Pyung Lee

PKL4FR

Project 3 Discussion

1a)

1)
$$\frac{\partial c}{\partial t} = \frac{C_i^{l+1} - C_i^l}{\Delta t} = D\left[\frac{C_{i+1}^l - 2C_i^l + C_{i-1}^l}{\Delta x^2}\right] + k_{flux}\mu n\left(b + \frac{v_1 C_i^l}{k_1 + C_i^l}\right) - \left[\frac{\gamma C_i^l}{C_i^l + k_4}\right]$$

* Interior point

$$C_i^{l+1} = C_i^l + \frac{\Delta t D}{\Delta x^2}\left[\frac{C_{i+1}^l - 2C_i^l + C_{i-1}^l}{1}\right] + \Delta t k_{flux}\mu n\left[b + \frac{v_1 C_i^l}{k_1 + C_i^l}\right] - \left[\Delta t \frac{\gamma C_i^l}{C_i^l + k_4}\right]$$

* Boundary

$$\frac{\partial C_0^l}{\partial x} = \frac{C_1^l - C_{-1}^l}{2\Delta x} \rightarrow C_{-1}^l = C_1^l - 2\Delta x \frac{\partial C_0^l}{\partial x} \qquad X = 0$$

2

$$\hookrightarrow \frac{\partial C_0^l}{\partial x}(2\Delta x) + C_{-1}^l = C_1^l \qquad X = L$$

Plug into above equation to find finite equation at boundary points.

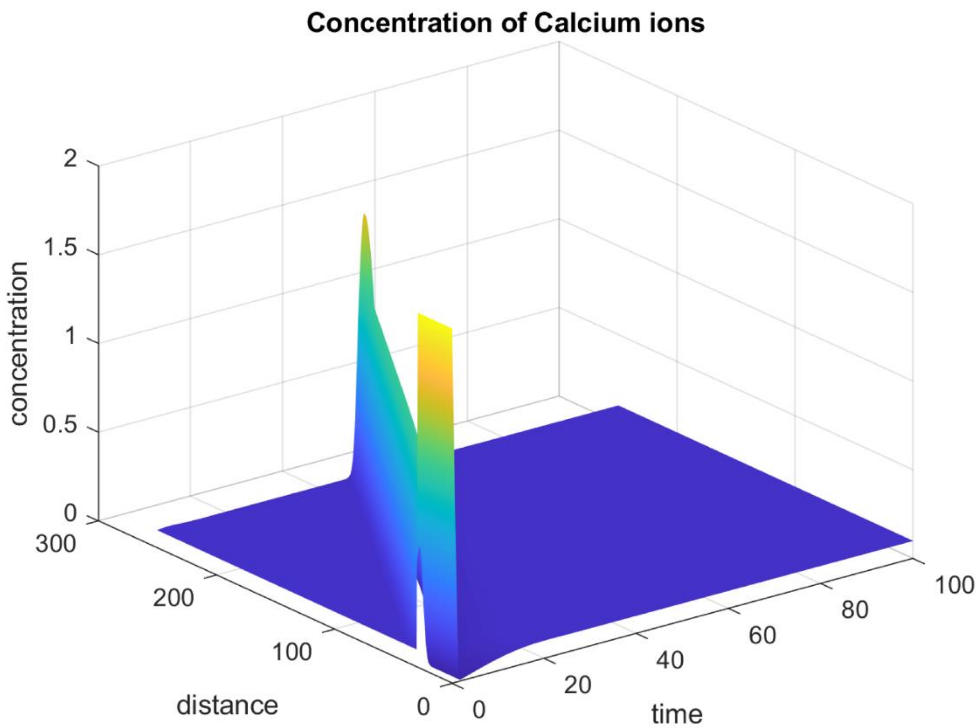
X = 0

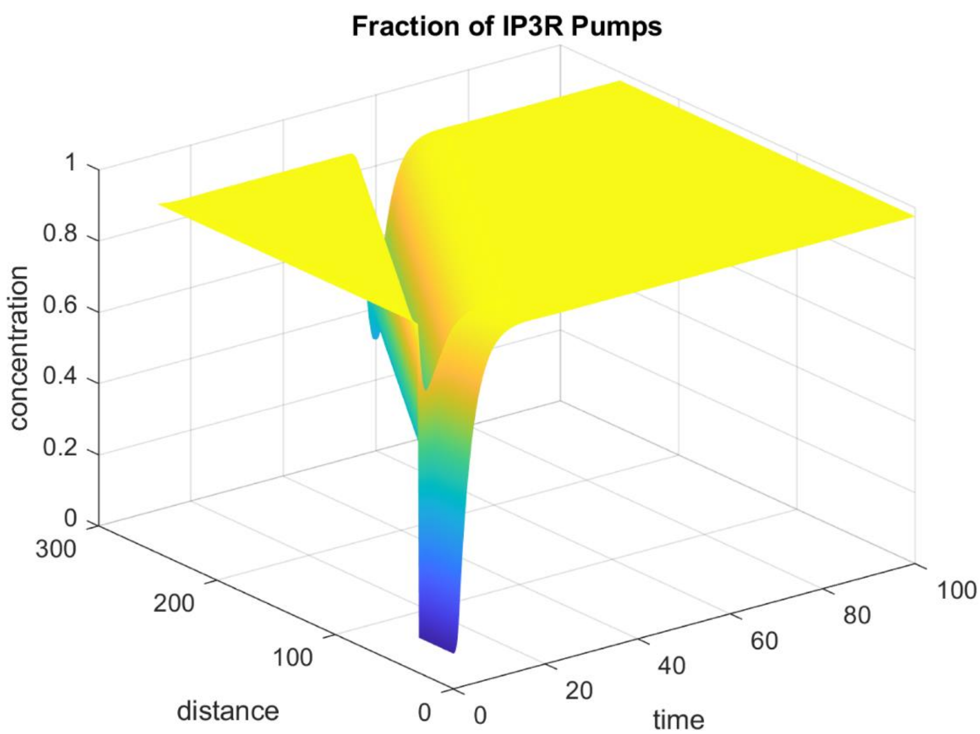
$$C_i^{l+1} = C_i^l + \frac{\Delta t D}{\Delta x^2}\left[C_{i+1}^l - 2C_i^l + C_{i+1}^l\right] + \Delta t k_{flux}\mu n\left[b + \frac{v_1 C_i^l}{k_1 + C_i^l}\right] - \left[\Delta t \frac{\gamma C_i^l}{C_i^l + k_4}\right]$$

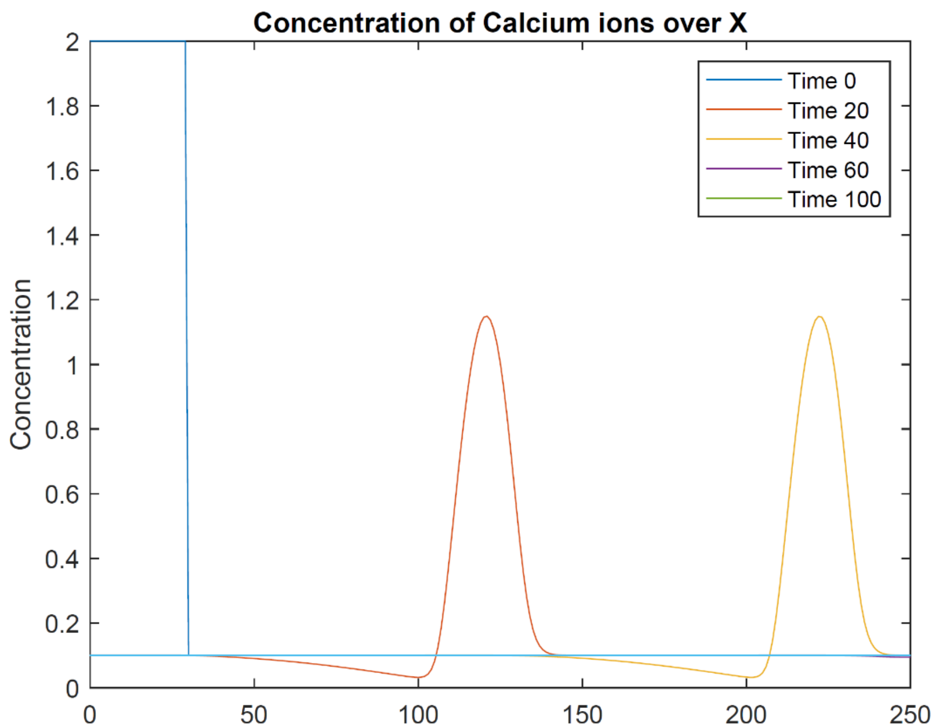
X = L

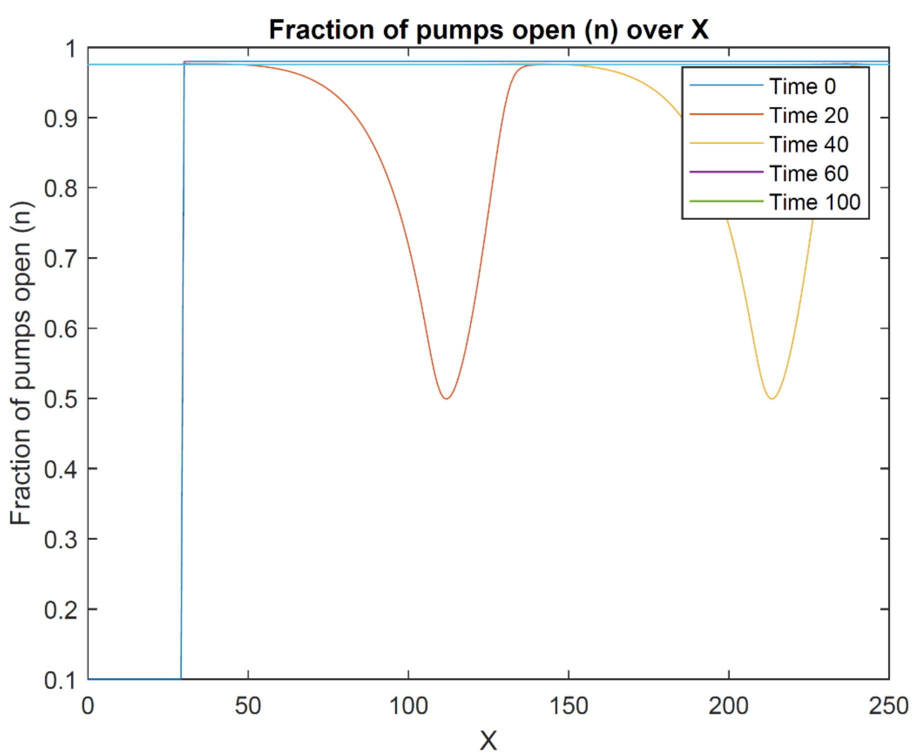
$$C_i^{l+1} = C_i^l + \frac{\Delta t D}{\Delta x^2}\left[C_{i-1}^l - 2C_i^l + C_{i-1}^l\right] + \Delta t k_{flux}\mu n\left[b + \frac{v_1 C_i^l}{k_1 + C_i^l}\right] - \left[\Delta t \frac{\gamma C_i^l}{C_i^l + k_4}\right]$$

