the equation

$$
\begin{aligned}
D_{\mathbf{u}} f(\mathbf{a}) &= \nabla f(\mathbf{a}) \cdot \mathbf{u} \\
&= \|\nabla f(\mathbf{a})\| \, \|\mathbf{u}\| \cos\theta \\
&= \|\nabla f(\mathbf{a})\| \cos\theta
\end{aligned}
$$

where θ is the angle between $\mathbf{u}$ and the gradient. (Recall that $\mathbf{u}$ is a unit vector, meaning that $\|\mathbf{u}\| = 1$.)

A Walk in the Equation Park (1)

- Here is the general case:

```
#CALCULATE REACTION
PAR   <- 0.5*(540+440*sin(2*pi*t/365-1.4));
layer_mid_depth <- (k-1)*del_Z + del_Z/2;
layer_PAR <- PAR*exp(-light_extinction*(layer_mid_depth));
C_Uptake <- maxUptake*(layer_PAR/(layer_PAR+ksPAR))*PHYTO.3d[k,i,j];
Degradation <- degRate*(PHYTO.3d[k,i,j])^2
Reaction <- -Degradation + C_Uptake;

#CALCULATE ADVECTION
flux_advection_Z_high = vp*PHYTO.3d[k,i,j]
flux_advection_Z_low = vp*PHYTO.3d[k-1,i,j]
volume = (del_X*del_Y*del_Z)
Advection = (Norm_L*flux_advection_Z_low*xy_area +
Norm_H*flux_advection_Z_high*xy_area)/-volume
```

A Walk in the Equation Park (2)

- Continued from previous slide:

```
#CALCULATE DIFFUSION
flux_diffu_X_high = -D_coeff*((PHYTO.3d[k,i+1,j]-PHYTO.3d[k,i,j])/del_X)
flux_diffu_X_low = -D_coeff*((PHYTO.3d[k,i,j]-PHYTO.3d[k,i-1,j])/del_X)
flux_diffu_Y_high = -D_coeff*((PHYTO.3d[k,i,j+1]-PHYTO.3d[k,i,j])/del_Y)
flux_diffu_Y_low = -D_coeff*((PHYTO.3d[k,i,j]-PHYTO.3d[k,i,j-1])/del_Y)
flux_diffu_Z_high = -D_coeff*((PHYTO.3d[k+1,i,j]-PHYTO.3d[k,i,j])/del_Z)
flux_diffu_Z_low = -D_coeff*((PHYTO.3d[k,i,j]-PHYTO.3d[k-1,i,j])/del_Z)
Diffusion = (Norm_H*flux_diffu_X_high*yz_area + Norm_L*flux_diffu_X_low*yz_area +
Norm_H*flux_diffu_Y_high*xz_area + Norm_L*flux_diffu_Y_low*xz_area +
Norm_H*flux_diffu_Z_high*xy_area + Norm_L*flux_diffu_Z_low*xy_area)/-volume};

dPHYTO.3d[k,i,j] <-  Advection + Diffusion + Reaction
```

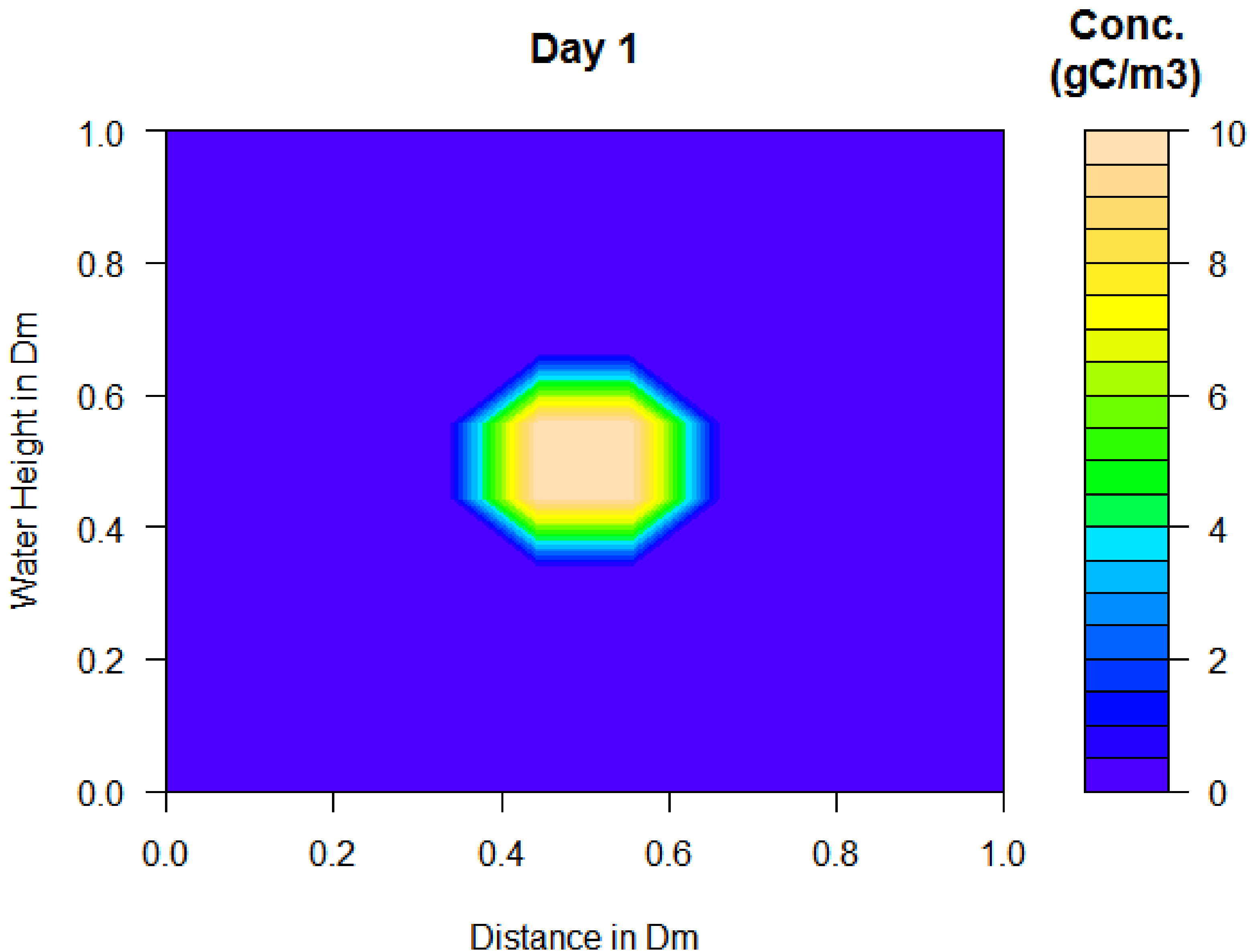
A Walk in the Equation Park (3)

- A Set of Boundary Layer Conditions:

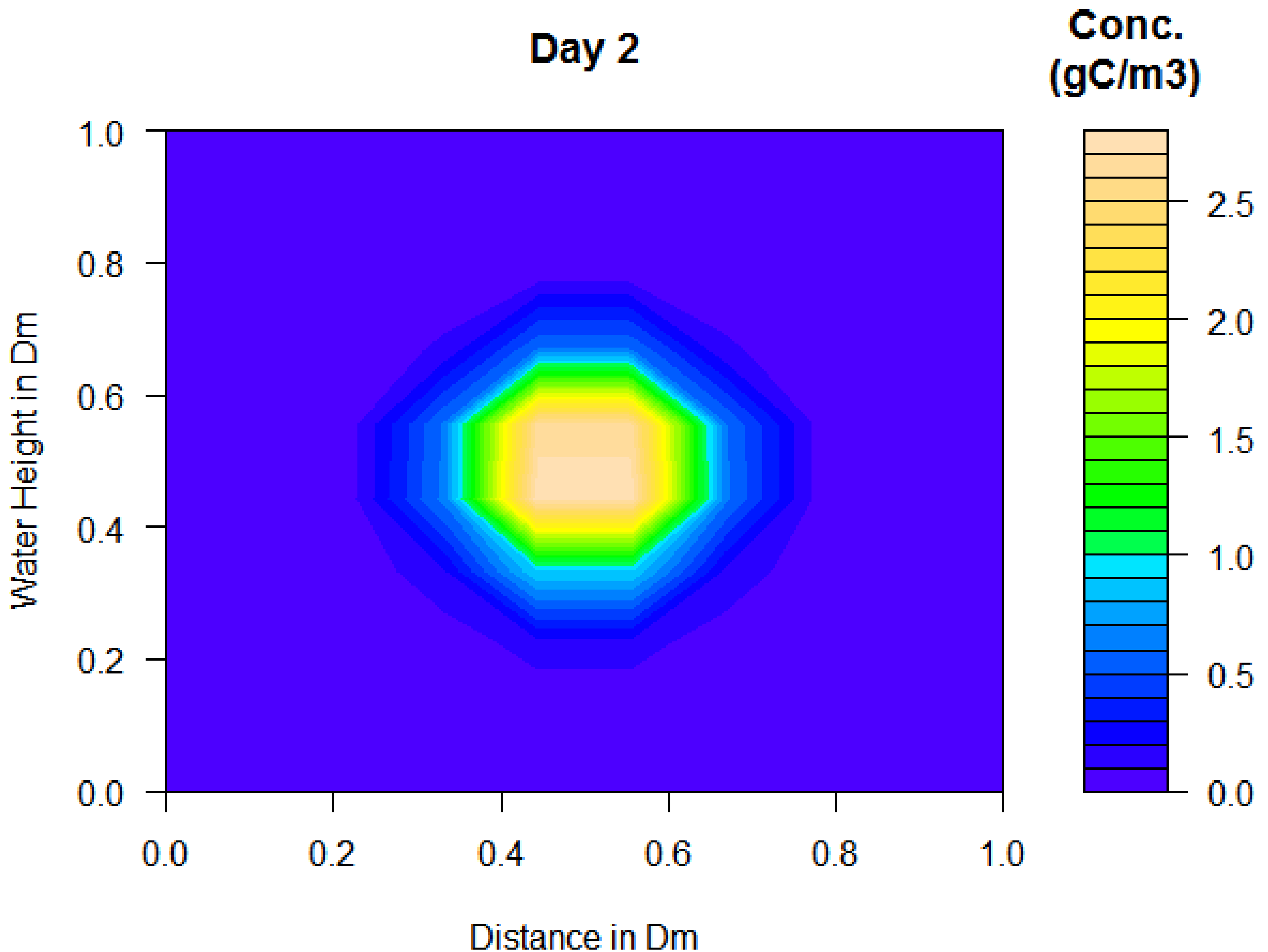
```
# calculate advection and diffusion for each box w.r.t. specific boundary layer conditions(27)
if(i==1 & j==1 & k==1){⇔};
if(i==X_extent & j==1 & k==1){⇔};
if(i==X_extent & j==Y_extent & k==1){⇔};
if(i==1 & j==Y_extent & k==1){⇔};
if(j==1 & k==1 & i!=1 & i!=X_extent){⇔};
if(i==X_extent & k==1 & j!=1 & j!=Y_extent){⇔};
if(j==Y_extent & k==1 & i!=1 & i!=X_extent){⇔};
if(i==1 & k==1 & j!=Y_extent & j!=1){⇔};
if(k==1 & i!=1 & i!=X_extent & j!=1 & j!=Y_extent){⇔}; #End Of Top Boxes
if(i==1 & j==1 & k==Z_extent){⇔};
if(i==X_extent & j==1 & k==Z_extent){⇔};
if(i==X_extent & j==Y_extent & k==Z_extent){⇔};
if(i==1 & j==Y_extent & k==Z_extent){⇔};
if(j==1 & k==Z_extent & i!=1 & i!=X_extent){⇔};
if(i==X_extent & k==Z_extent & j!=1 & j!=Y_extent){⇔};
if(j==Y_extent & k==Z_extent & i!=1 & i!=X_extent){⇔};
if(i==1 & k==Z_extent & j!=1 & j!=Y_extent){⇔};
if(k==Z_extent & i!=1 &i!=X_extent & j!=1 &j!=Y_extent){⇔};#End Of Bottom Boxes
if(i==1 & j==1 & k!=1 & k!=Z_extent){⇔};
if(i==X_extent & j==1 & k!=1 & k!=Z_extent){⇔};
if(j==1 & i!=1 & i!=X_extent & j!=1 & j!=Y_extent){⇔}; #End of Front Side; where j==1
if(i==1 & j==Y_extent & k!=1 &k!=Z_extent){⇔};
if(i==X_extent & j==Y_extent & k!=1 & k!=Z_extent){⇔};
if(j==Y_extent & i!=1 & i!=X_extent & k!=1 & k!=Z_extent){⇔}; # End Back Side; where j==Y_extent
if(i==1 & j!=1 & j!=Y_extent & k!=1 & k!=Z_extent){⇔}; # End Left Side; where i==1
if(i==X_extent & j!=1 & j!=Y_extent & k!=1 & k!=Z_extent){⇔}; # End Right Side; where i==X_extent
if(i!=1 & i!=X_extent & j!=1 & j!=Y_extent & k!=1 & k!=Z_extent){⇔};
```

A Visualization of Early Spatial Dynamics

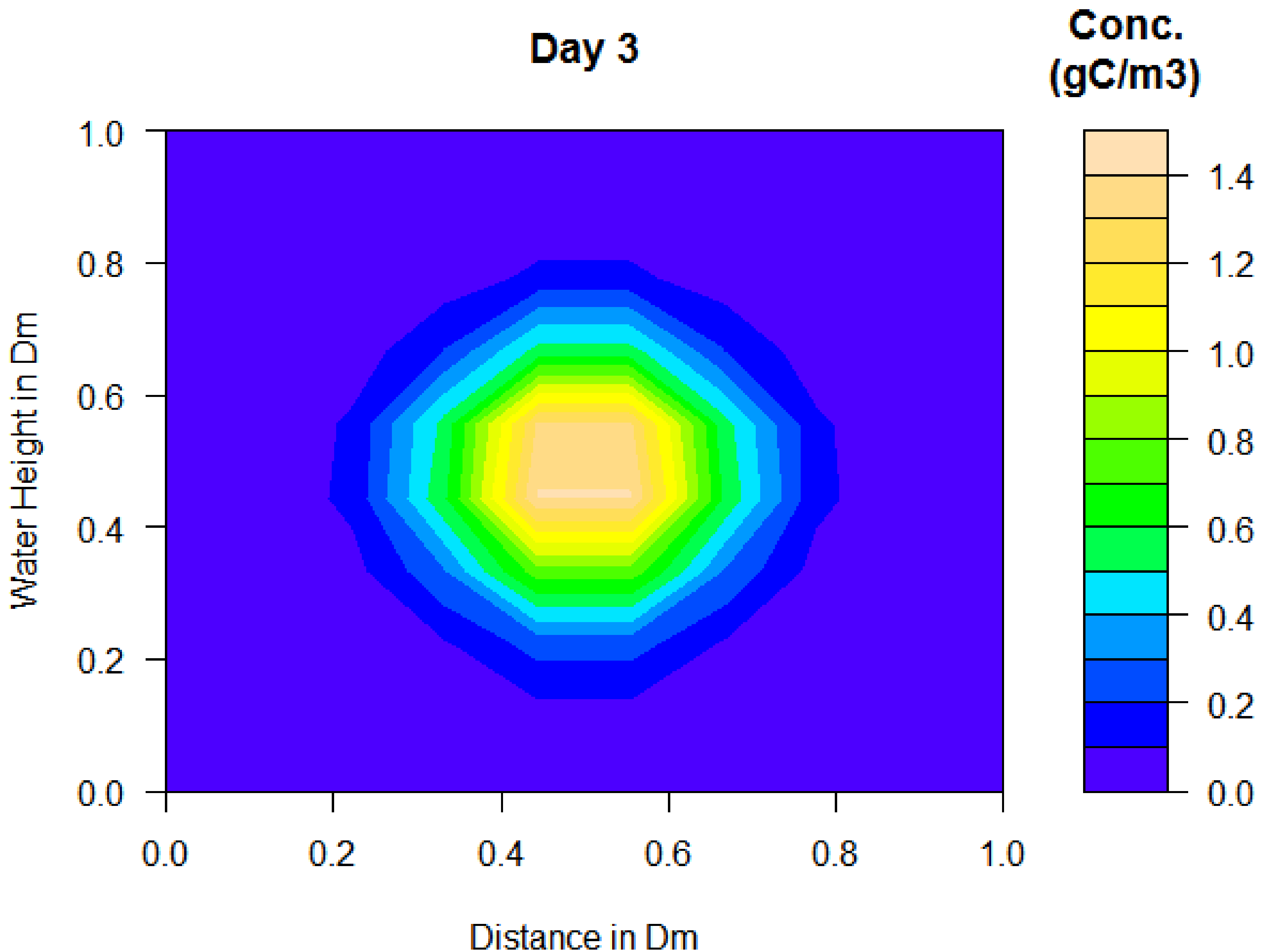
- I varied the sinking rate and examined the spatial distribution of phytoplankton over time
  - When the sinking rate is low enough that phytoplankton diffuses from subsurface up to an area of higher available light, a top down gradient develops
  - When the sinking rate is greater that ~4 phytoplankton never make it to the surface and a sub-surface population develops
  - What follows is a series where VP = 0.1 and D = .2