1b)


Concentration of Calcium ions
concentration
2
1.5
1
0.5
0
300
200
100
0
distance
0
20
40
60
80
100
time


Fraction of IP3R Pumps
concentration
1
0.8
0.6
0.4
0.2
0
300
200
100
0
distance
0
20
40
60
80
100
time


Concentration of Calcium ions over X
Concentration
Time 0
Time 20
Time 40
Time 60
Time 100
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2
0
50
100
150
200
250

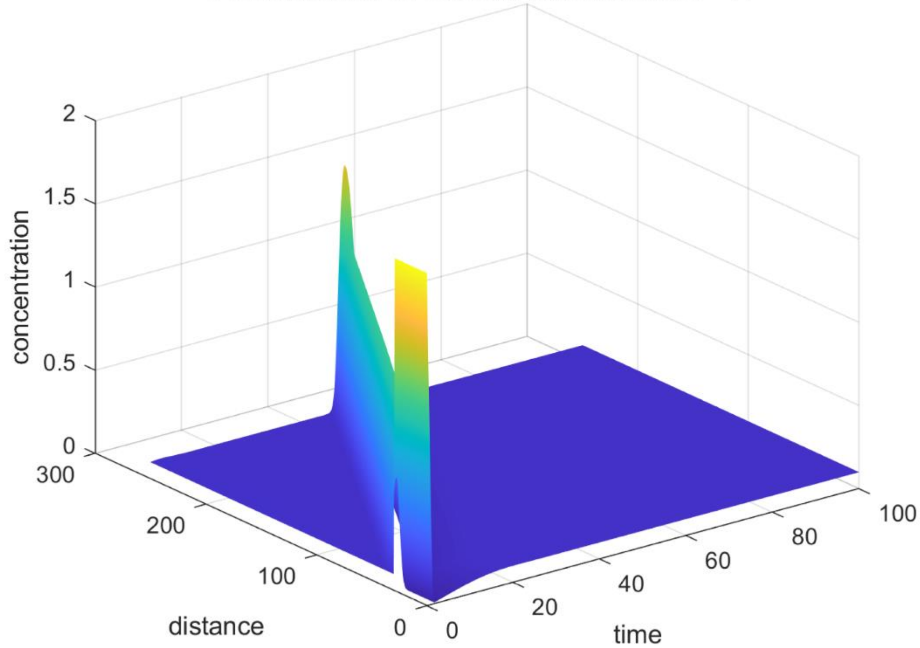

Fraction of pumps open (n) over X
Fraction of pumps open (n)
Time 0
Time 20
Time 40
Time 60
Time 100
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
0
50
100
150
200
250
X

%% PART B
%Q: How would you describe the behavior of c(t,x)?
%A: There is a hiccup of increased concentration when time and distance both increases, but as time continues, the concentration returns to its initial concentration.

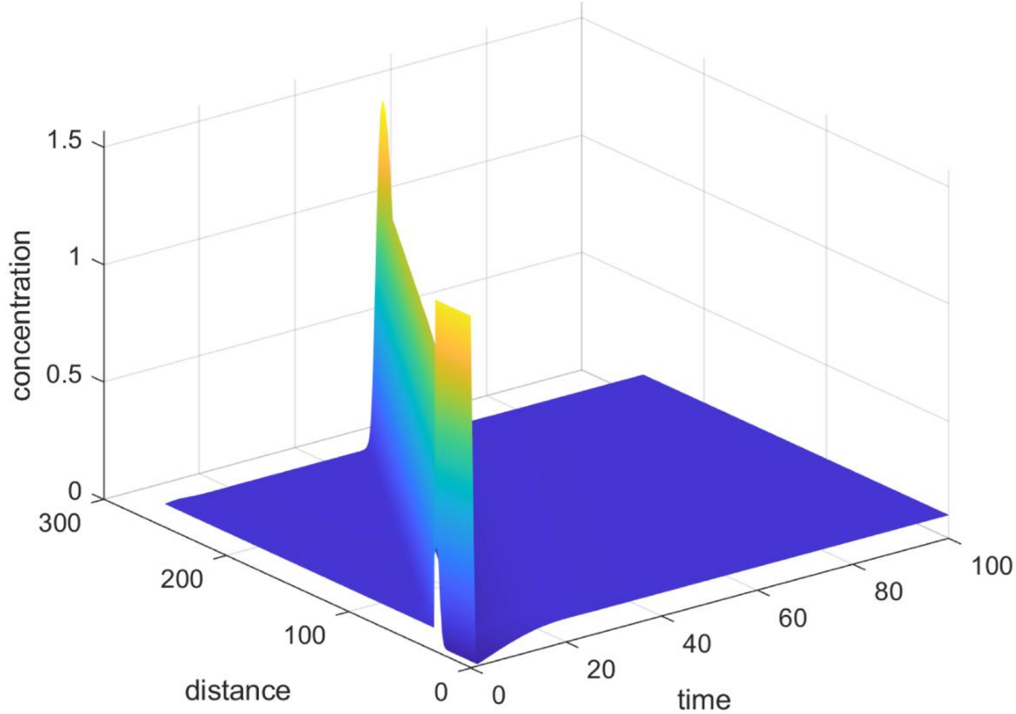
%Q: How would you physically explain what is happening considering both C and N?
%A: Initially there is a steady increase of concentration because of the fixed fraction of channels that are open. But when a level of calcium ion is met, the more open channels are open making the concentration spike. This is the SPIKE seen on the graph. When a high concentration is
reached, the channel is closed and the concentration steadily decreases to a finite level as calcium ions are pumped out into the ER.

1c)

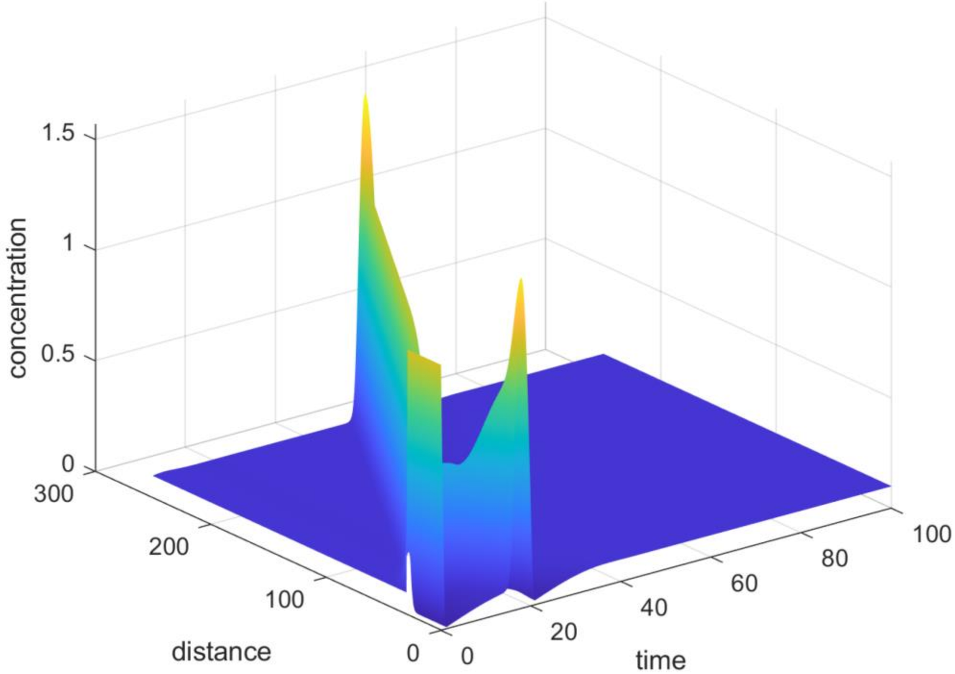
Concentration of Calcium ions ... Initial c = 2



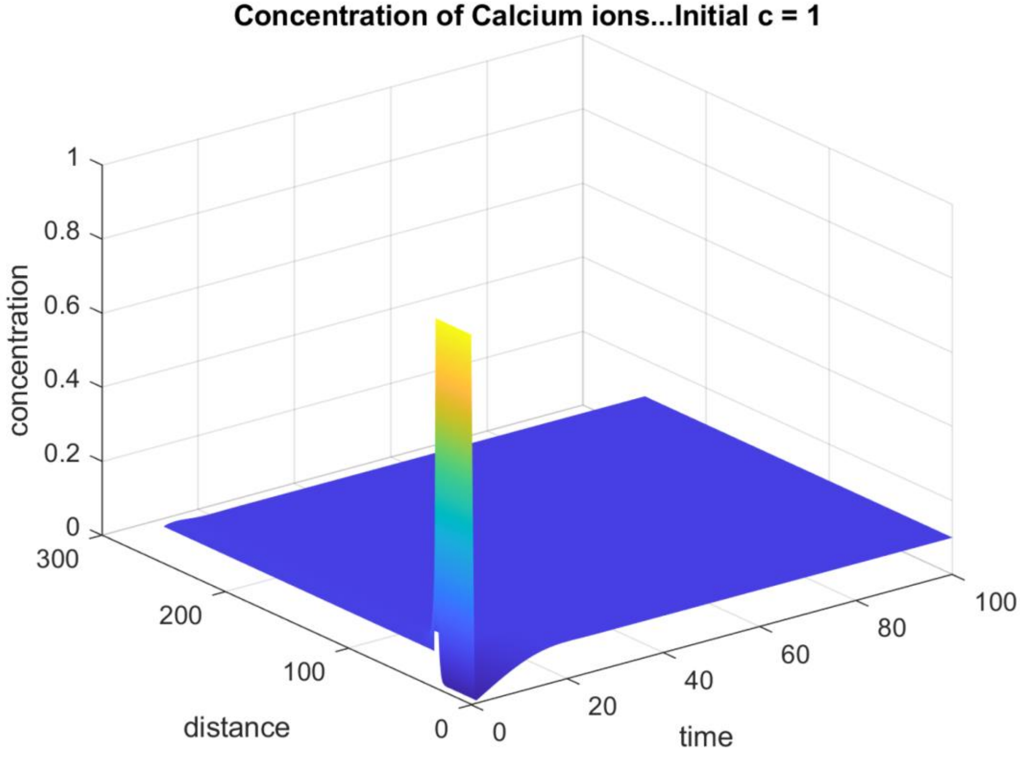
Concentration of Calcium ions ... Initial c = 1.5



Concentration of Calcium ions ... Initial c = 1.2

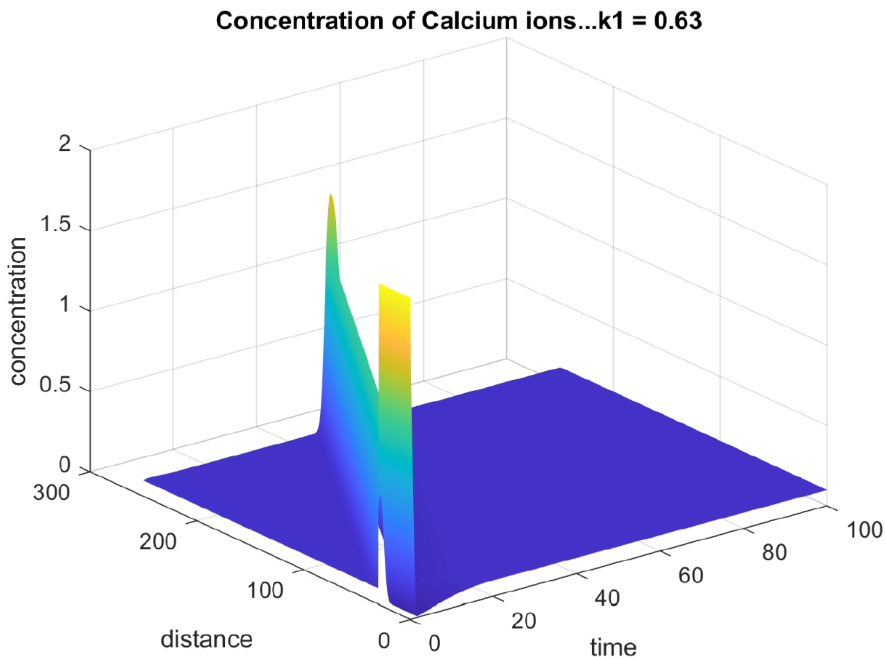


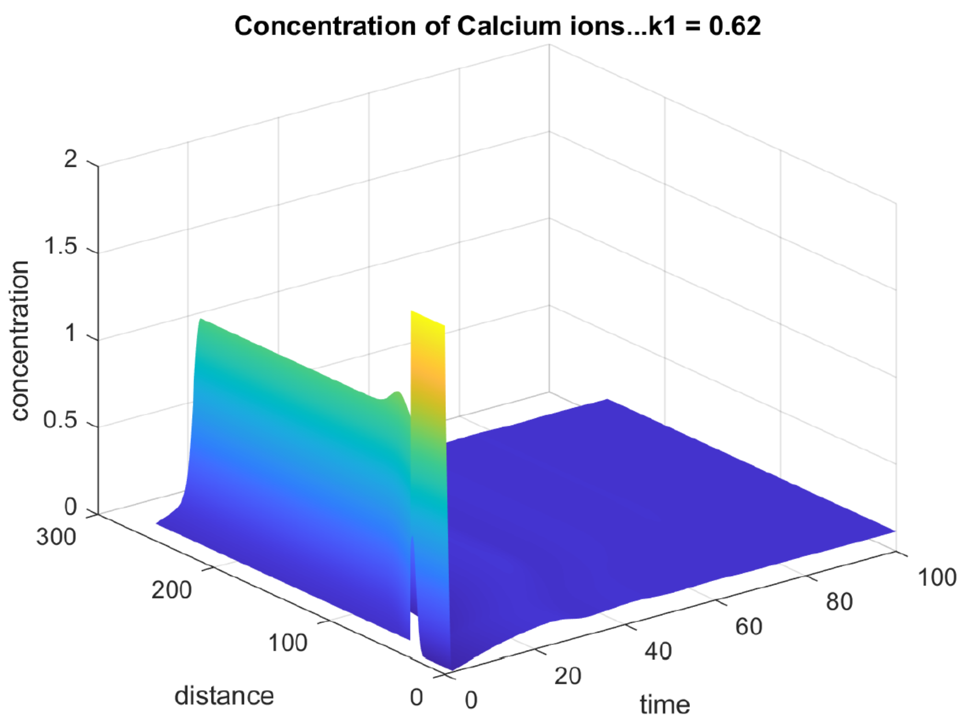
Concentration of Calcium ions...Initial c = 1

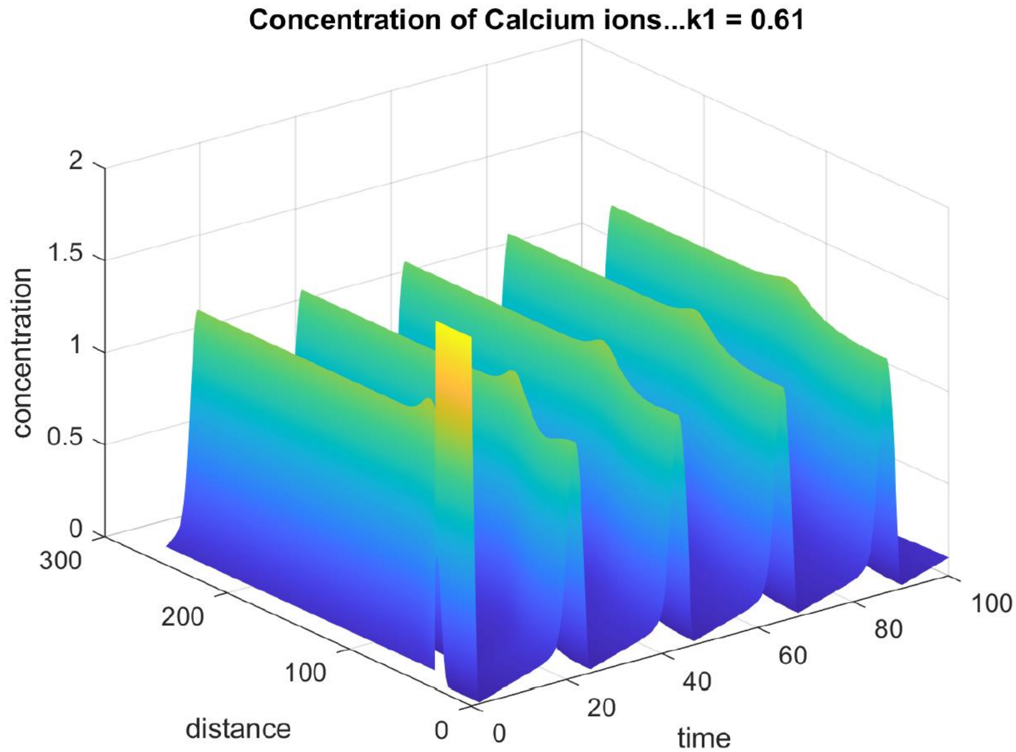


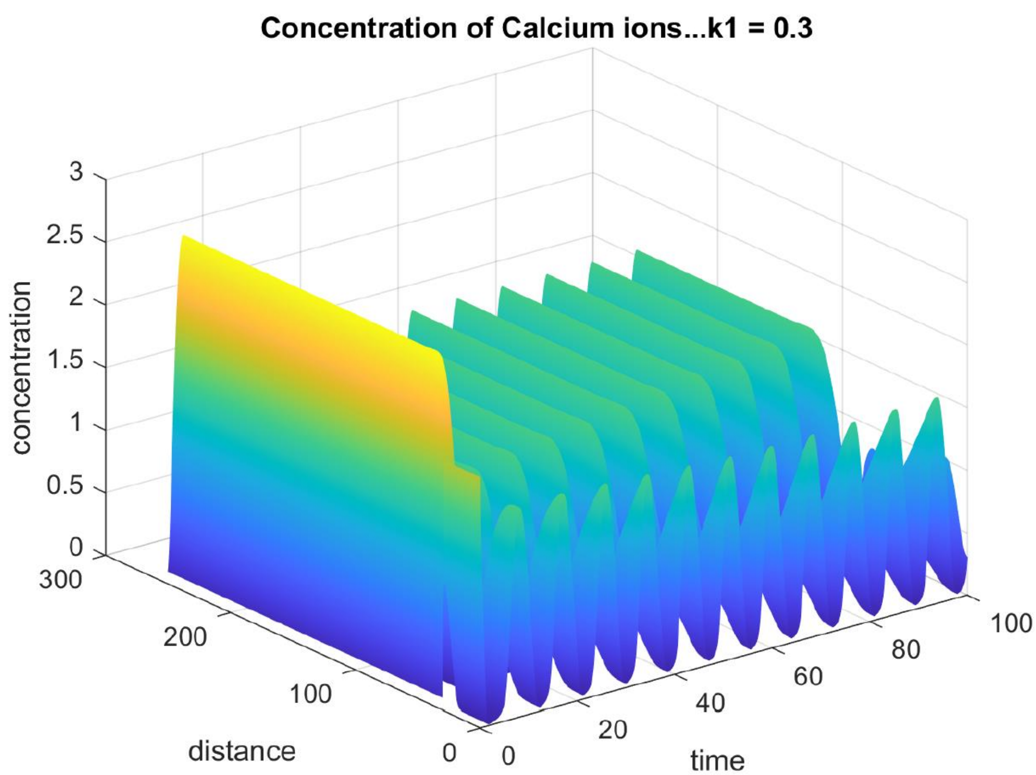
%%PART C
%Q: Investigate the effect of changing the concentration burst. What effects do you see?
%A: Changing the initial concentration to 1.5, there wasn’t a big change from the initial condition of n = 2. There was a larger spike as the distance increased. For the n = 1.2 graph, there was a second spike in the lower distances as time progressed, resulting in a maximum spike later in time. For n = 1, there was a single concentration spike at the lower distances only, and then the concentration equilibrized. It did not have a concentration spike for the later distances as time progressed.