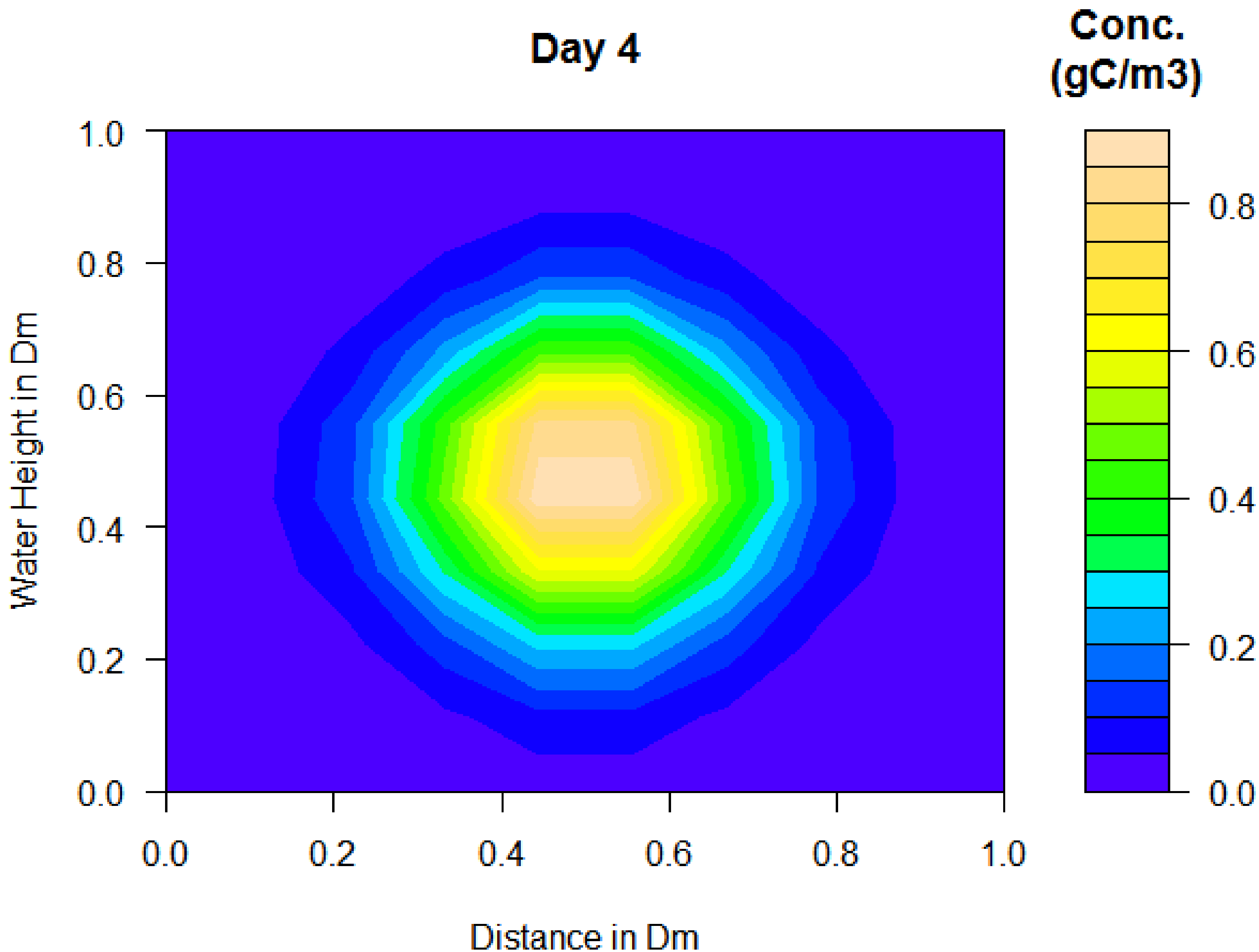
Day 1
Conc.
(gC/m3)
Water Height in Dm
Distance in Dm
1.0
0.8
0.6
0.4
0.2
0.0
10
8
6
4
2
0

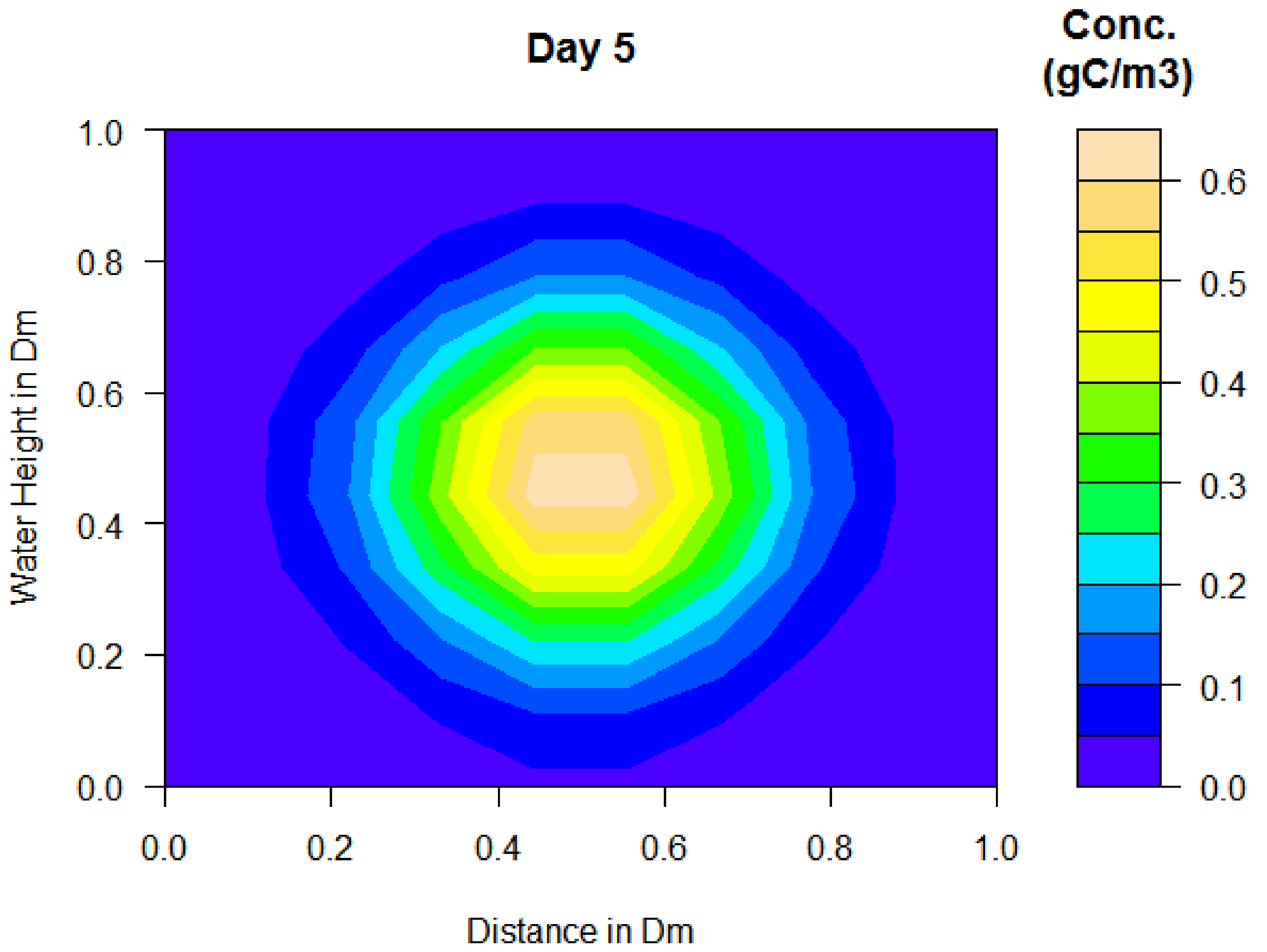


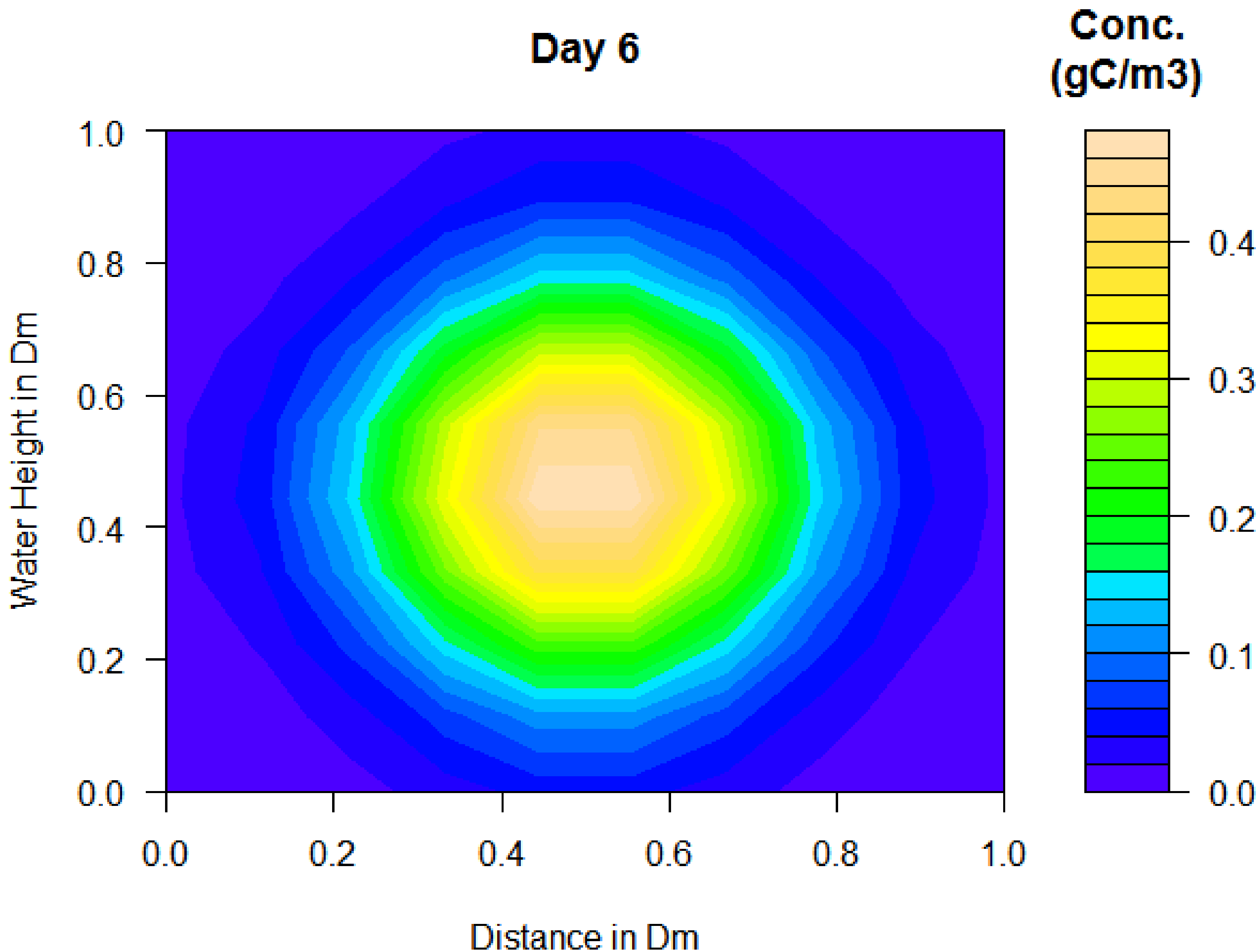
Day 2
Conc.
(gC/m3)
1.0
0.8
0.6
0.4
0.2
0.0
Water Height in Dm
0.0
0.2
0.4
0.6
0.8
1.0
Distance in Dm
2.5
2.0
1.5
1.0
0.5
0.0

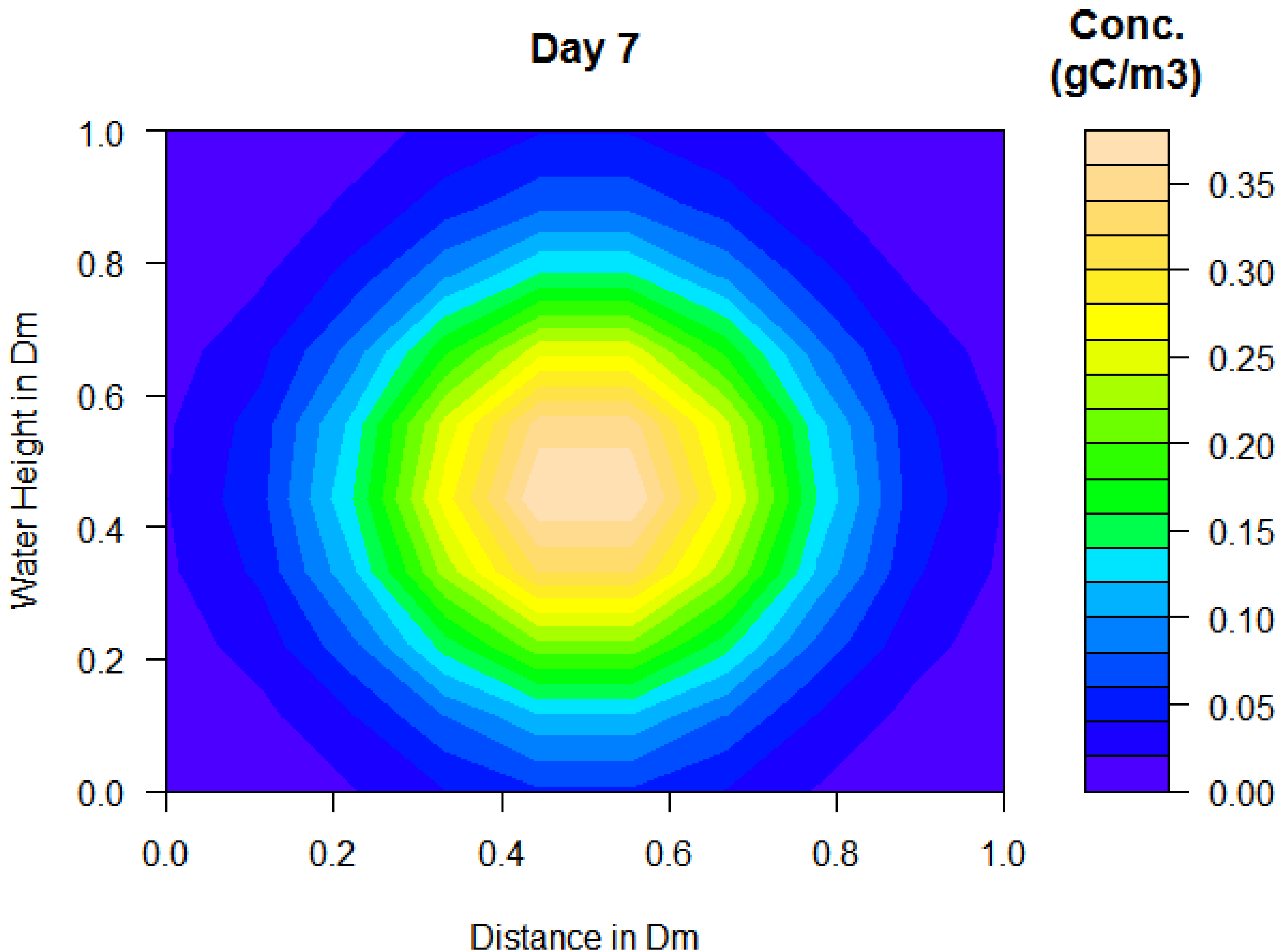


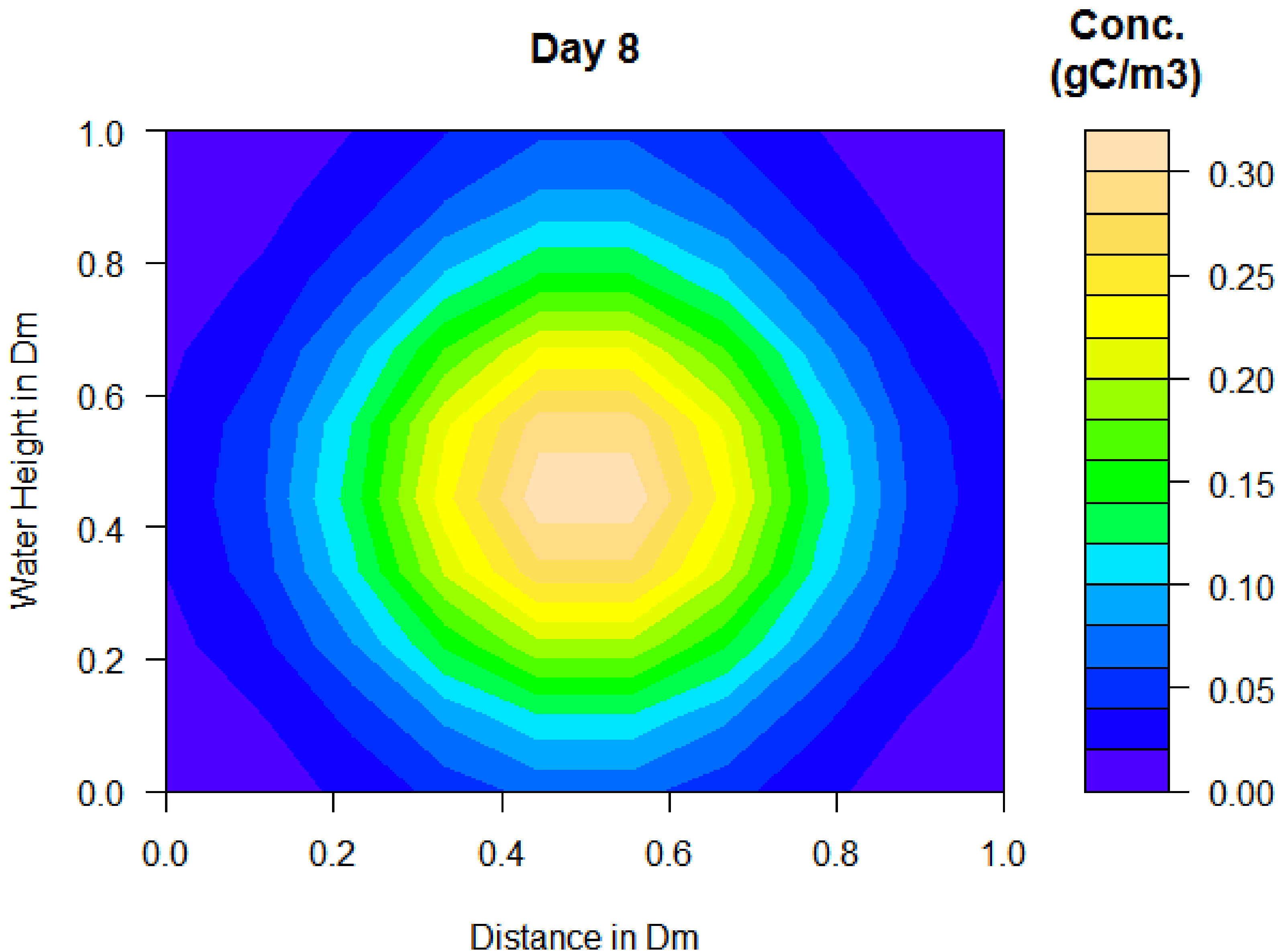
Day 3
Conc.
(gC/m3)
Water Height in Dm
Distance in Dm
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0