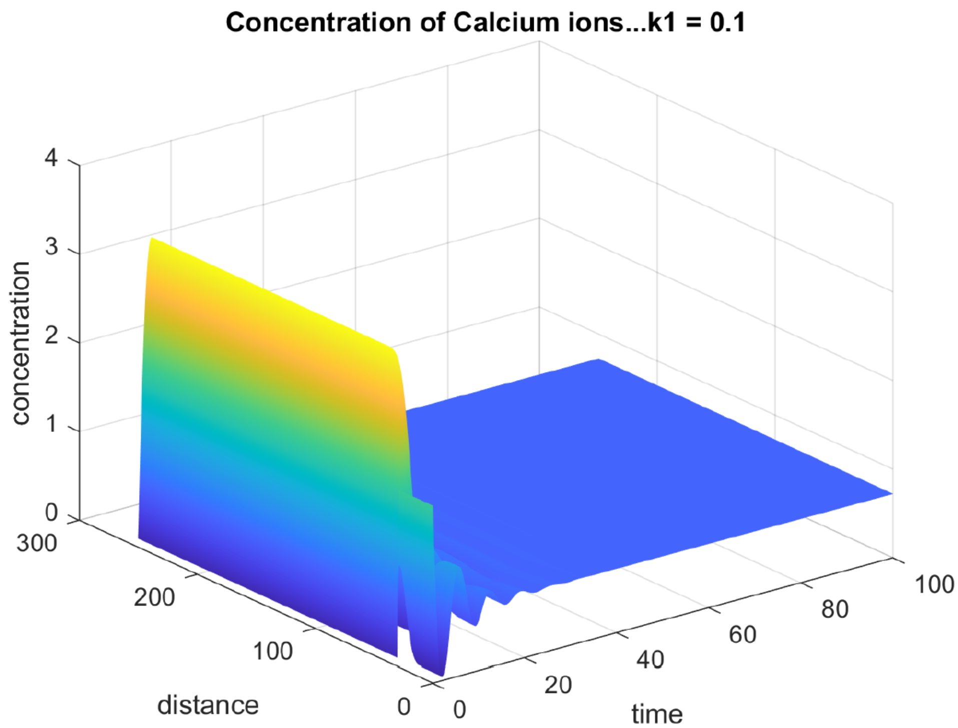
1d)

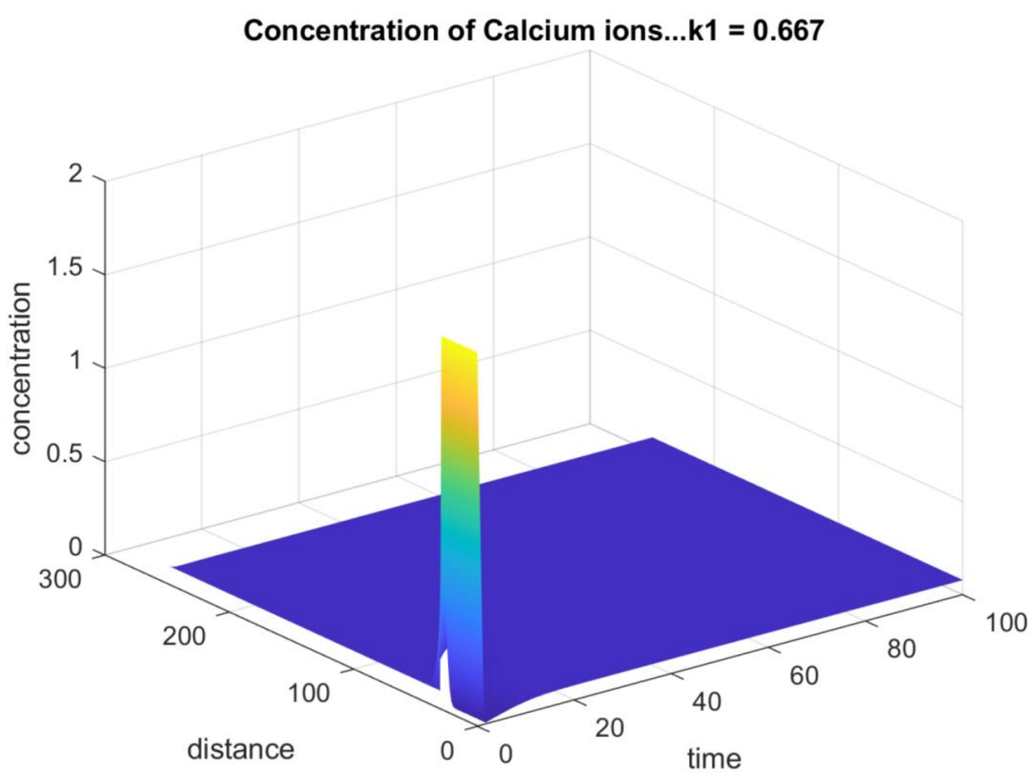

Concentration of Calcium ions...k1 = 0.63
concentration
0
0.5
1
1.5
2
300
200
100
0
distance
0
20
40
60
80
100
time


Concentration of Calcium ions...k1 = 0.62
concentration
0
0.5
1
1.5
2
300
200
100
0
distance
0
20
40
60
80
100
time


Concentration of Calcium ions...k1 = 0.61
concentration
distance
time
0
0.5
1
1.5
2
300
200
100
0
0
20
40
60
80
100

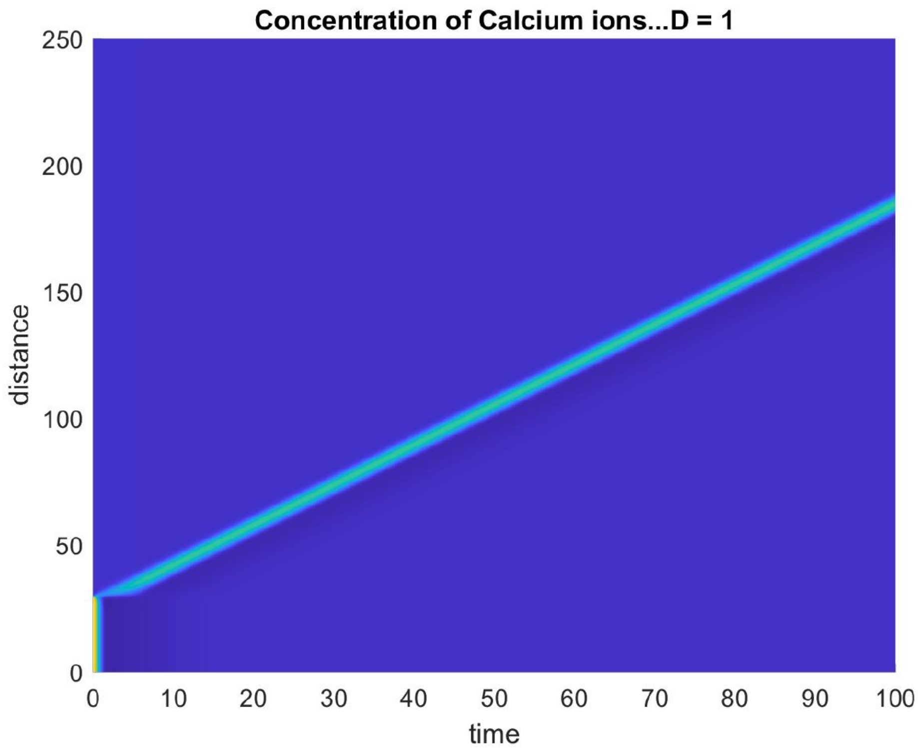

Concentration of Calcium ions...k1 = 0.3
concentration
distance
time
0
0.5
1
1.5
2
2.5
3
300
200
100
0
0
20
40
60
80
100

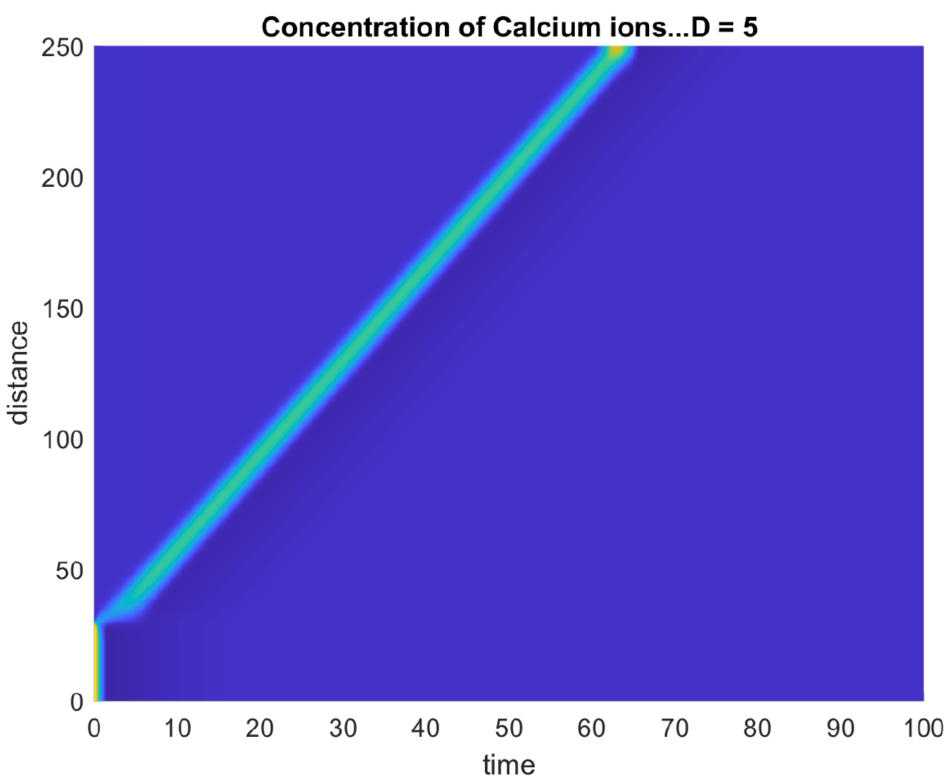

Concentration of Calcium ions...k1 = 0.1
4
3
2
1
0
concentration
300
200
100
0
distance
0
20
40
60
80
100
time

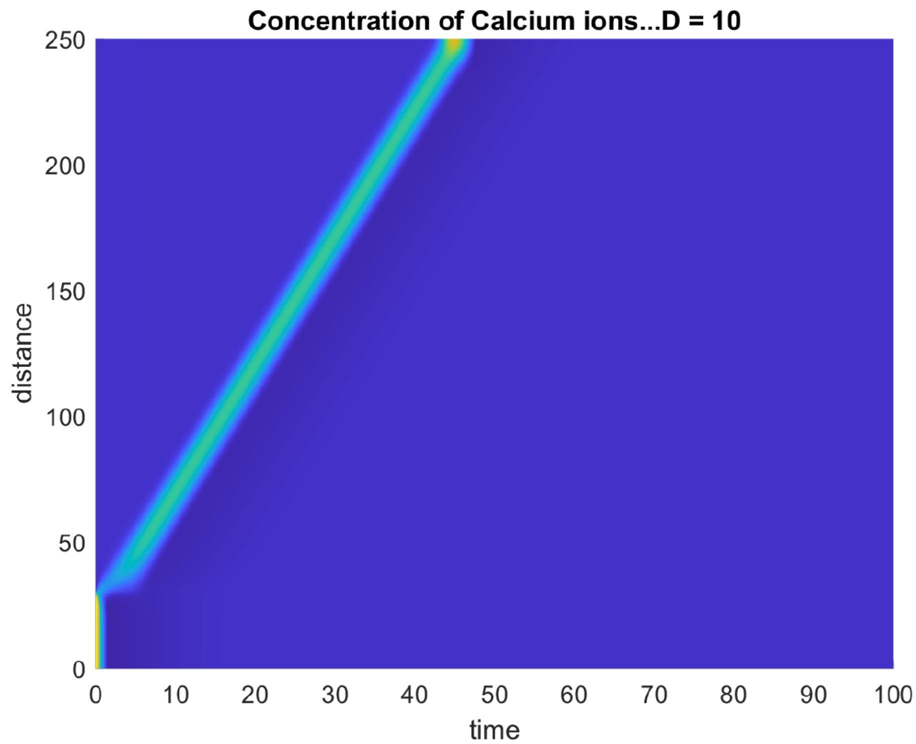

Concentration of Calcium ions...k1 = 0.667
2
1.5
1
0.5
0
concentration
300
200
100
0
distance
0
20
40
60
80
100
time

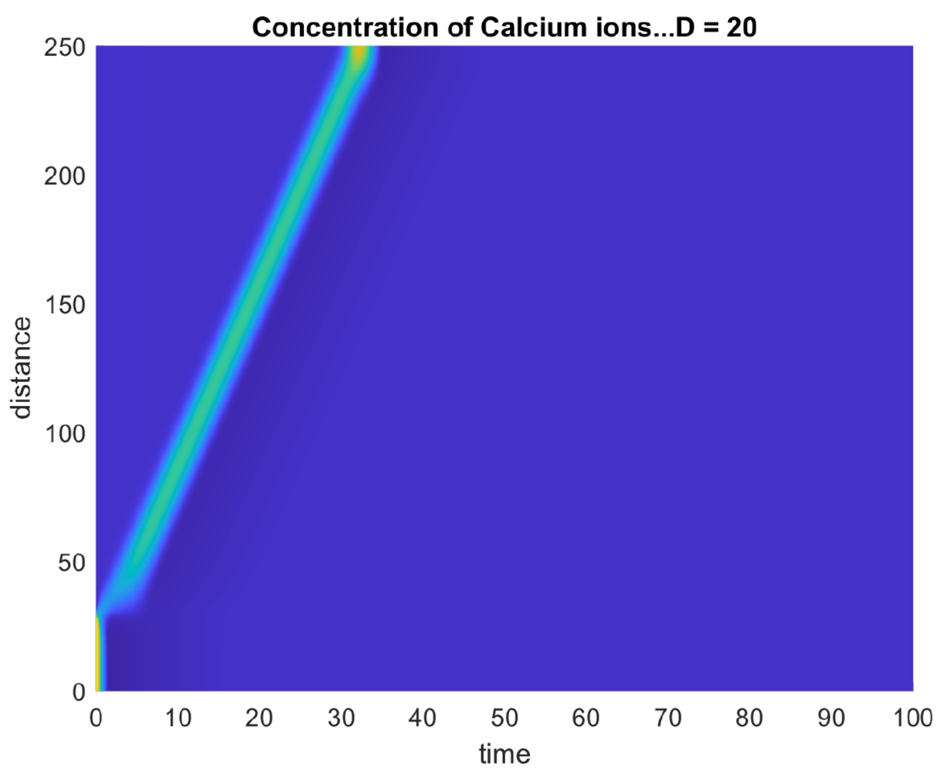
```
%% PART D
%Q: Investigate the effect of changing k1. What effects do you
see?
%A: When K1 is lowered to 0.62, the concentration spike happened
all around the same time (more or less) along the distance as
opposed to being spread out among distance in time. When K1 was
lowered to 0.61, multiple spikes were shone in the concentration
graph. These spikes occurred the same time among all the
distances like when K1 = 0.62, but now there were 3 or 4 more
spikes the were shown. When K1 = 0.3, a larger initial spike of
concentration was seen around the initial time for all
distances. When time decreased, there was a “oscillation” like
spikes for all distances seen throughout time. When K1 = 0.1,
there was a large initial spike for all distances at the initial
time, but then concentration for all distances quickly decreased
to an equilibrized concentration. When K1 = 0.667, there was
only an initial concentration spike at the lower distances and
no where else. This spike quickly decreased as time progressed.
```

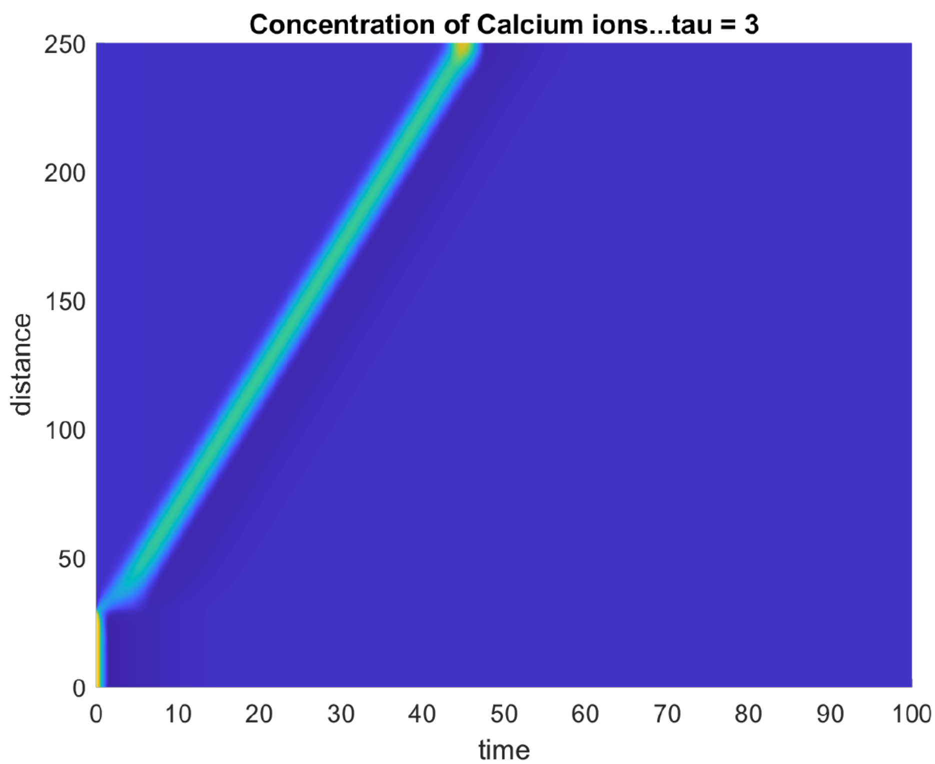
1e)

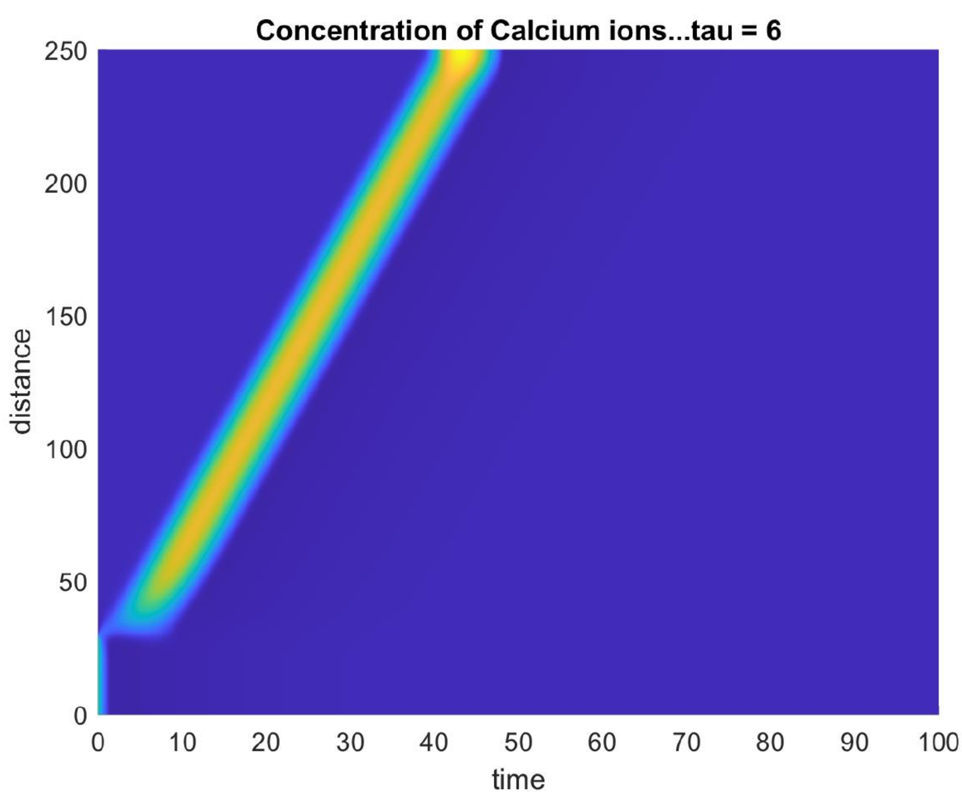

Concentration of Calcium ions...D = 1
distance
time
250
200
150
100
50
0
0
10
20
30
40
50
60
70
80
90
100