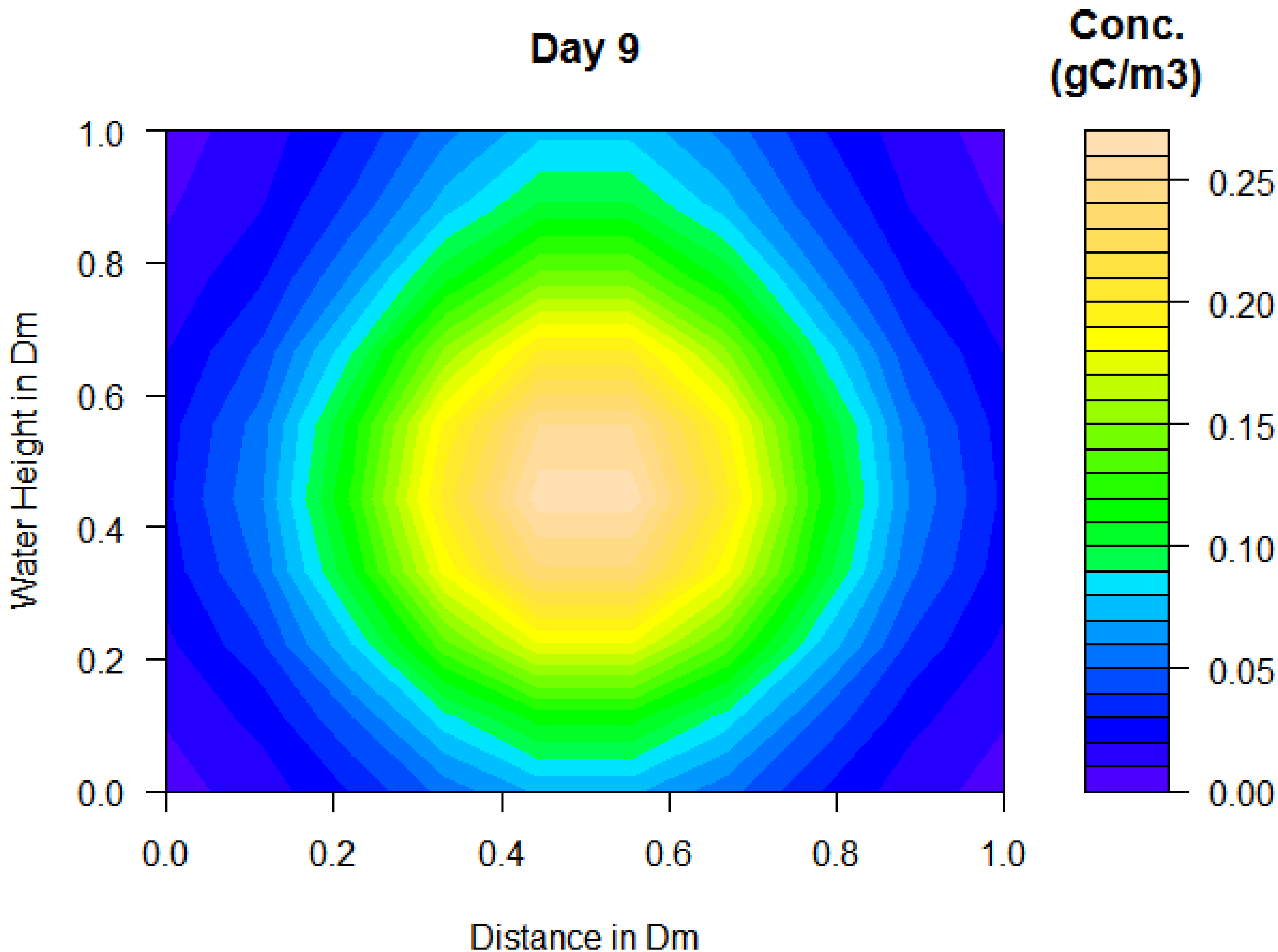

Day 4
Conc.
(gC/m3)
Water Height in Dm
Distance in Dm
0.0
0.2
0.4
0.6
0.8
1.0

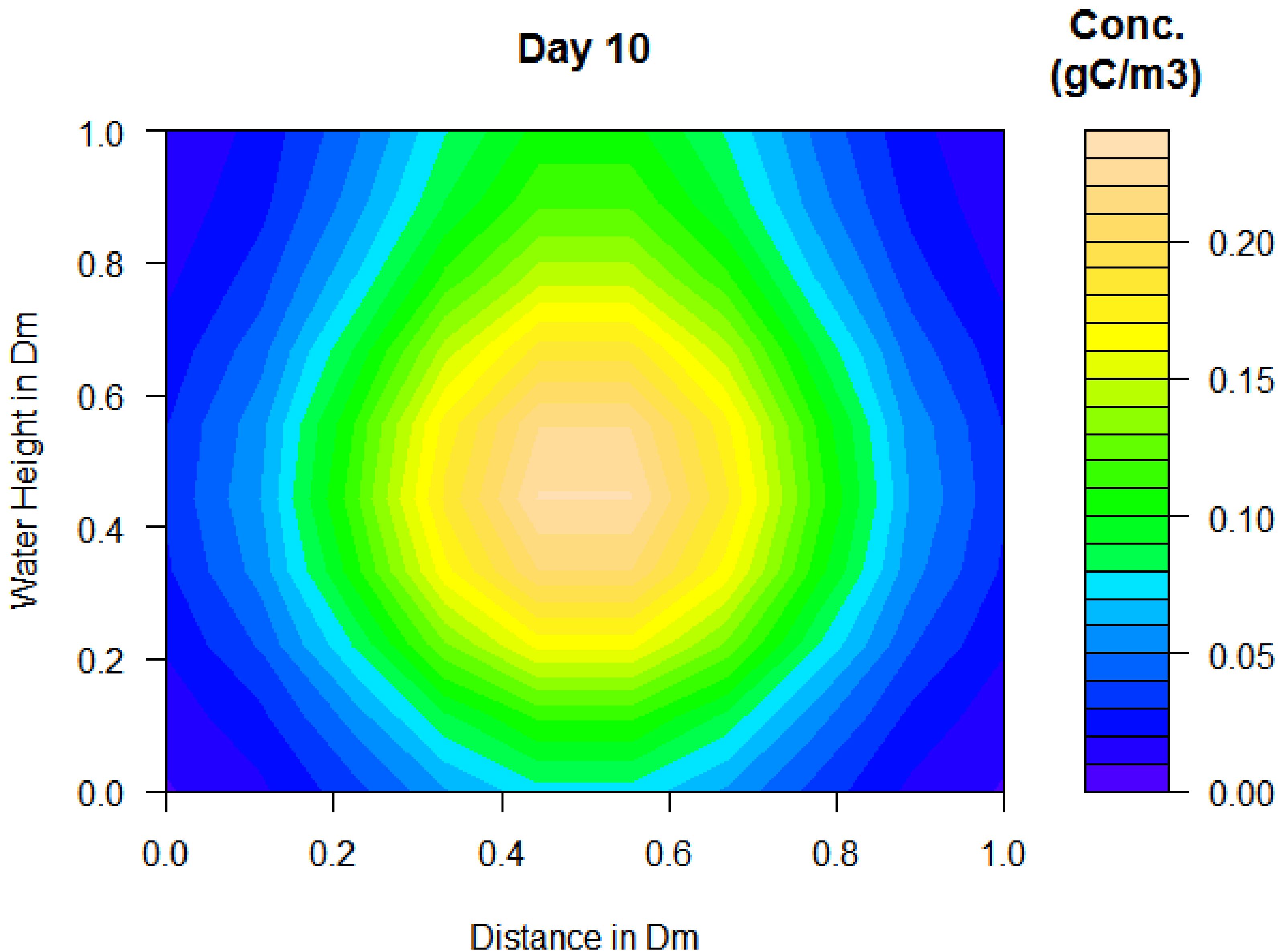

Day 5
Conc.
(gC/m3)
Water Height in Dm
Distance in Dm
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0
0.6
0.5
0.4
0.3
0.2
0.1
0.0

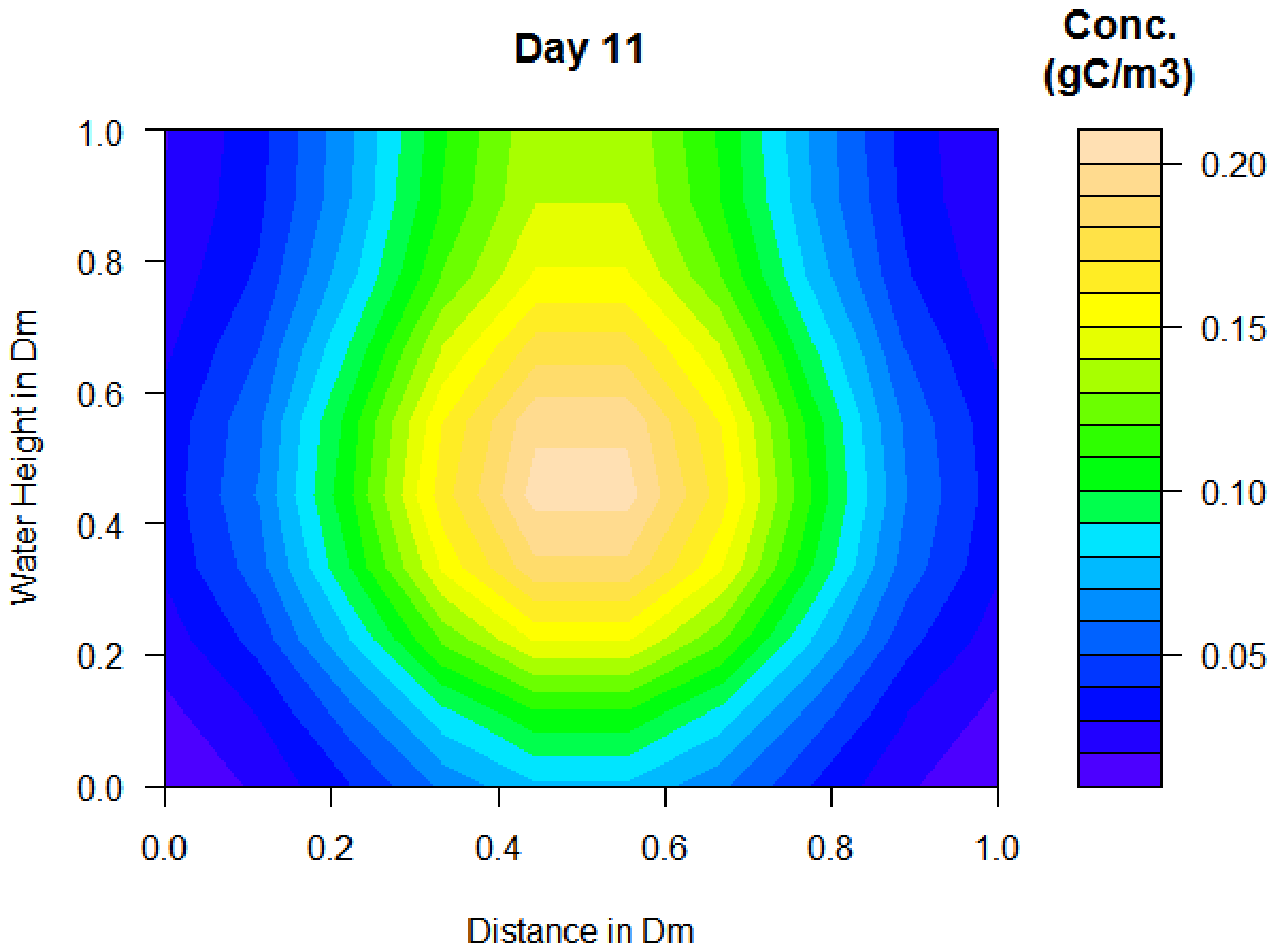

Day 6
Conc.
(gC/m3)
Water Height in Dm
Distance in Dm
0.0
0.2
0.4
0.6
0.8
1.0
0.1
0.3


Day 7
Conc.
(gC/m3)
Water Height in Dm
Distance in Dm
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00

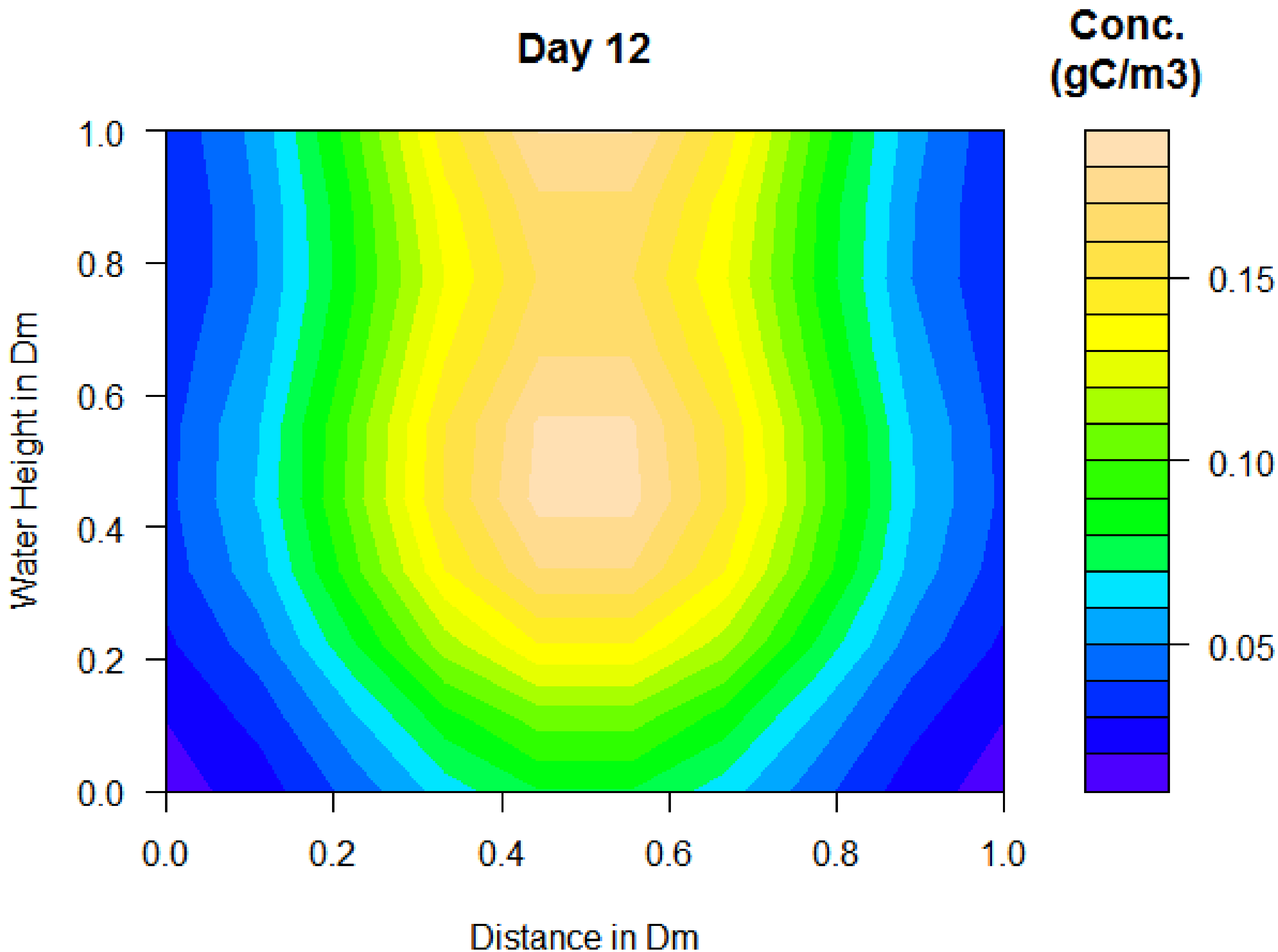

Day 8
Conc.
(gC/m3)
1.0
0.8
0.6
0.4
0.2
0.0
Water Height in Dm
0.0
0.2
0.4
0.6
0.8
1.0
Distance in Dm
0.30
0.25
0.20
0.15
0.10
0.05
0.00


Day 9
Conc.
(gC/m3)
1.0
0.8
0.6
0.4
0.2
0.0
Water Height in Dm
0.0
0.2
0.4
0.6
0.8
1.0
Distance in Dm
0.25
0.20
0.15
0.10
0.05
0.00

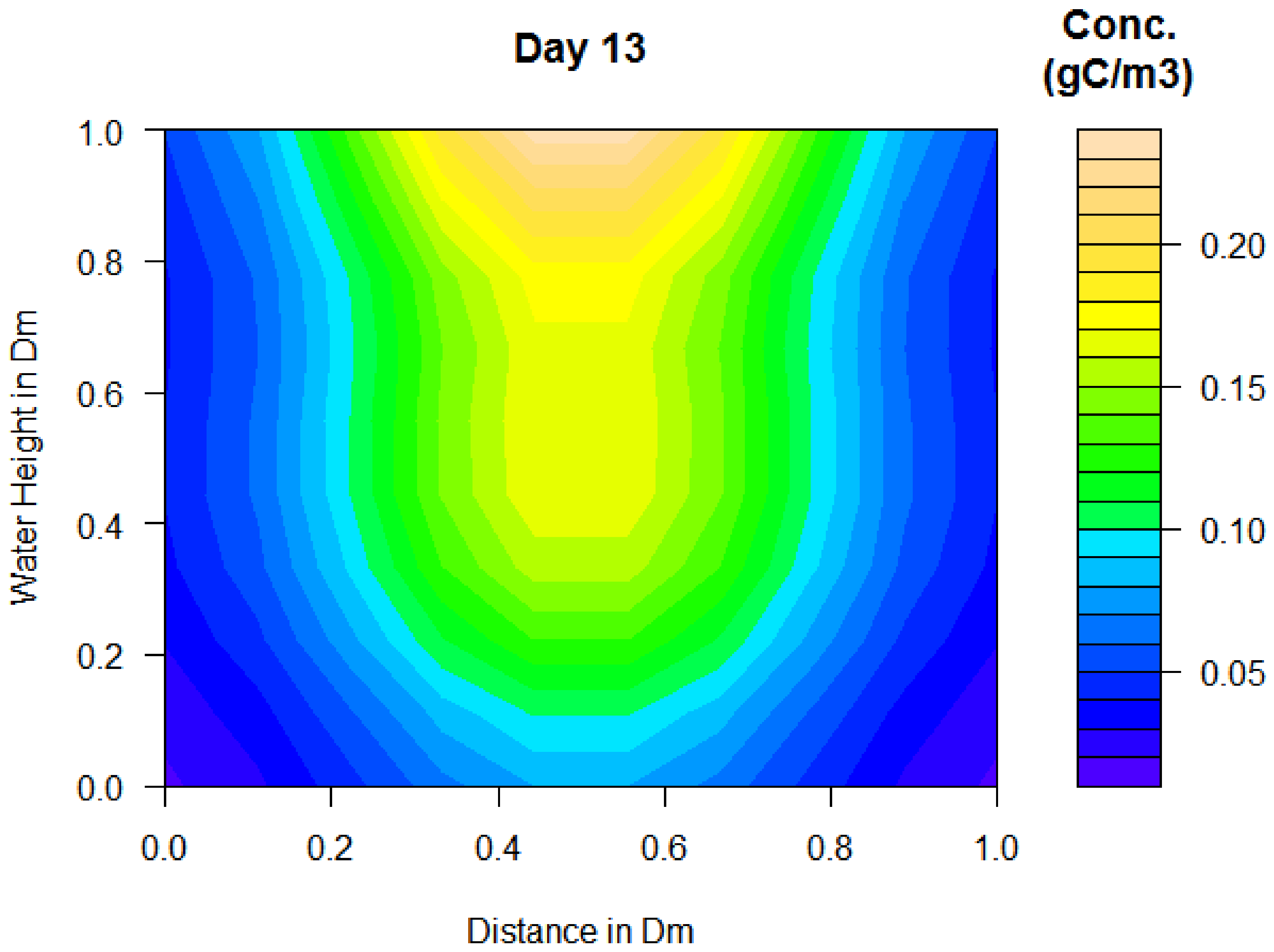

Day 10
Conc.
(gC/m3)
Water Height in Dm
Distance in Dm
0.0
0.2
0.4
0.6
0.8
1.0
0.00
0.05
0.10
0.15
0.20