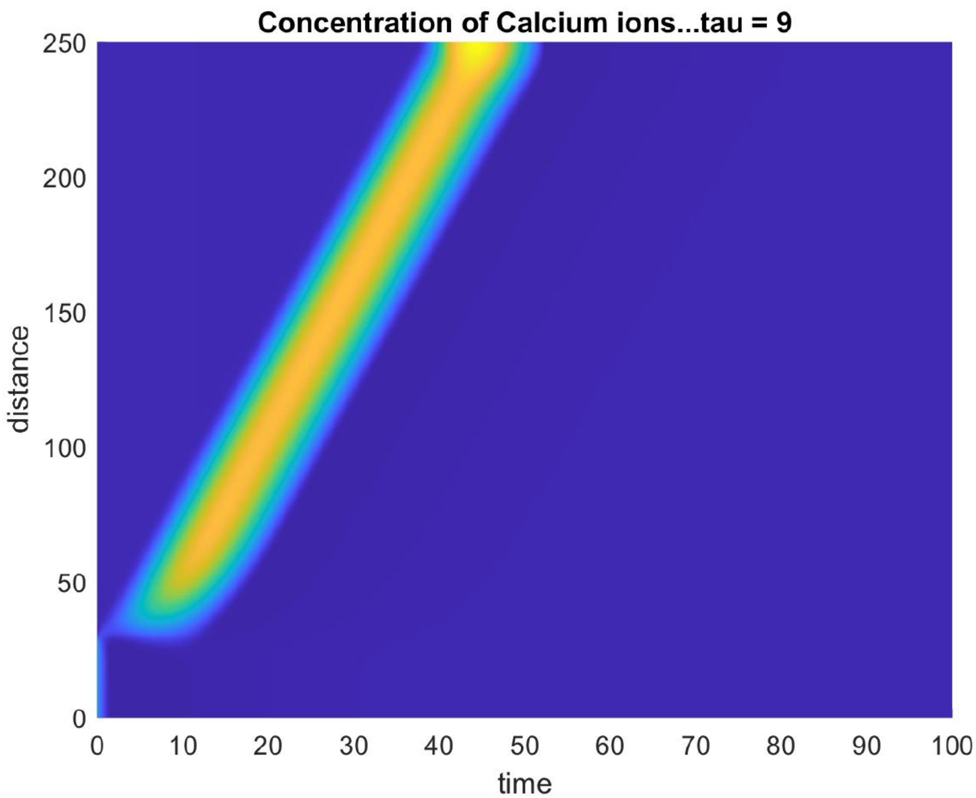

Concentration of Calcium ions...D = 5
distance
time
250
200
150
100
50
0
0
10
20
30
40
50
60
70
80
90
100


Concentration of Calcium ions...D = 10
distance
time
0
50
100
150
200
250
0
10
20
30
40
50
60
70
80
90
100


Concentration of Calcium ions...D = 20
distance
time
0
50
100
150
200
250
0
10
20
30
40
50
60
70
80
90
100


Concentration of Calcium ions...tau = 3
distance
time
250
200
150
100
50
0
0
10
20
30
40
50
60
70
80
90
100

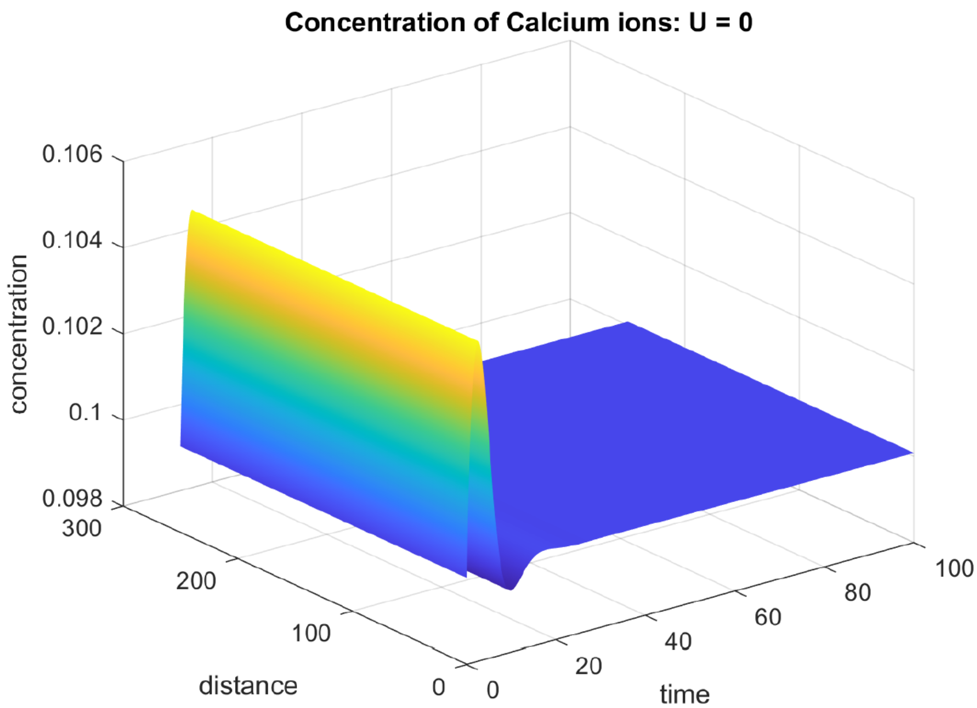

Concentration of Calcium ions...tau = 6
distance
time
250
200
150
100
50
0
0
10
20
30
40
50
60
70
80
90
100


Concentration of Calcium ions...tau = 9
distance
time
0
50
100
150
200
250
0
10
20
30
40
50
60
70
80
90
100

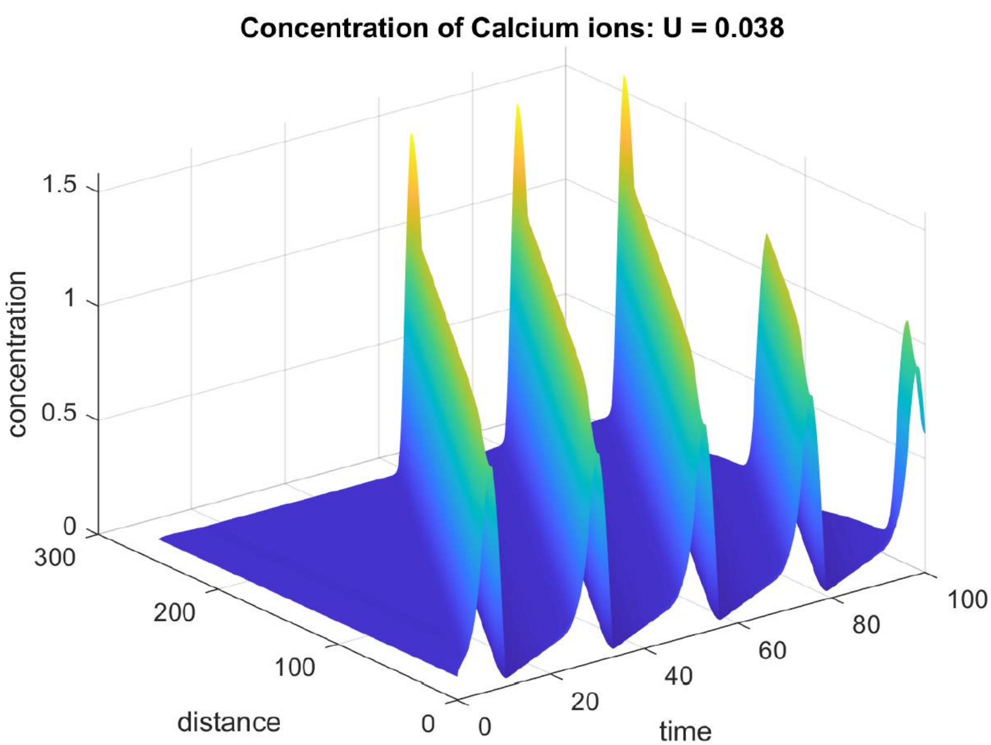
```
%% PART E

%Q: What parameters can be changed to affect the traveling speed
of the phenomenon seen in part b?
%A: There were two parameters that affected the diffusion rate.
The first is D. This parameter was changed from D = 1 to D = 20.
From these plots, as D gets bigger in size, the slope also
steadily increases. This shows that it takes less time to
diffuse from cell to cell. The diffusion rate is higher. Tau was
also changed from a value from 3 to 9. The graph shoes as tau
increases, the length of time it takes to diffuse out of a
certain distance increase (the thickness of the line increases).
This could mean that when tau is a higher value then it takes a
longer time for the concentration of ions to leave the cell;
rather the ions linger in the cell for an extended period.
```

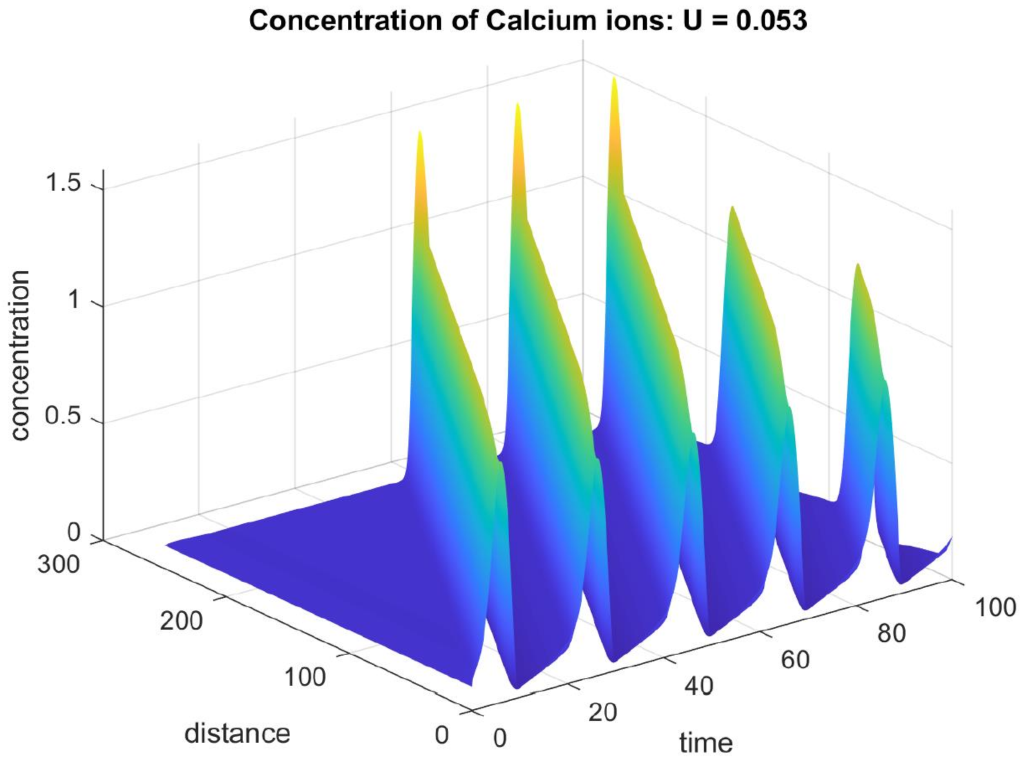
2b)

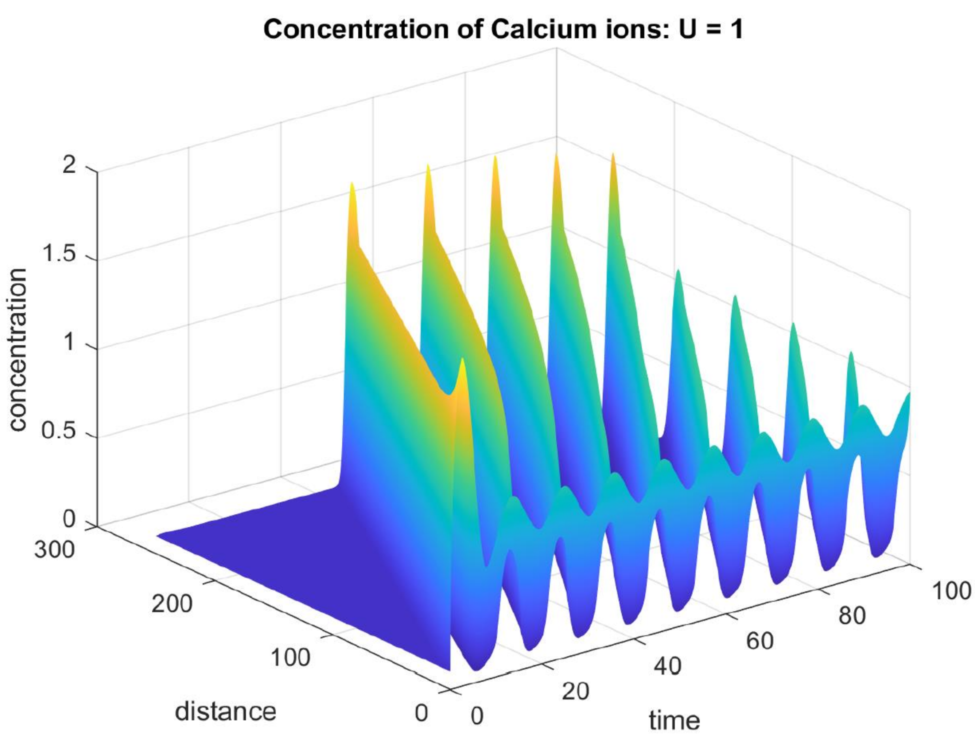


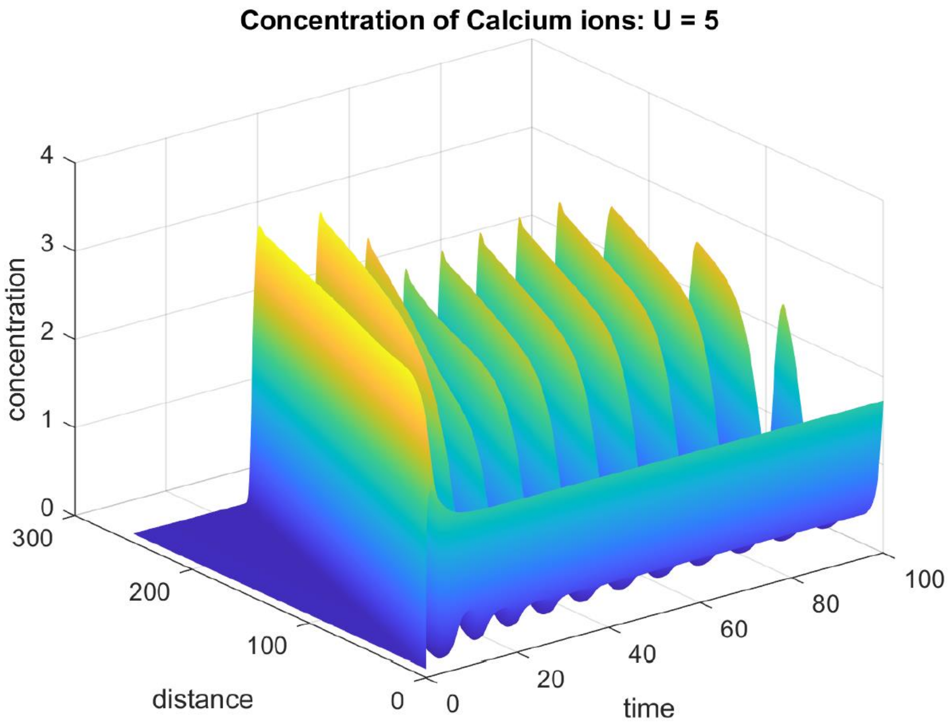
Concentration of Calcium ions: U = 0
0.106
0.104
0.102
0.1
0.098
concentration
300
200
100
0
distance
0
20
40
60
80
100
time

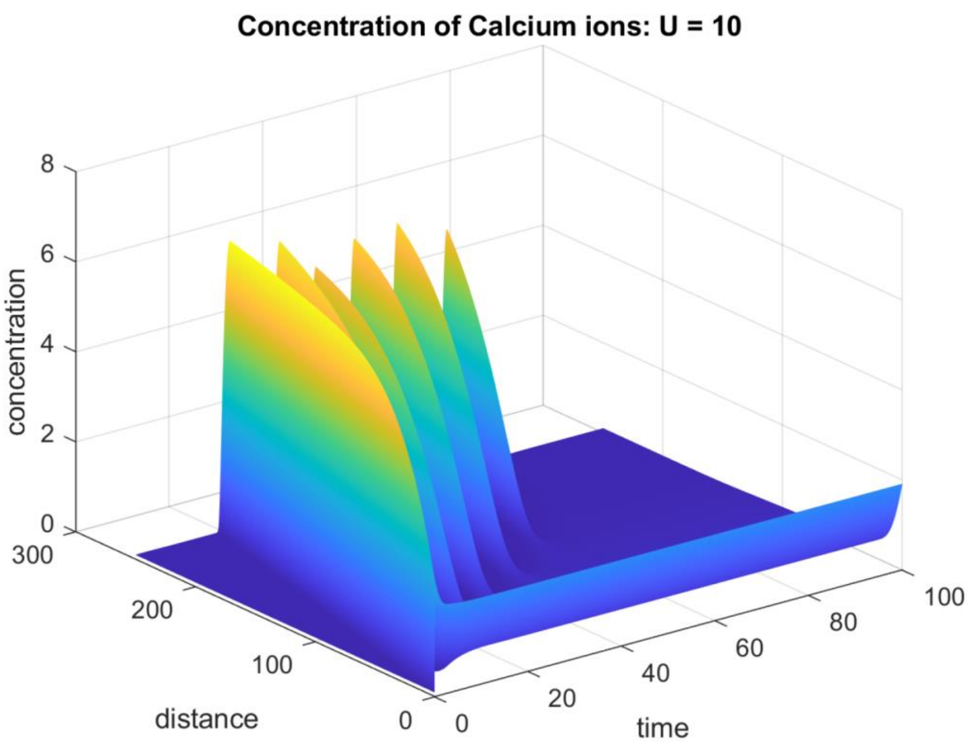


Concentration of Calcium ions: U = 0.038
1.5
1
0.5
0
concentration
300
200
100
0
distance
0
20
40
60
80
100
time


Concentration of Calcium ions: U = 0.053
concentration
distance
time
1.5
1
0.5
0
300
200
100
0
0
20
40
60
80
100


Concentration of Calcium ions: U = 1
concentration
distance
time
2
1.5
1
0.5
0
300
200
100
0
0
20
40
60
80
100


Concentration of Calcium ions: U = 5
concentration
distance
time
0
1
2
3
4
300
200
100
0
0
20
40
60
80
100