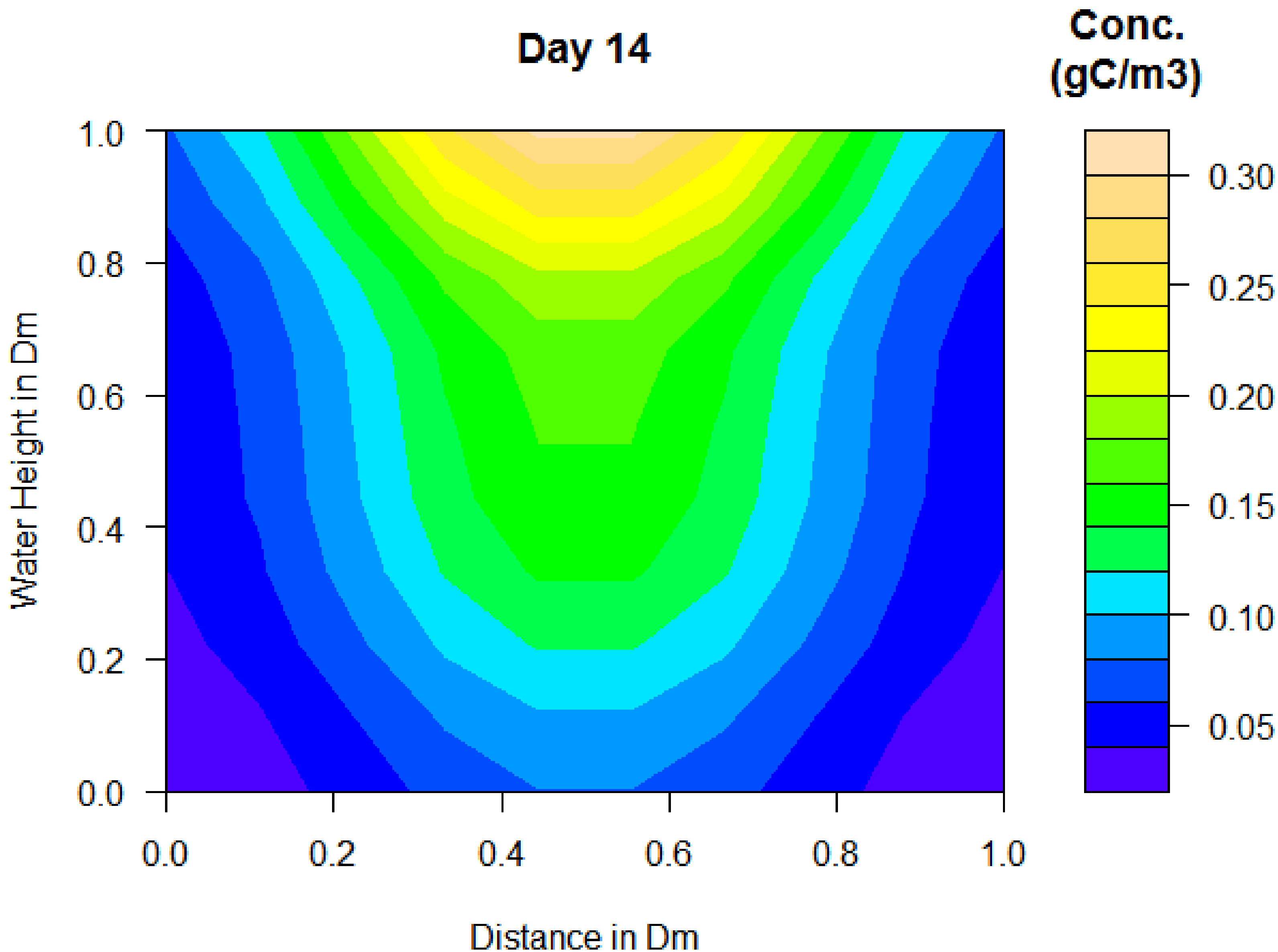


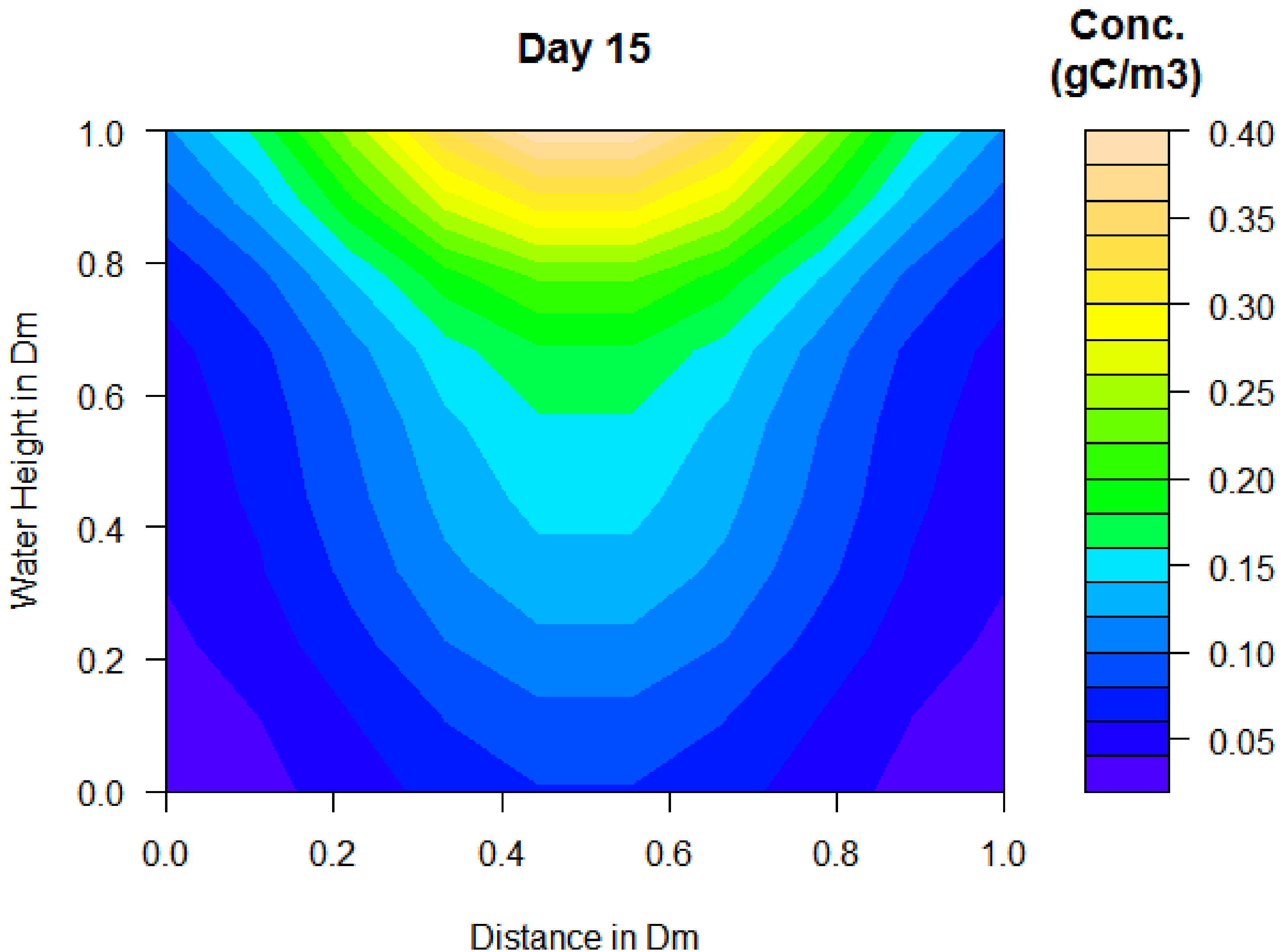
Day 11
Conc. (gC/m3)
1.0
0.8
0.6
0.4
0.2
0.0
Water Height in Dm
0.0
0.2
0.4
0.6
0.8
1.0
Distance in Dm
0.20
0.15
0.10
0.05

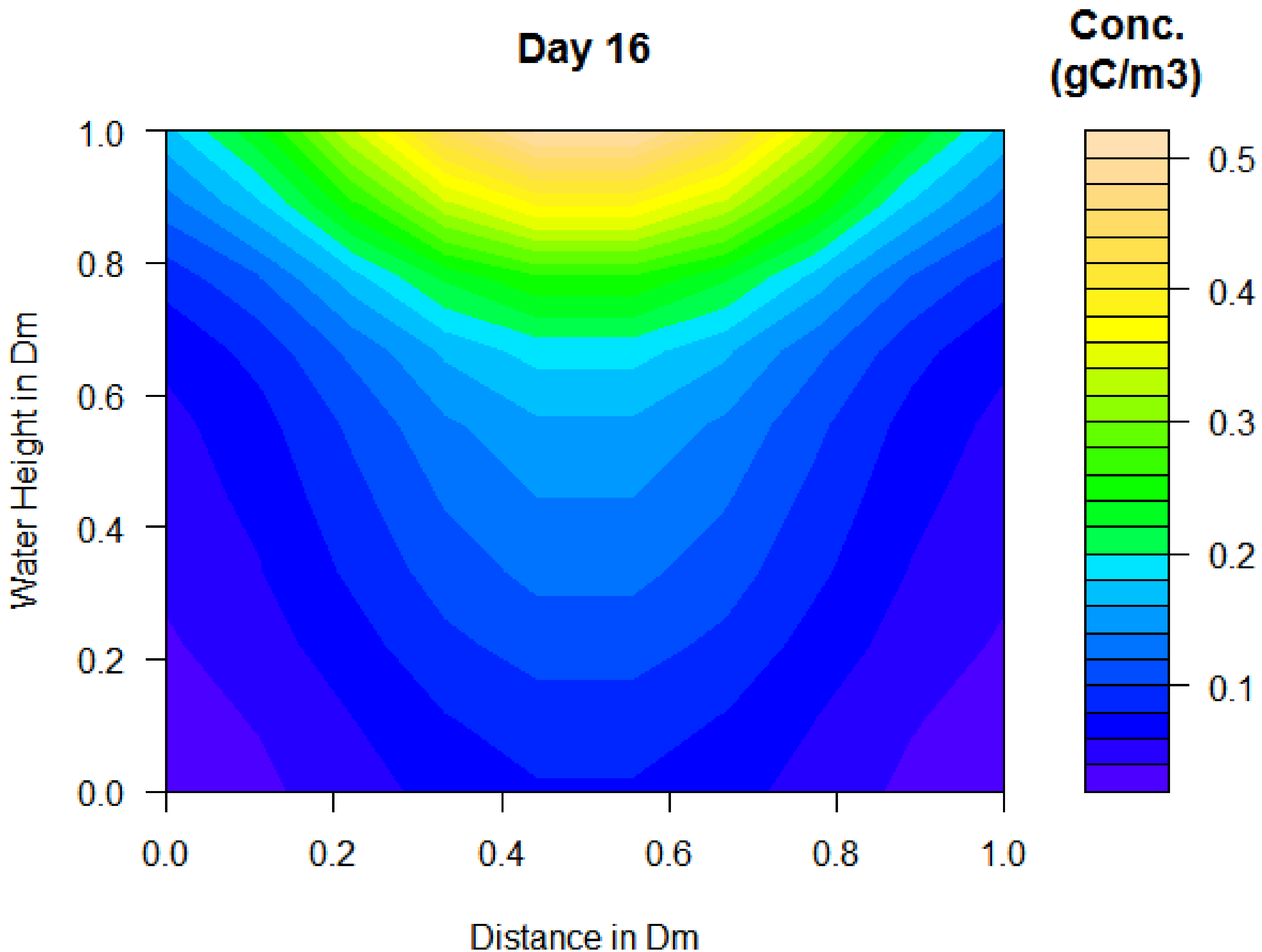


Day 12
Conc. (gC/m3)
1.0
0.8
0.6
0.4
0.2
0.0
Water Height in Dm
0.0
0.2
0.4
0.6
0.8
1.0
Distance in Dm
0.15
0.10
0.05

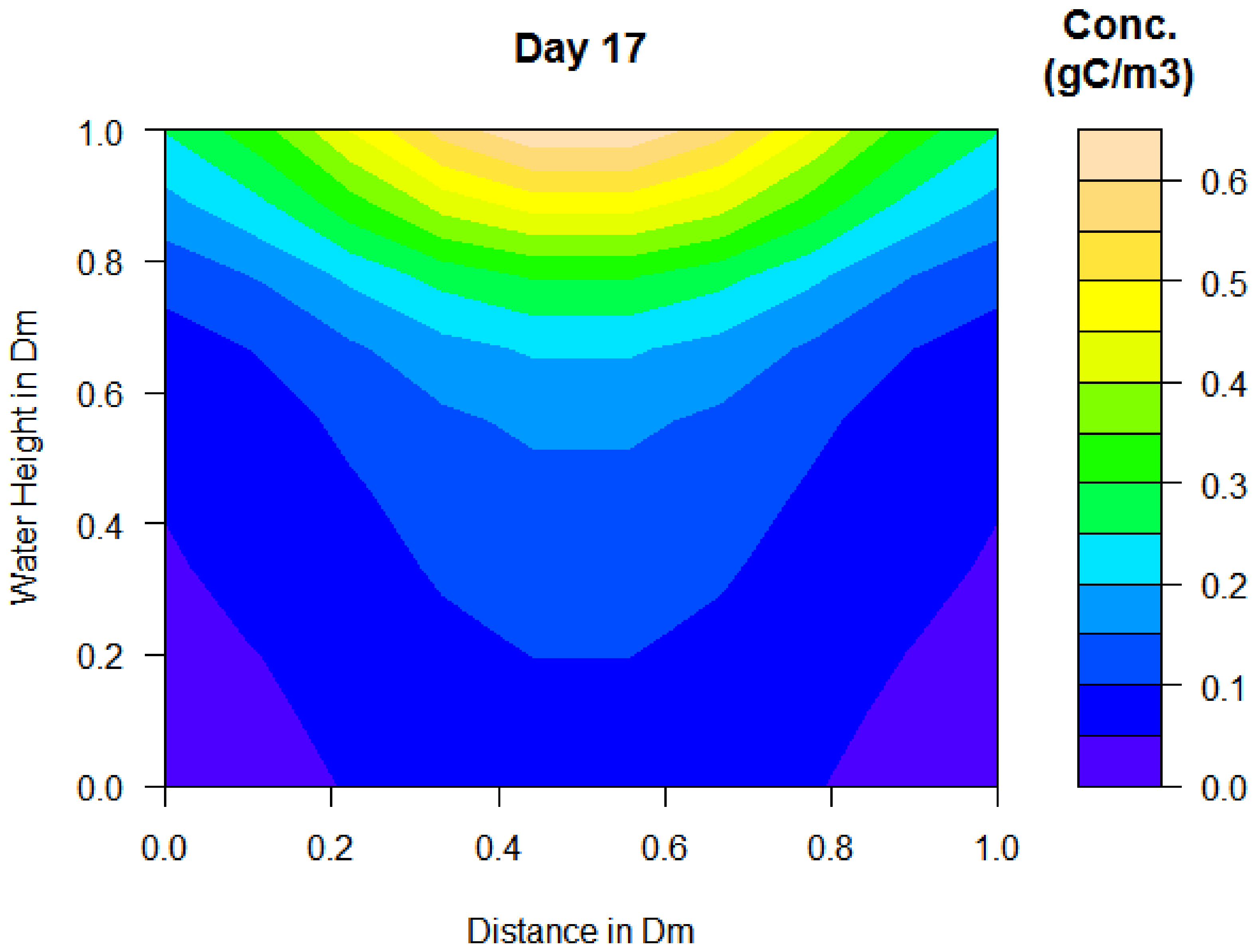

Day 13
Conc.
(gC/m3)
1.0
0.8
0.6
0.4
0.2
0.0
Water Height in Dm
0.0
0.2
0.4
0.6
0.8
1.0
Distance in Dm
0.20
0.15
0.10
0.05

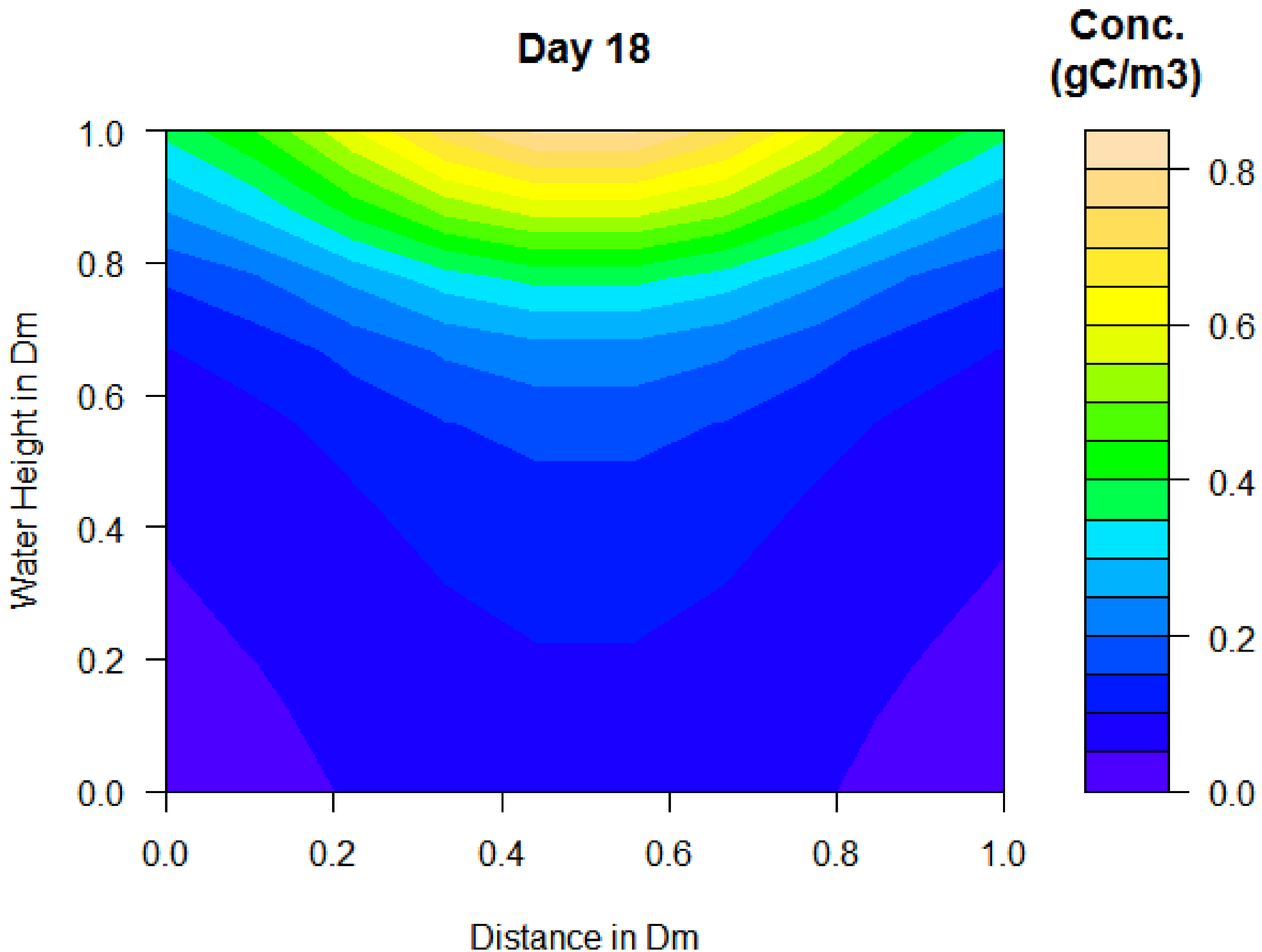

Day 14
Conc.
(gC/m3)
1.0
0.8
0.6
0.4
0.2
0.0
Water Height in Dm
0.0
0.2
0.4
0.6
0.8
1.0
Distance in Dm
0.30
0.25
0.20
0.15
0.10
0.05

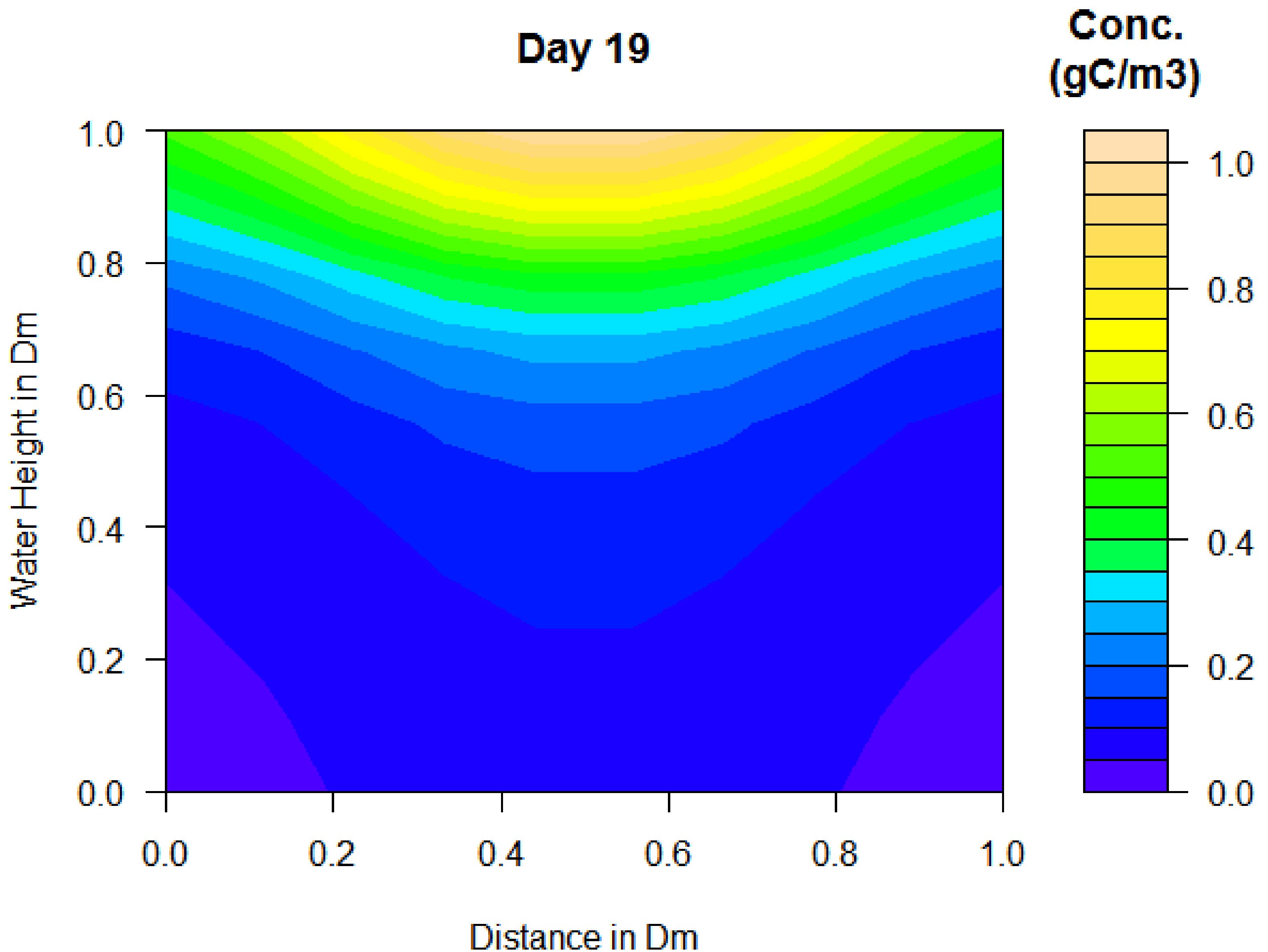

Day 15
Conc.
(gC/m3)
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
1.0
0.8
0.6
0.4
0.2
0.0
Water Height in Dm
0.0
0.2
0.4
0.6
0.8
1.0
Distance in Dm



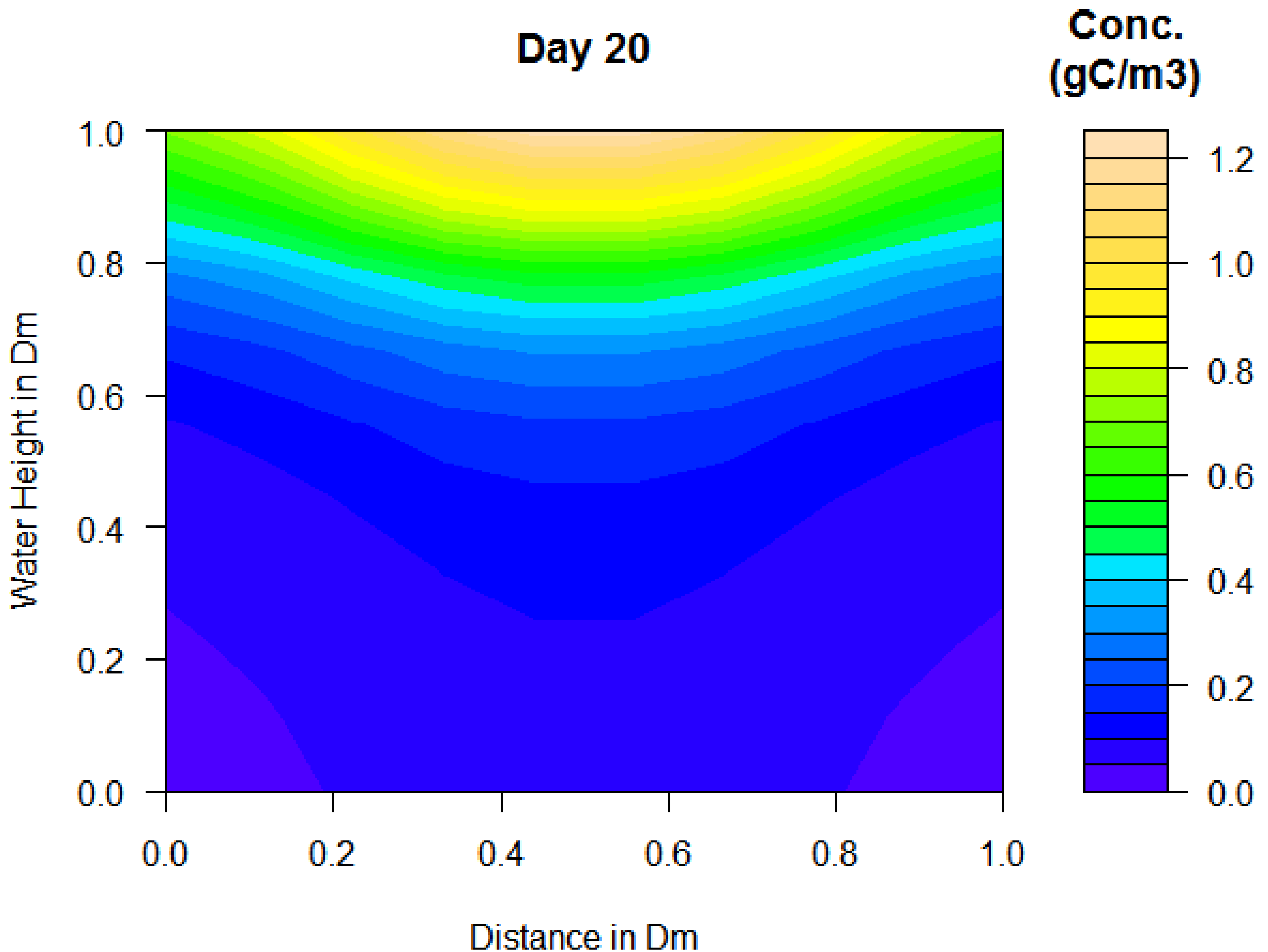
Day 16
Conc.
(gC/m3)
Water Height in Dm
Distance in Dm
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0
0.5
0.4
0.3
0.2
0.1


Day 17
Conc.
(gC/m3)
Water Height in Dm
Distance in Dm
0.0
0.2
0.4
0.6
0.8
1.0
0.0
0.1
0.2
0.3
0.4
0.5
0.6

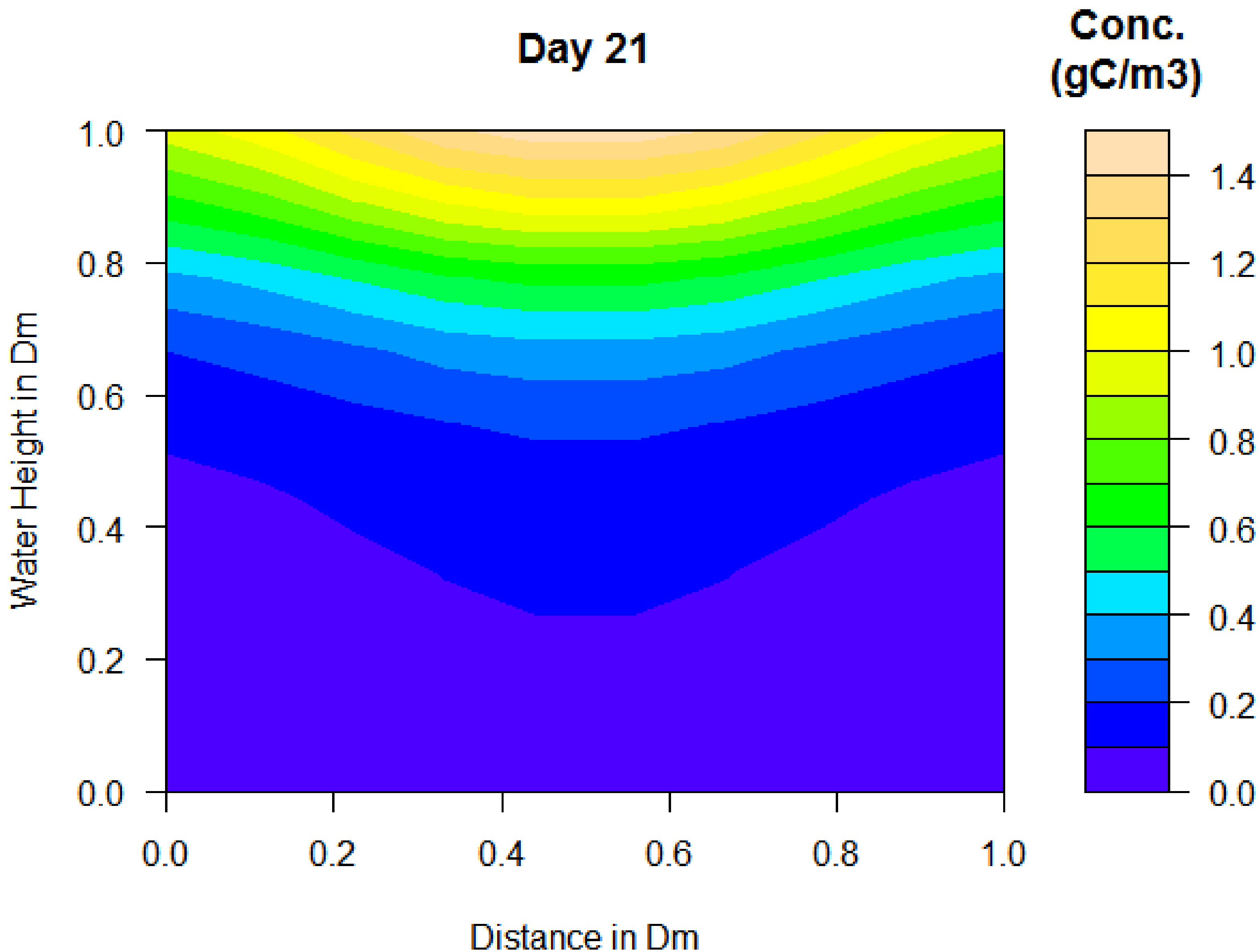

Day 18
Conc.
(gC/m3)
Water Height in Dm
Distance in Dm
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0
0.8
0.6
0.4
0.2
0.0

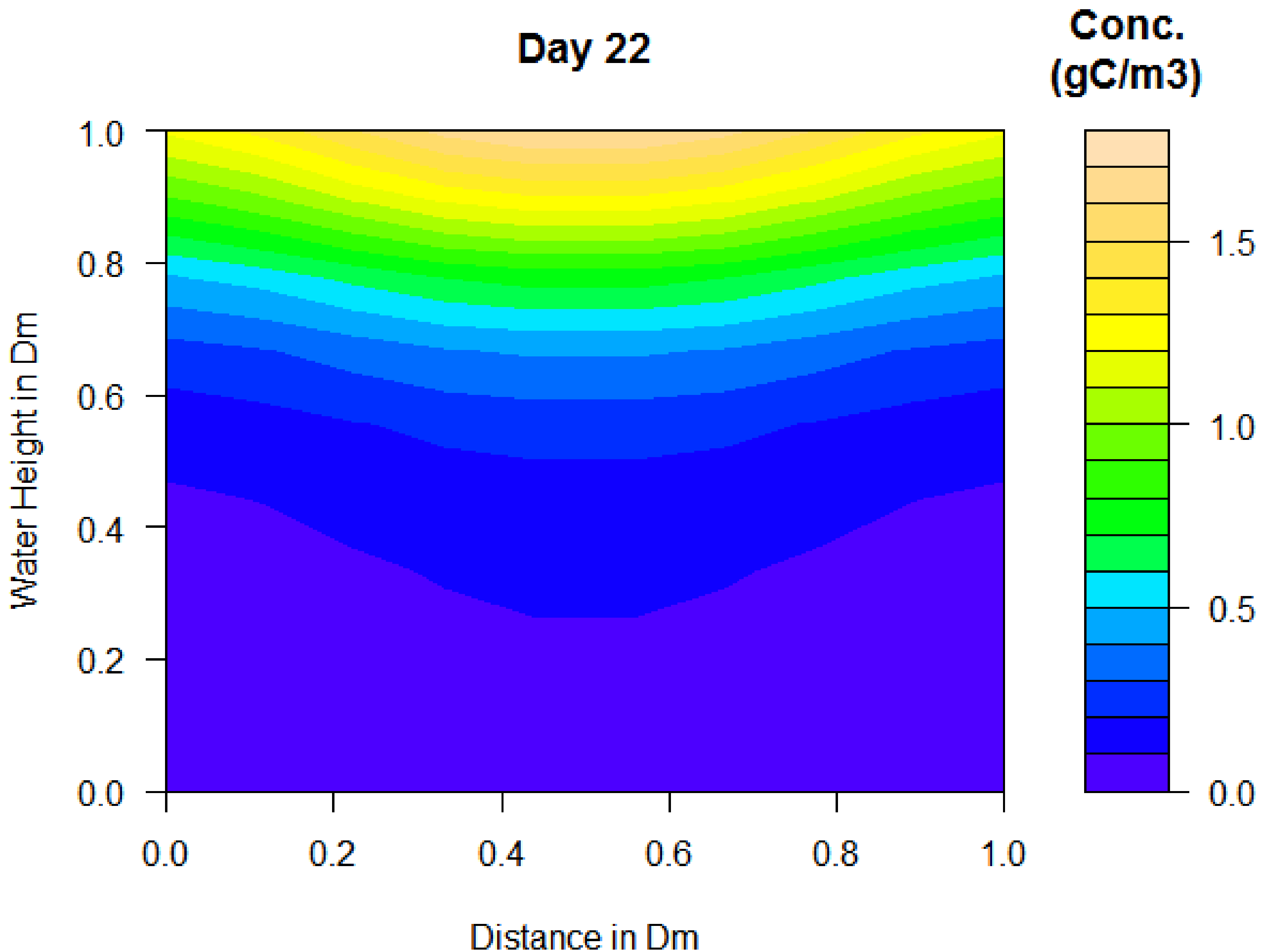


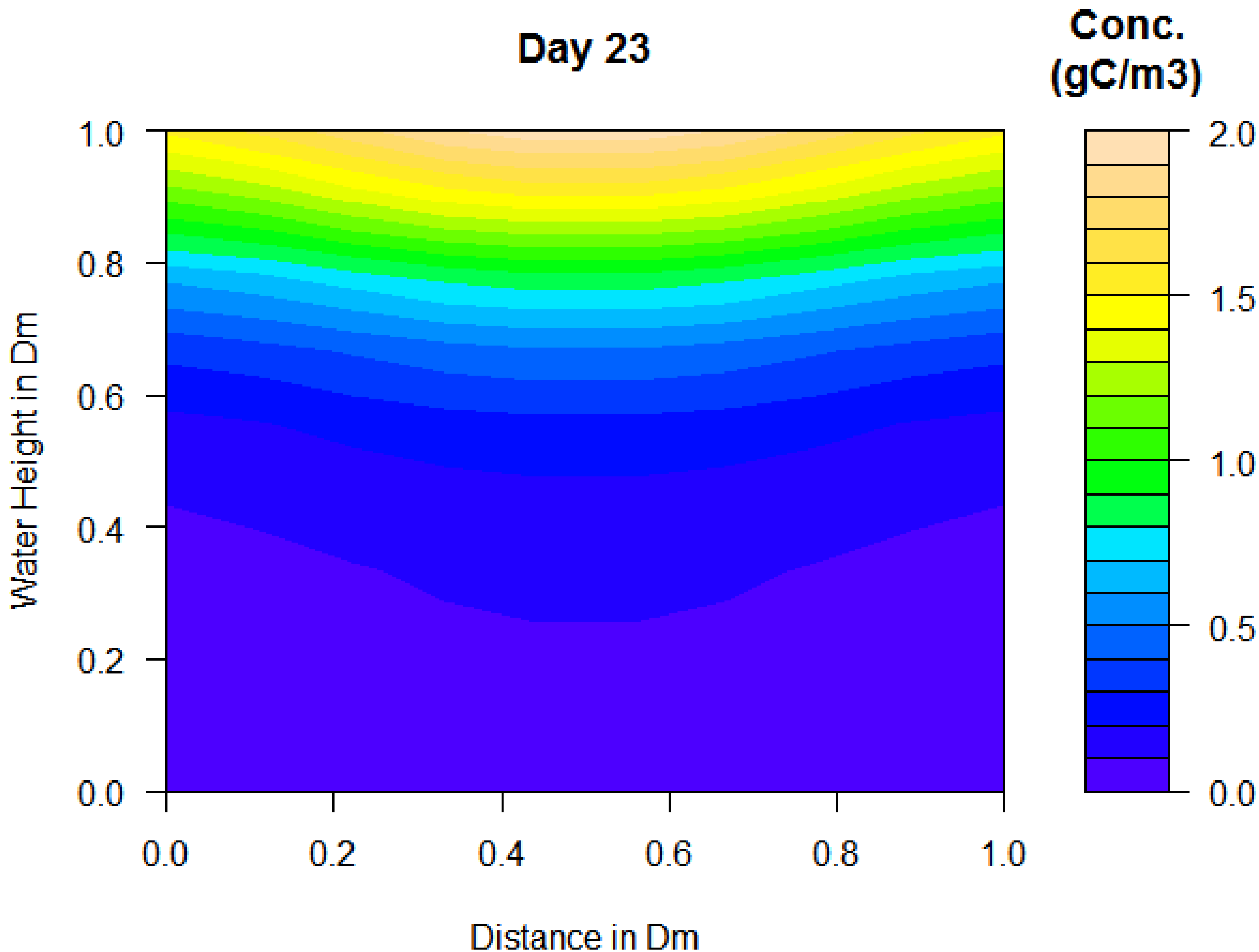
Day 19
Conc.
(gC/m3)
1.0
0.8
0.6
0.4
0.2
0.0
Water Height in Dm
Distance in Dm
0.0
0.2
0.4
0.6
0.8
1.0



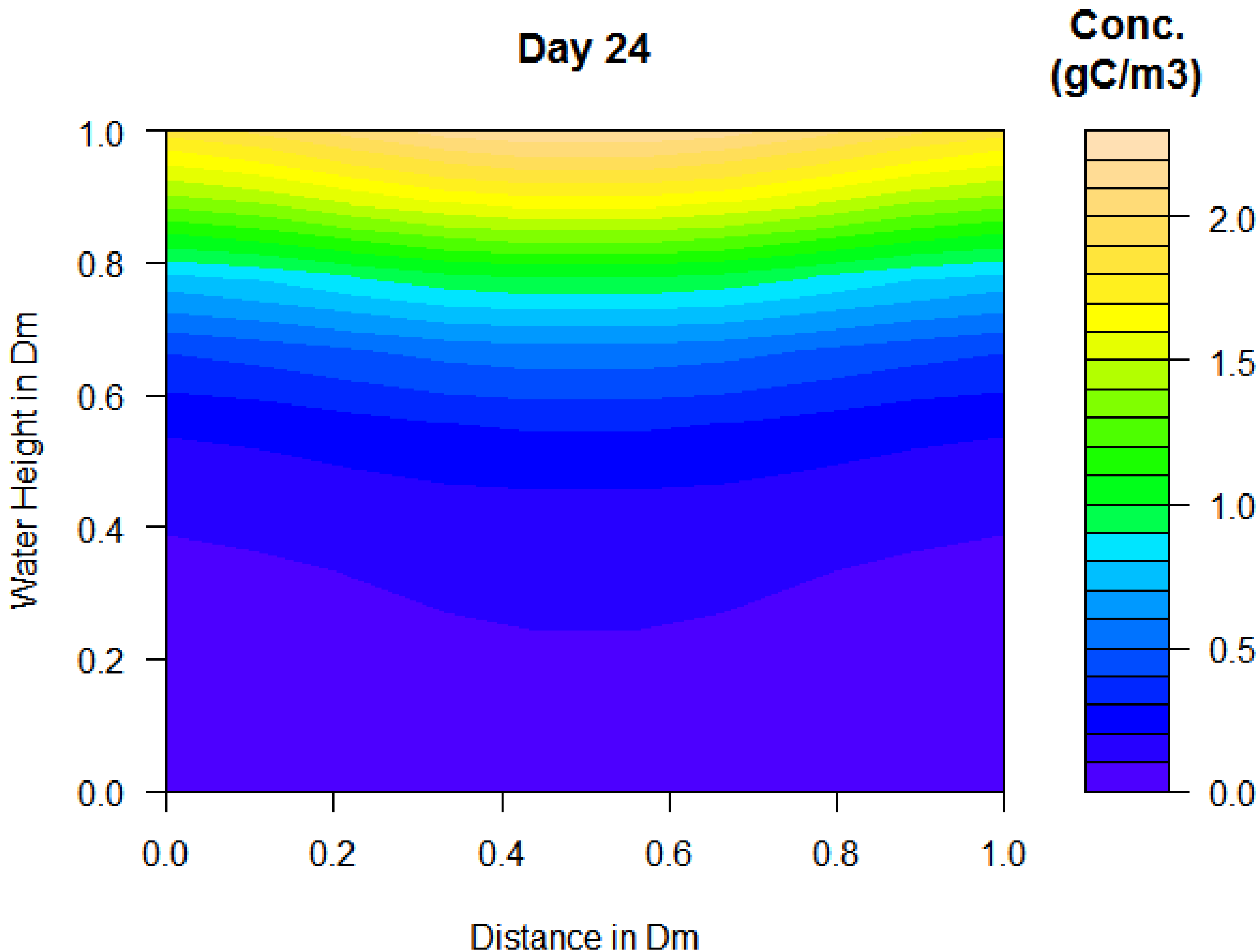
Day 20
Conc.
(gC/m3)
Water Height in Dm
Distance in Dm
0.0
0.2
0.4
0.6
0.8
1.0
1.2


Day 21
Conc.
(gC/m3)
Water Height in Dm
Distance in Dm
0.0
0.2
0.4
0.6
0.8
1.0
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0

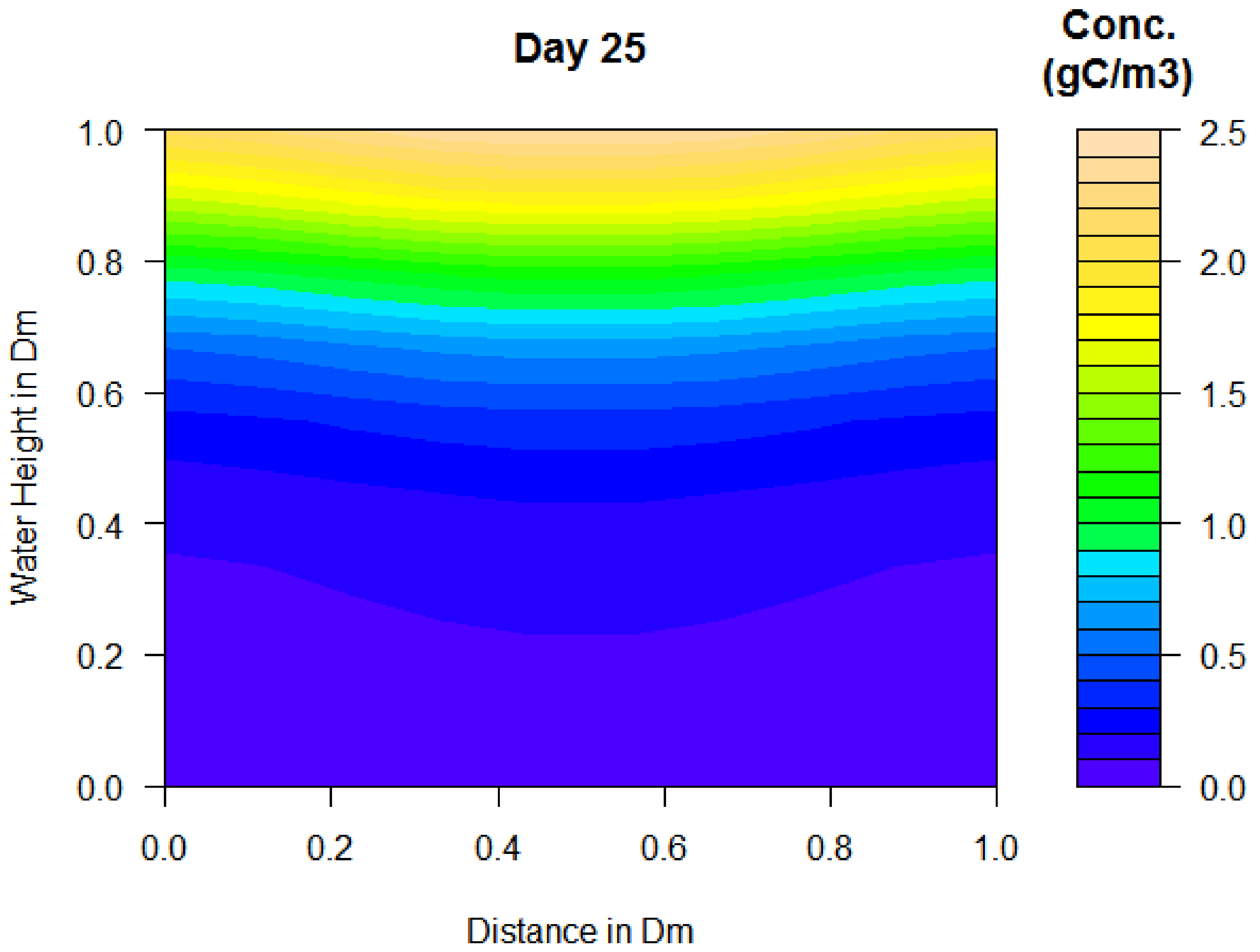

Day 22
Conc.
(gC/m3)
1.0
0.8
0.6
0.4
0.2
0.0
Water Height in Dm
0.0
0.2
0.4
0.6
0.8
1.0
Distance in Dm
1.5
1.0
0.5
0.0



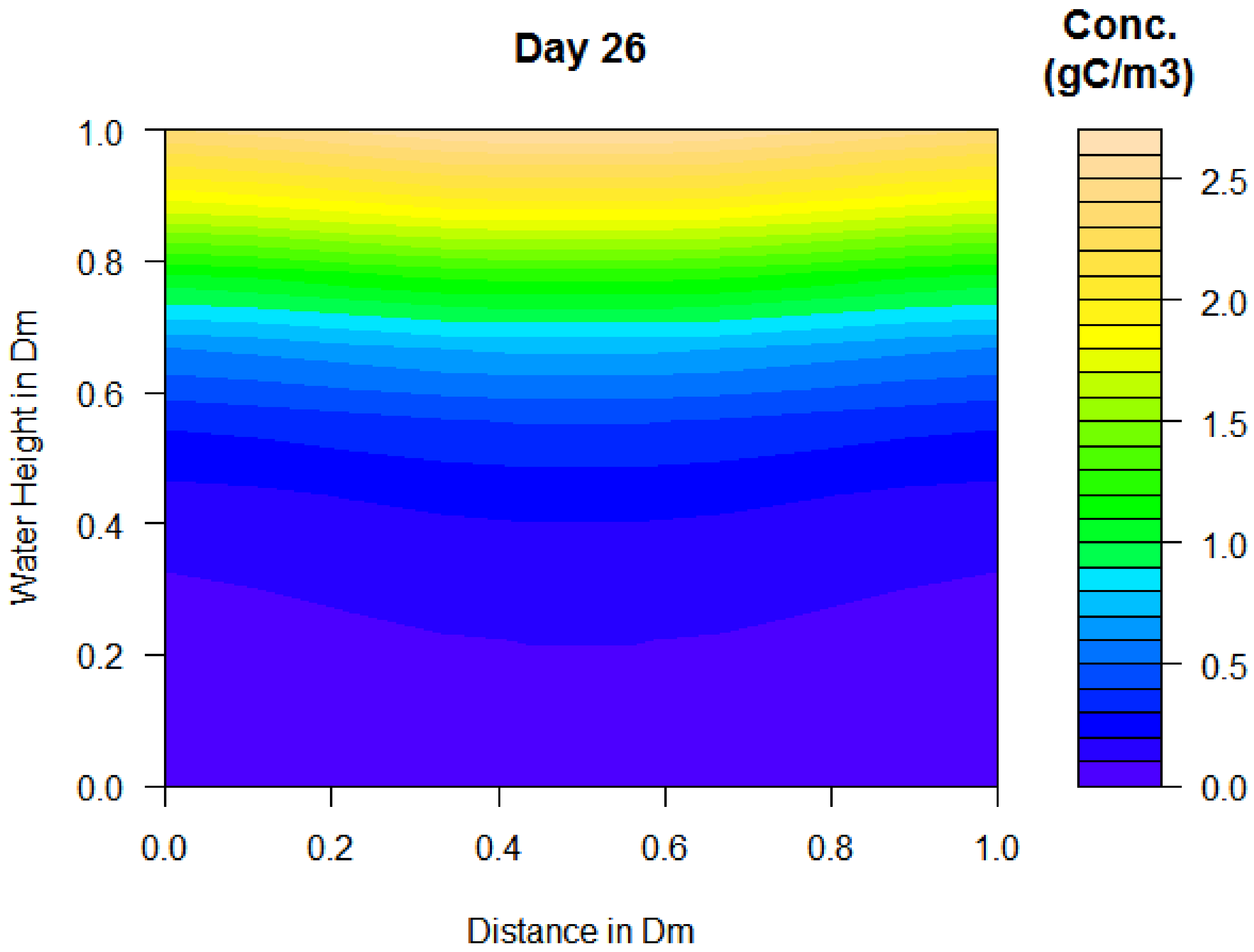
Day 23
Conc.
(gC/m3)
Water Height in Dm
Distance in Dm
0.0
0.2
0.4
0.6
0.8
1.0
0.0
0.5
1.0
1.5
2.0

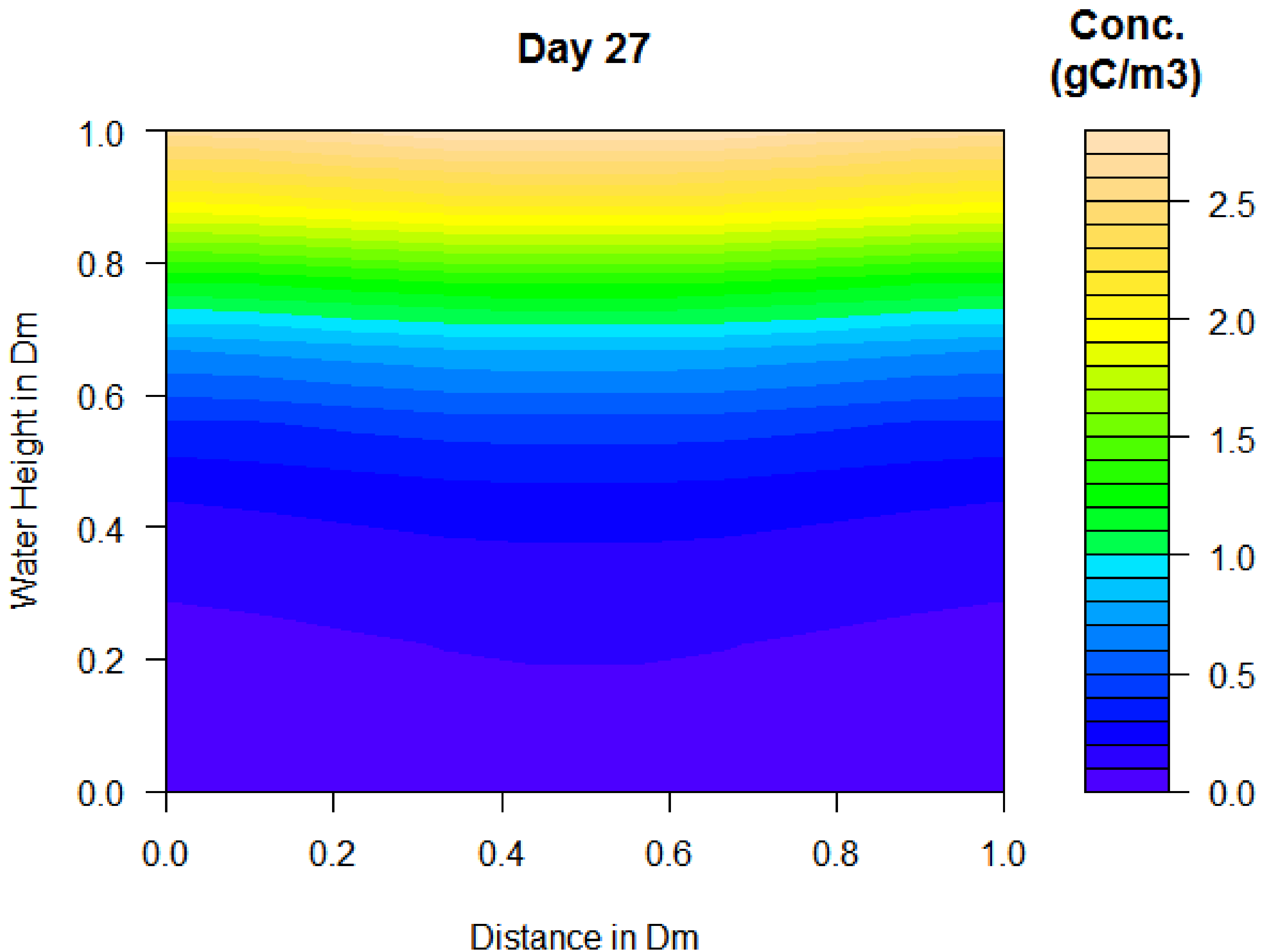


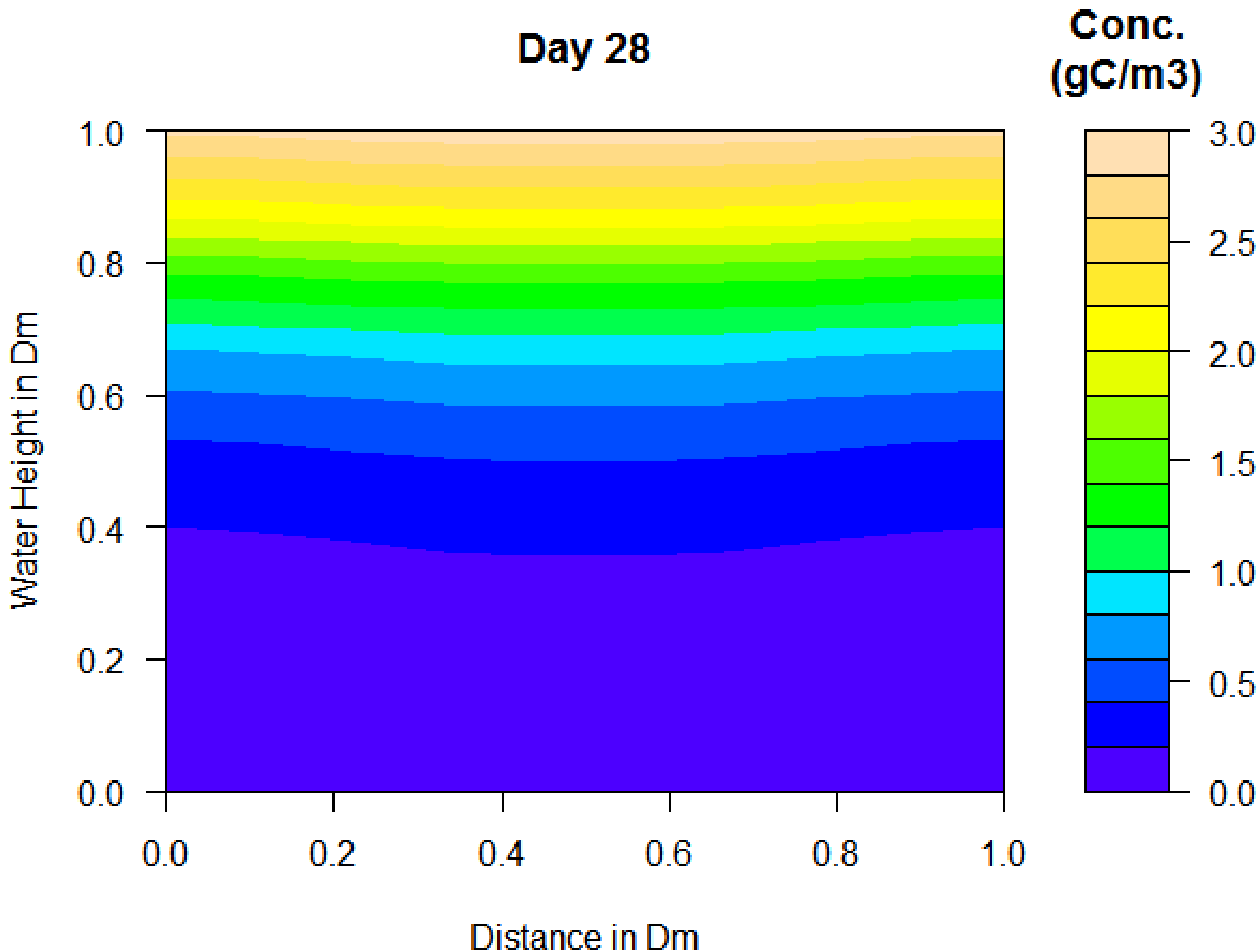
Day 24
Conc.
(gC/m3)
Water Height in Dm
Distance in Dm
0.0
0.2
0.4
0.6
0.8
1.0
0.0
0.5
1.0
1.5
2.0

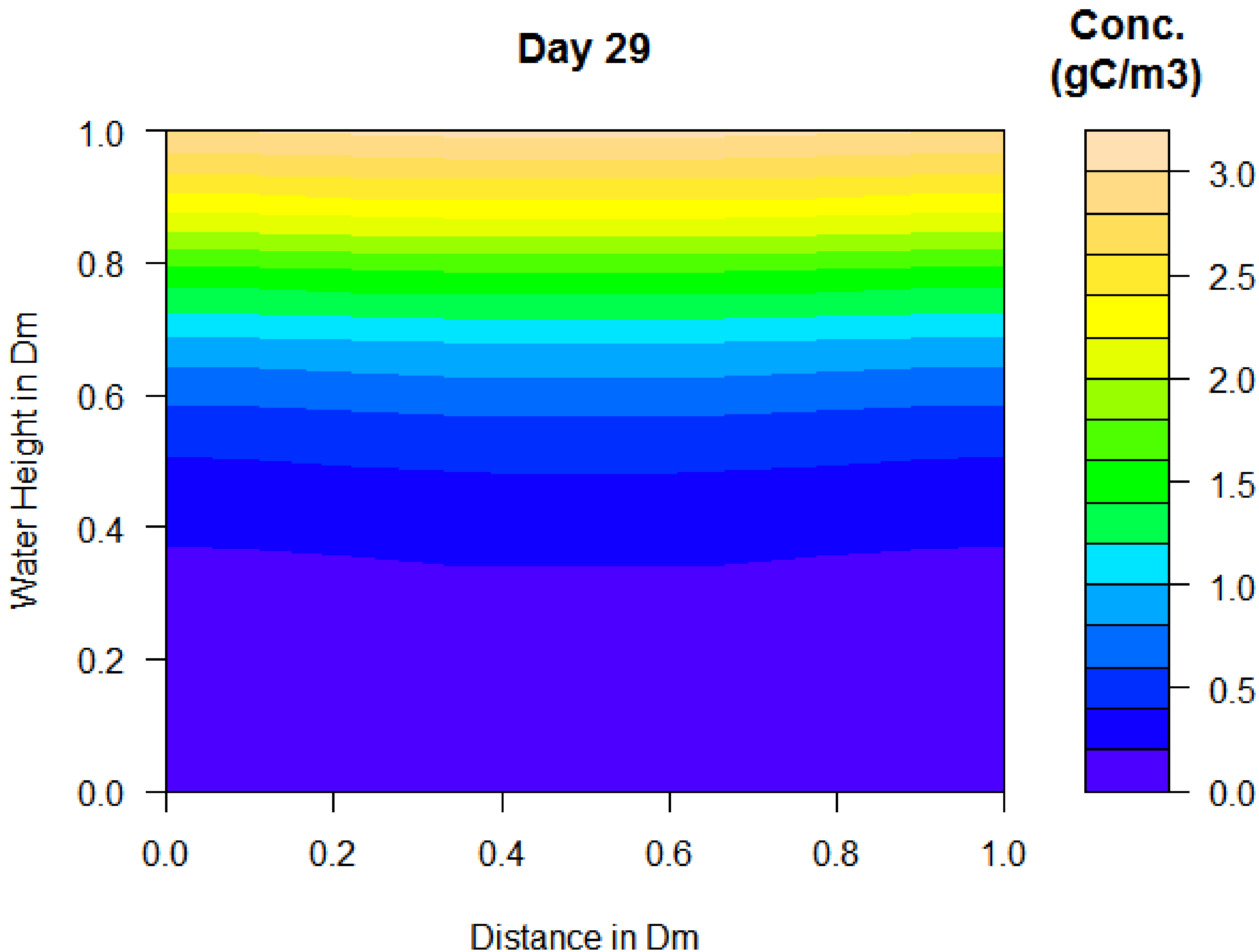


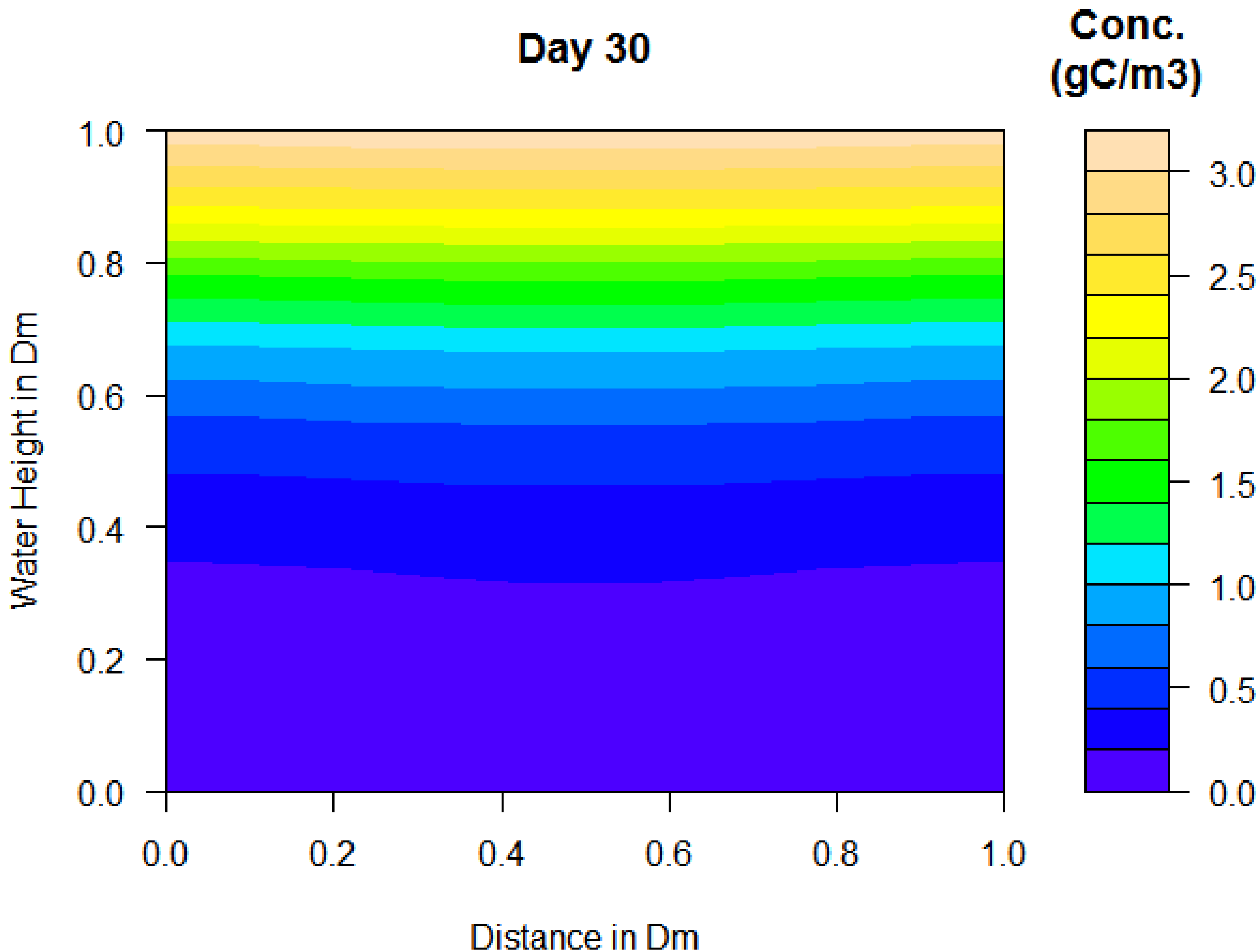
Day 25
Conc. (gC/m3)
Water Height in Dm
Distance in Dm
0.0
0.2
0.4
0.6
0.8
1.0
0.5
1.5
2.0
2.5

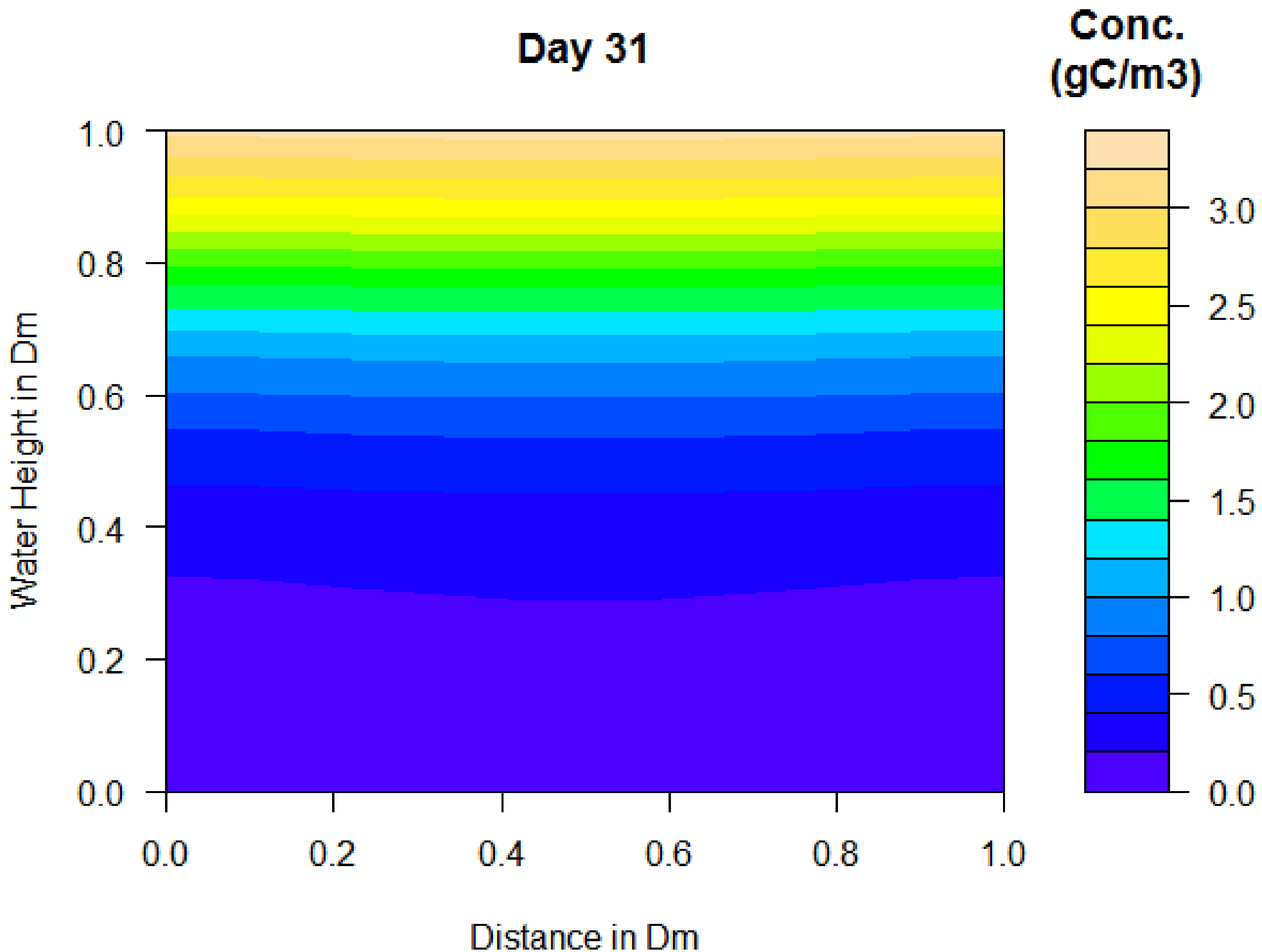

Day 26
Conc.
(gC/m3)
Water Height in Dm
Distance in Dm
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0
2.5
2.0
1.5
1.0
0.5
0.0


Day 27
Conc.
(gC/m3)
1.0
0.8
0.6
0.4
0.2
0.0
Water Height in Dm
0.0
0.2
0.4
0.6
0.8
1.0
Distance in Dm
2.5
2.0
1.5
1.0
0.5
0.0

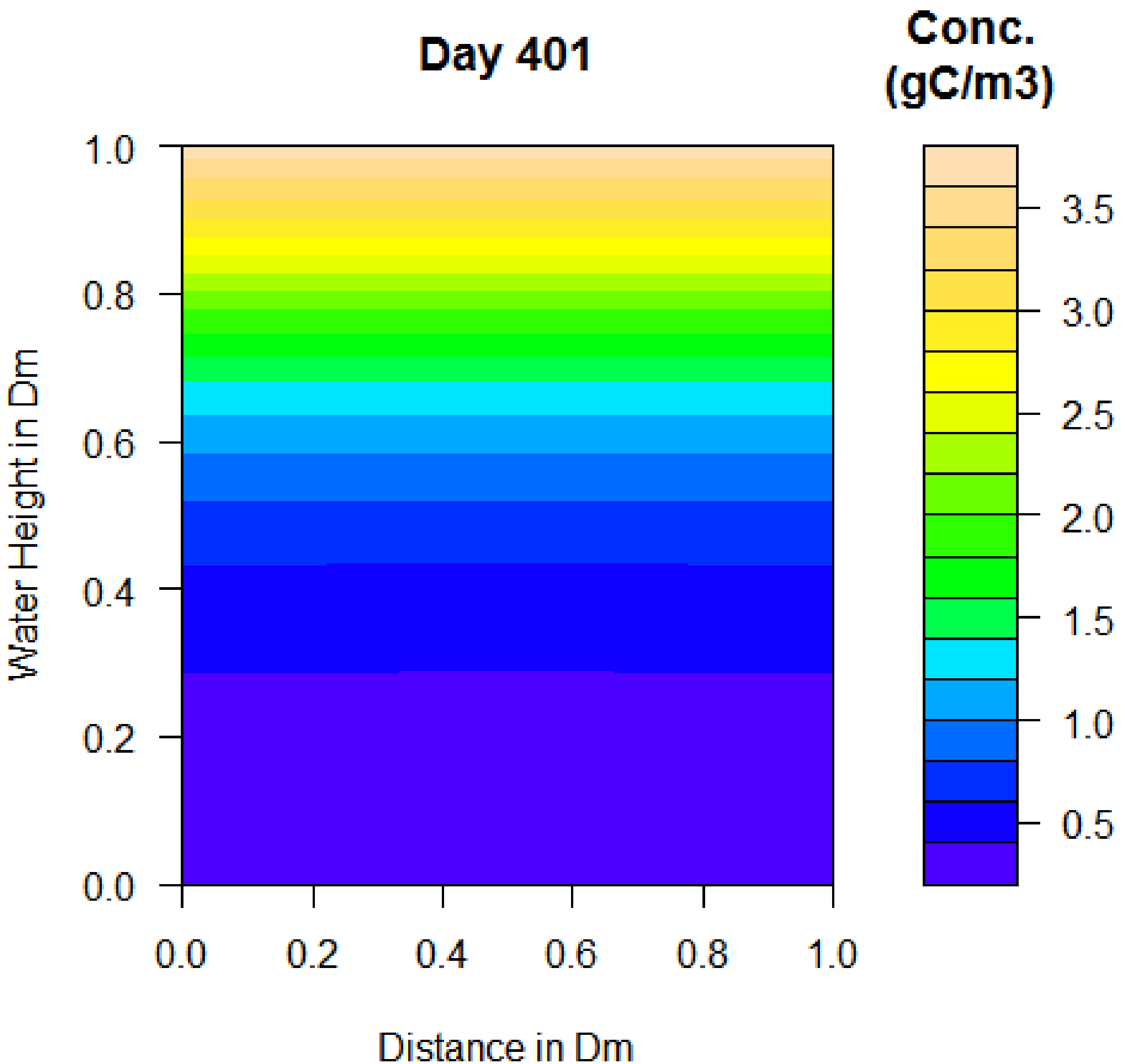

Day 28
Conc.
(gC/m3)
Water Height in Dm
Distance in Dm
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0
3.0
2.5
2.0
1.5
1.0
0.5
0.0

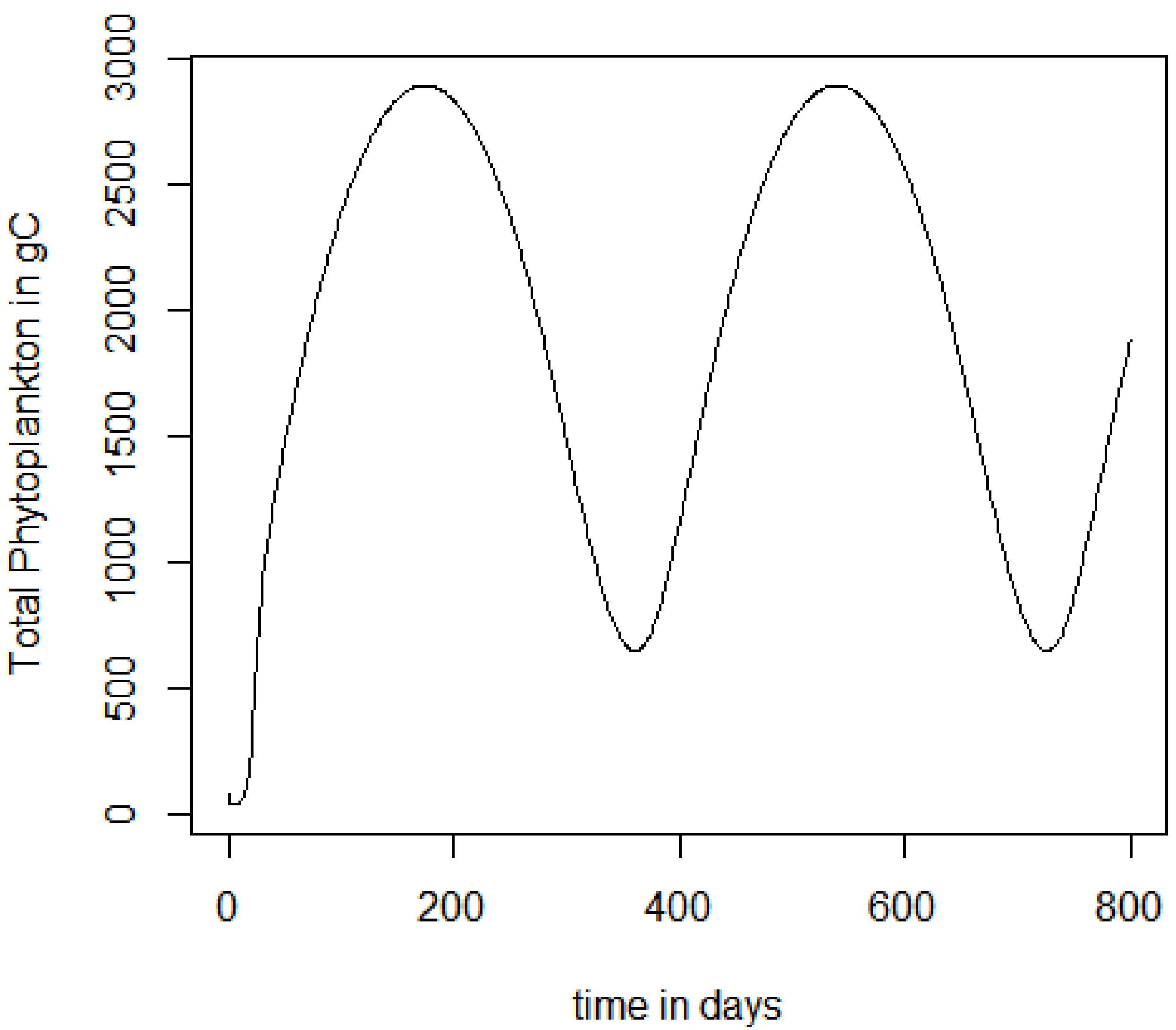

Day 29
Conc.
(gC/m3)
1.0
0.8
0.6
0.4
0.2
0.0
Water Height in Dm
0.0
0.2
0.4
0.6
0.8
1.0
Distance in Dm
3.0
2.5
2.0
1.5
1.0
0.5
0.0


Day 30
Conc.
(gC/m3)
1.0
0.8
0.6
0.4
0.2
0.0
Water Height in Dm
0.0
0.2
0.4
0.6
0.8
1.0
Distance in Dm
3.0
2.5
2.0
1.5
1.0
0.5
0.0



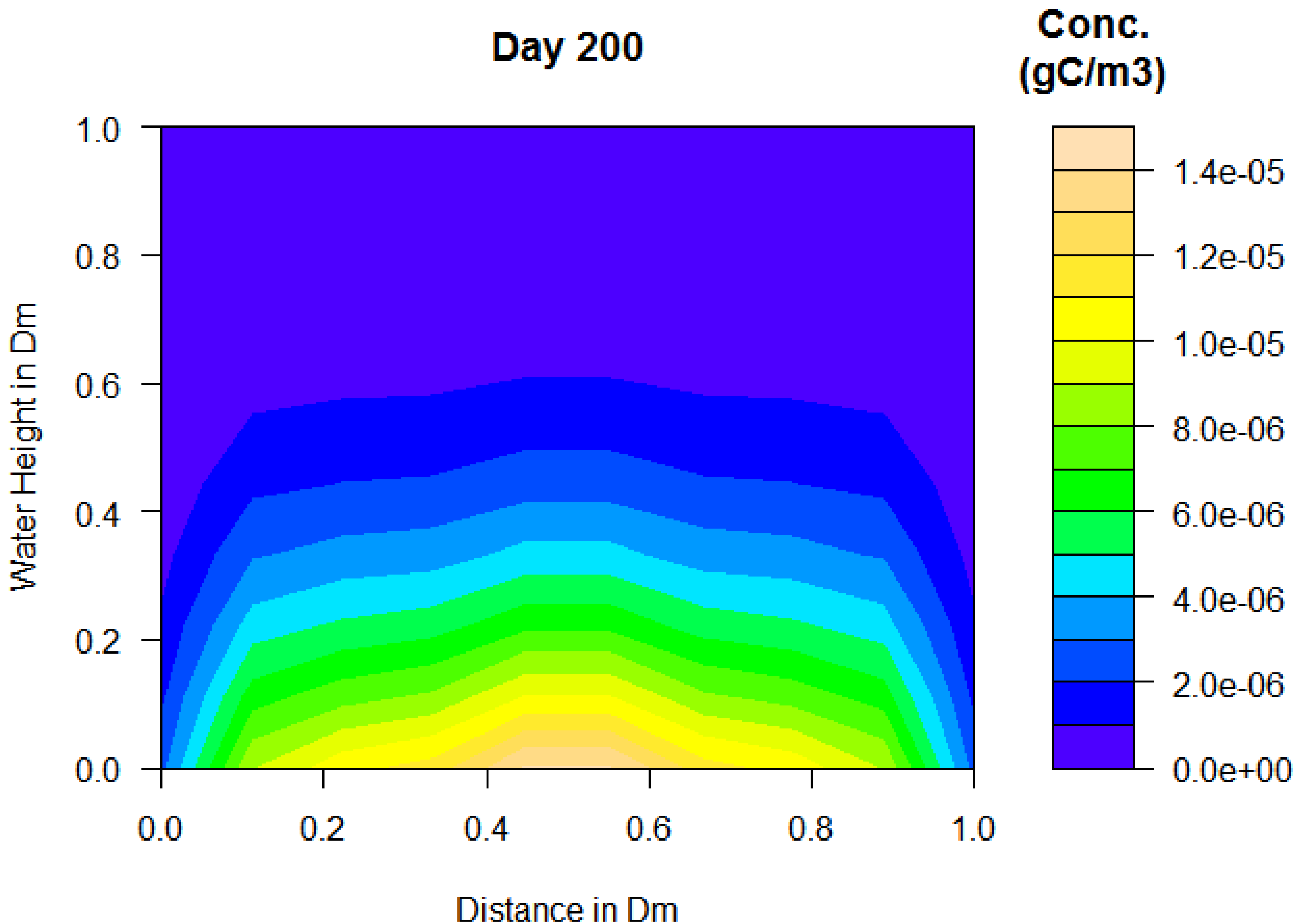
Day 31
Conc.
(gC/m3)
Water Height in Dm
Distance in Dm
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0
3.0
2.5
2.0
1.5
1.0
0.5
0.0


Day 401
Conc. (gC/m3)
1.0
0.8
0.6
0.4
0.2
0.0
Water Height in Dm
0.0
0.2
0.4
0.6
0.8
1.0
Distance in Dm
3.5
3.0
2.5
2.0
1.5
1.0
0.5

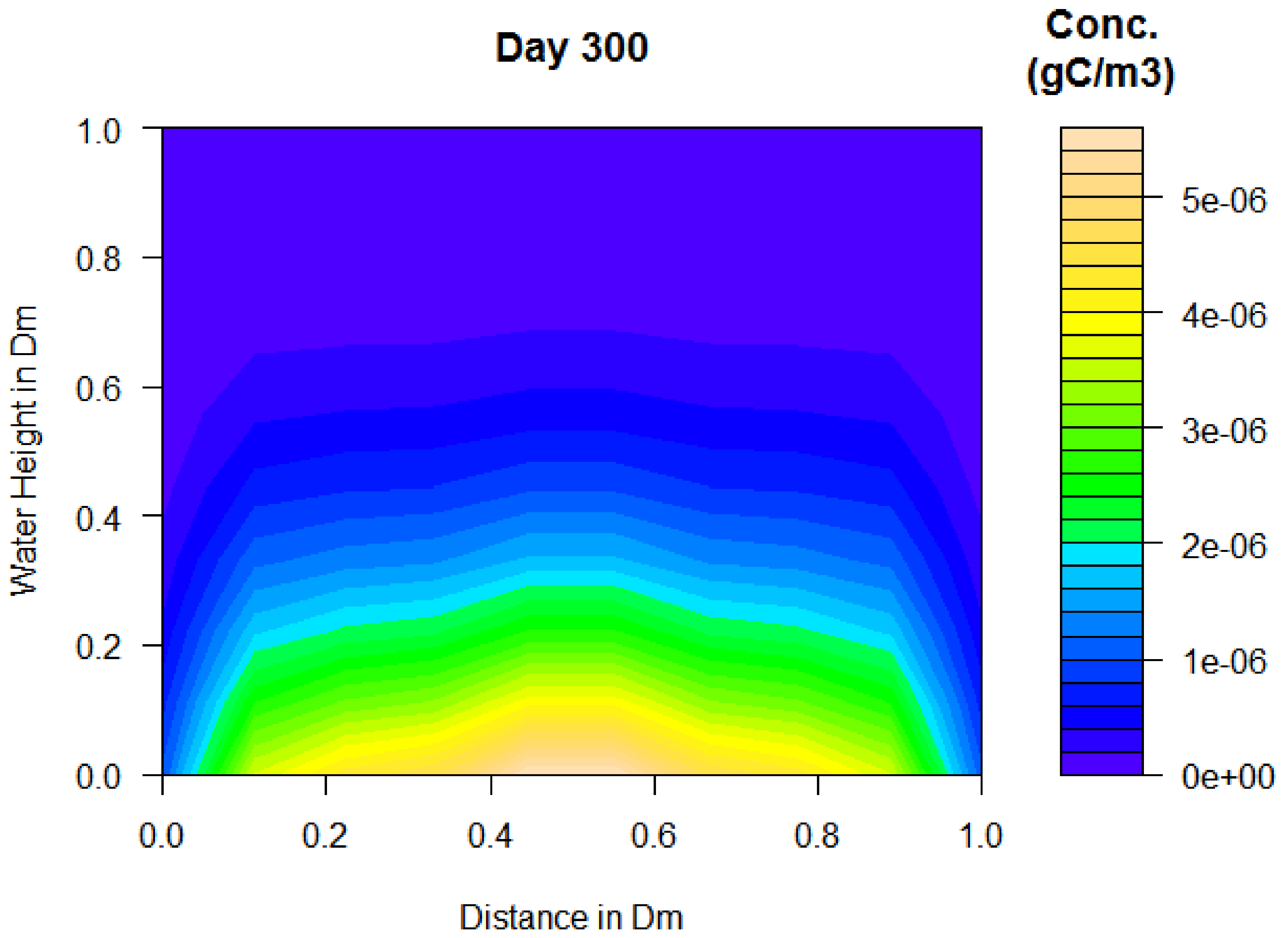

Total Phytoplankton in gC
0
500
1000
1500
2000
2500
3000
0
200
400
600
800
time in days

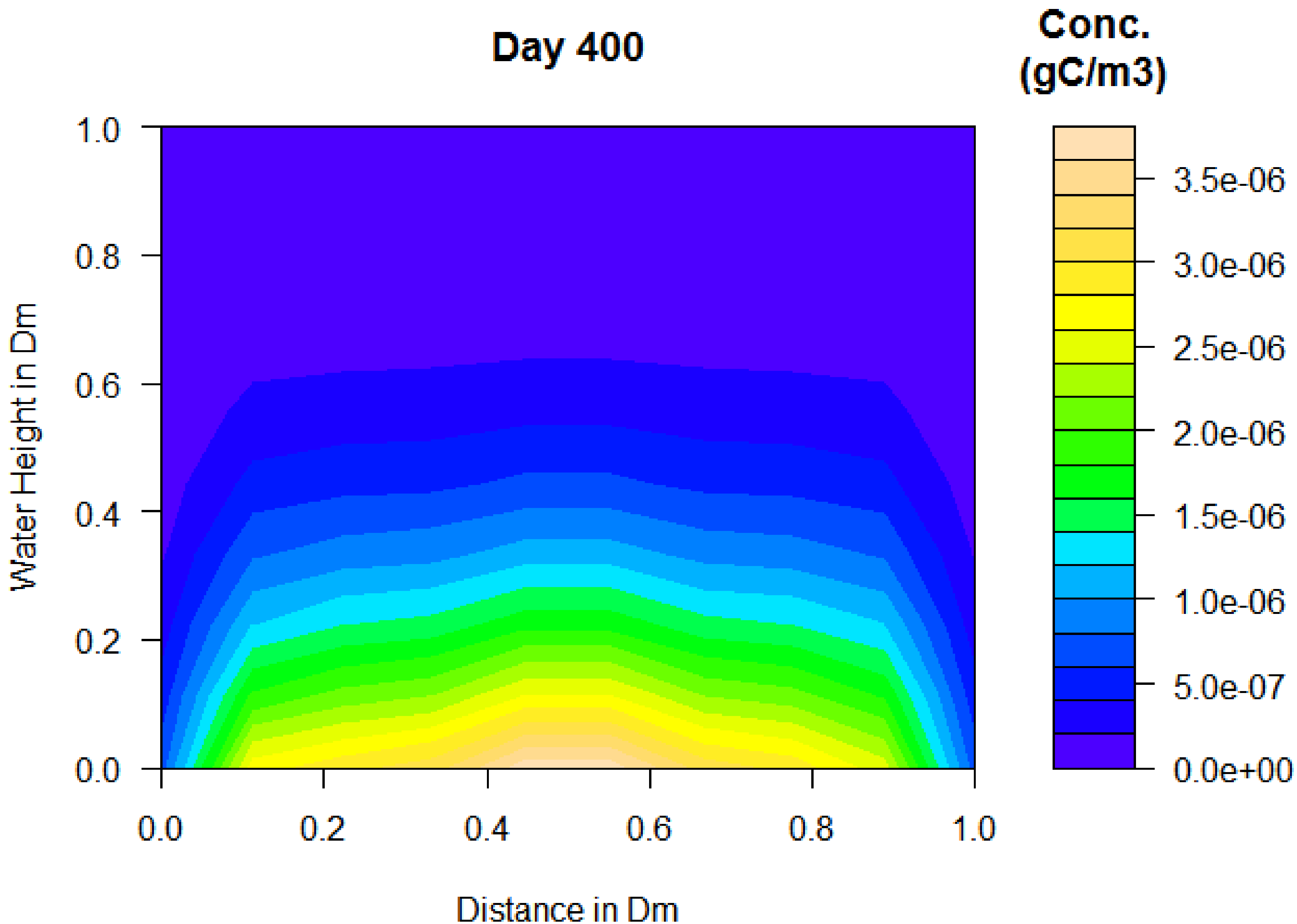
When Sinking Rate = 10 m/d

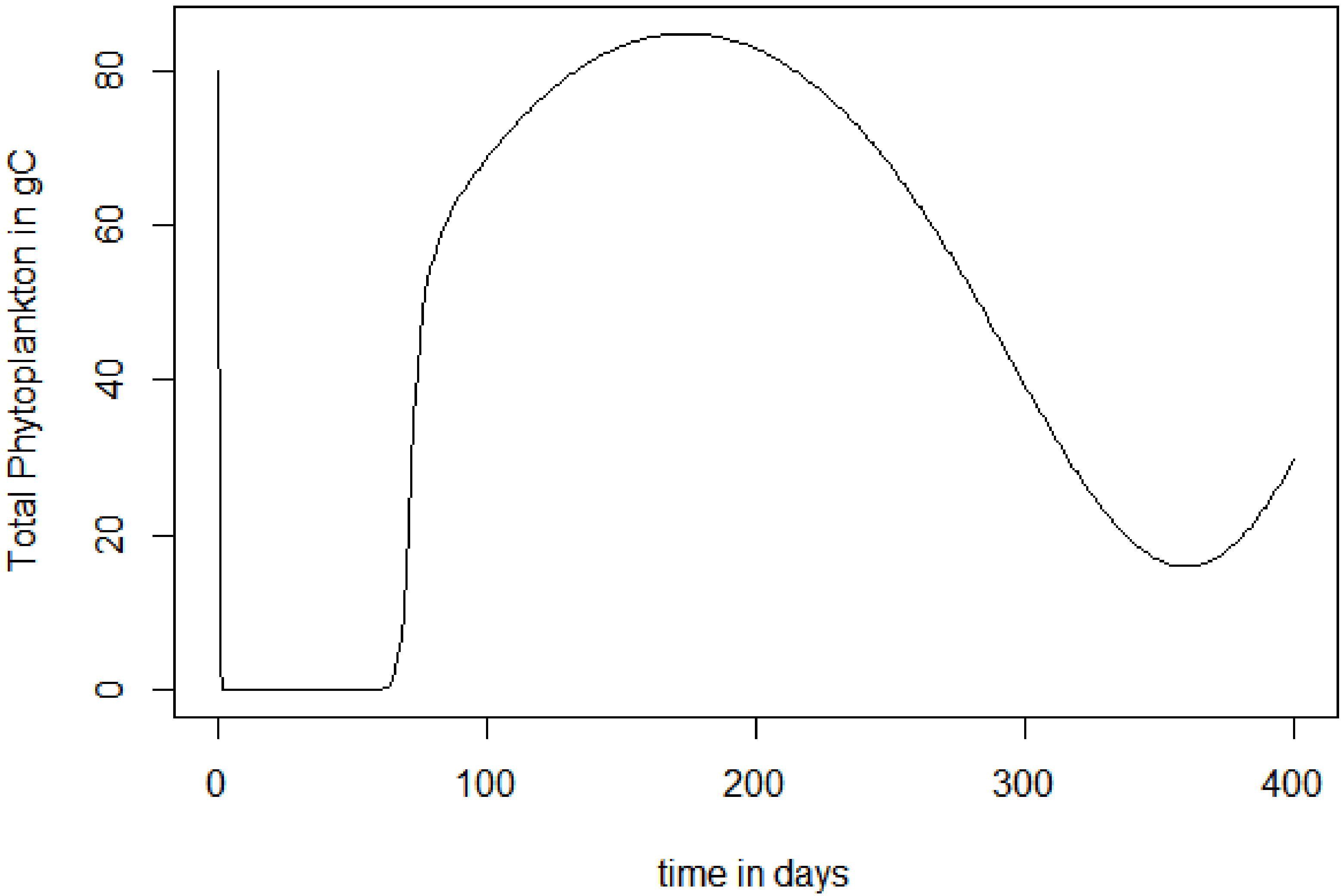
- Phytoplankton never make it to the surface, and remain sub-surface with concentrations cycling annually



Day 200
Conc.
(gC/m3)
1.4e-05
1.2e-05
1.0e-05
8.0e-06
6.0e-06
4.0e-06
2.0e-06
0.0e+00
Water Height in Dm
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0
Distance in Dm


Day 300
Conc.
(gC/m3)
1.0
0.8
0.6
0.4
0.2
0.0
Water Height in Dm
0.0
0.2
0.4
0.6
0.8
1.0
Distance in Dm
5e-06
4e-06
3e-06
2e-06
1e-06
0e+00


Day 400
Conc.
(gC/m3)
Water Height in Dm
Distance in Dm
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0
3.5e-06
3.0e-06
2.5e-06
2.0e-06
1.5e-06
1.0e-06
5.0e-07
0.0e+00


Total Phytoplankton in gC
0
20
40
60
80
0
100
200
300
400
time in days

Future Work and Areas of Uncertainty

- Elucidating effects of varying initial concentration fields
- Examining a larger range of diffusion coefficients
- Fine tuning degradation rate/formulation
- Work to characterize what factors affect sinking rate
- The inclusion of horizontal advection in the model
- The inclusion of turbulence considerations to the formulation of a vector field of advective speed

Questions, Comments, Thoughts or Concerns??