Concentration of Calcium ions: U = 10
concentration
distance
time
0
2
4
6
8
300
200
100
0
0
20
40
60
80
100

```
%% Q2 PART B

%Q: Describe how the behavior of the system changes with
different input flow rates u.
%A: When U = 0, there is one concentration spike since those are
the initial conditions. When U = 0.038 - 0.053, there are a few
spikes present in the later distances that seem to be around the
same concentration value. When U is 0.053 these spikes are
closer together. This makes sense because U is a constant flow
into the x = 0 boundary. When U =1. There are more concentration
spikes as time progresses resembling a wave like structure in
the graph. This is because there is a higher flow of
concentration being flowing in from the boundary. When U = 5 and
10, there are more concentration spikes present in time and
there is a relatively high concentration value for the lower
distances throughout all time after the initial condition. This
makes sense because now there is a higher flow of concentration
of calcium ions flowing that the closed pumps can’t take out of
the cytosol in time.
```

3a)

* Semi-implicit

$$C_i^{\ell+1} = C_i^{\ell} + \frac{\Delta t D}{\Delta x^2}\left[C_{i+1}^{\ell+1} - 2C_i^{\ell+1} + C_{i-1}^{\ell+1}\right] + \Delta t\, k_{flux}\, \mu n \left[b + \frac{v_1 C_i^{\ell}}{k_1 + C_i^{\ell}}\right] - \left[\frac{\Delta t\, \gamma C_i^{\ell}}{C_i^{\ell} + k_4}\right]$$

$$C_i^{\ell+1} - \lambda\left[C_{i+1}^{\ell+1} - 2C_i^{\ell+1} + C_{i-1}^{\ell+1}\right] = \Delta t\, k_{flux}\, \mu n \left[b + \frac{v_1 C_i^{\ell}}{k_1 + C_i^{\ell}}\right] - \left[\frac{\Delta t\, \gamma C_i^{\ell}}{C_i^{\ell} + k_4}\right]$$

* Boundary: $\frac{C_{i+1}^{\ell} - C_{i-1}^{\ell}}{2\Delta x} = \frac{\partial c}{\partial x}$

@ $x = 0$

$C_{-1}^{\ell+1} = C_1^{\ell+1} - 2\Delta x \cancel{\frac{\partial c}{\partial x}}^{0}$

$C_{-1}^{\ell+1} = C_1^{\ell+1}$

@ $x = L$

$C_1^{\ell+1} = C_{-1}^{\ell+1}$

Interior: $-\lambda C_{i+1}^{\ell+1} + (1+2\lambda)C_i^{\ell+1} - \lambda C_{i-1}^{\ell+1}$

$x=0$ boundary: $-2\lambda C_{i+1}^{\ell+1} + (1+2\lambda)C_i^{\ell+1}$

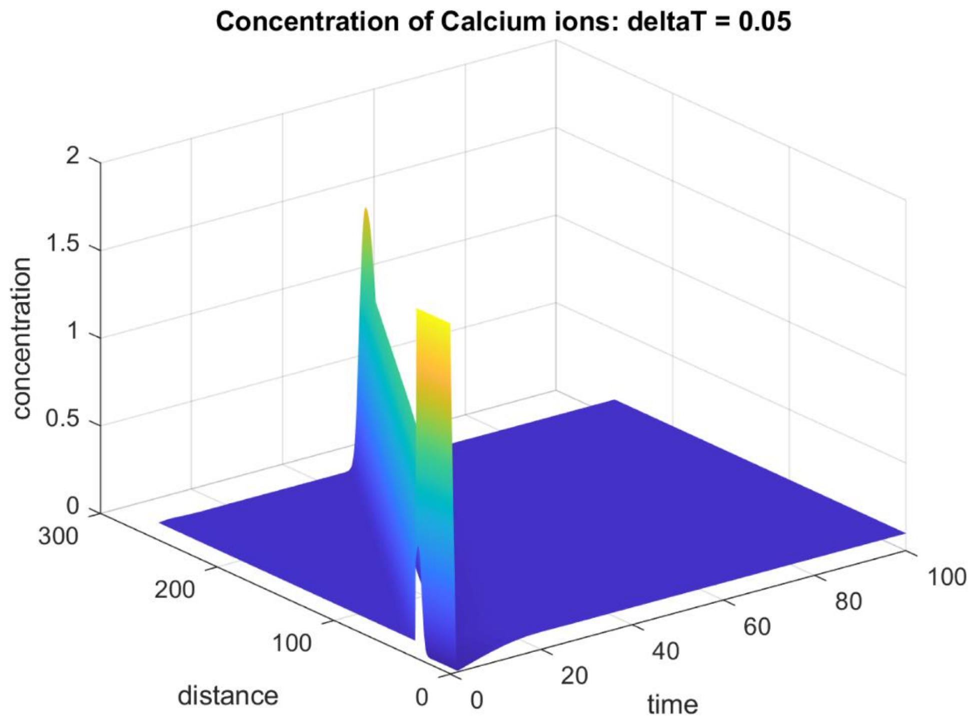
$x=L$ boundary: $(1+2\lambda)C_i^{\ell+1} - 2\lambda C_{i-1}^{\ell+1}$

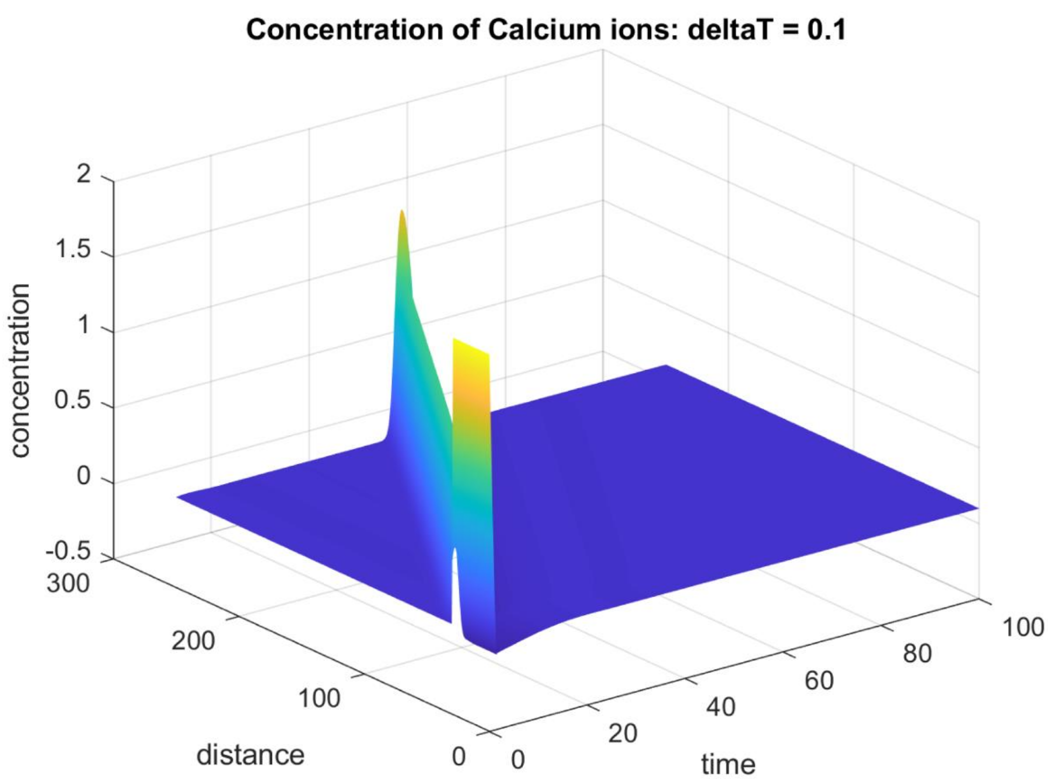
$-\lambda C_{i+1}^{i+1} + (1+2\lambda)C_i^{\ell+1} - \lambda C_{i-1}^{\ell+1} = \Delta t\, k_{flux}\, \mu n\left[b + \frac{v_1 C_i^{\ell}}{k_1 + C_i^{\ell}}\right] - \left[\frac{\Delta t\, \gamma C_i^{\ell}}{C_i^{\ell} + k_4}\right]$ → interior points

$-2\lambda C_{i+1}^{\ell+1} + (1+2\lambda)C_i^{\ell+1} =$ " → $x = 0$ boundary point

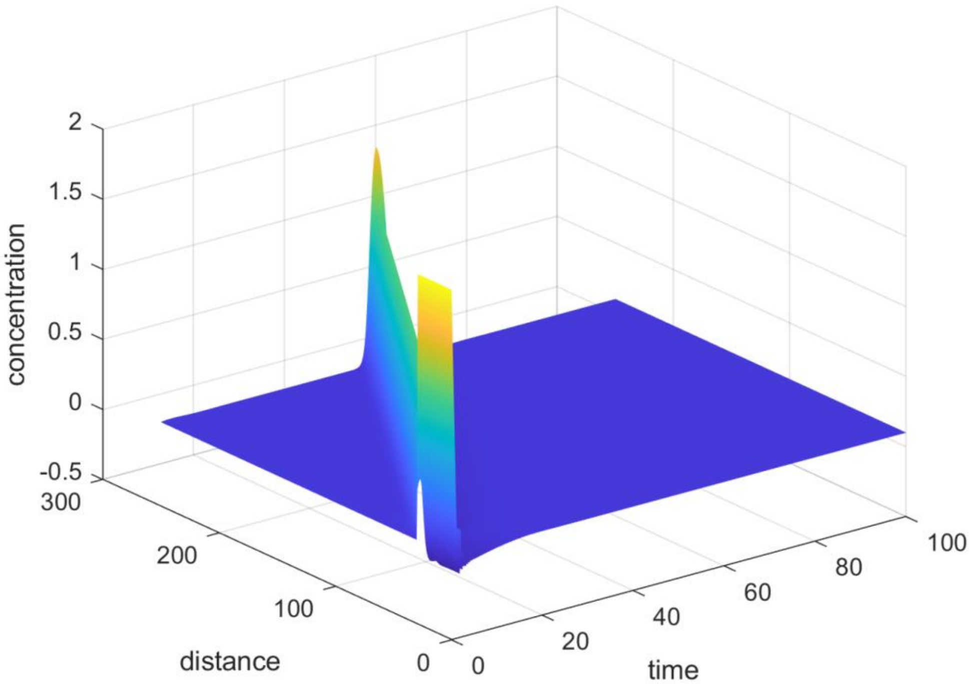
$(1+2\lambda)C_i^{\ell+1} - 2\lambda C_{i-1}^{\ell+1} =$ " → $x = L$ boundary point

3b)

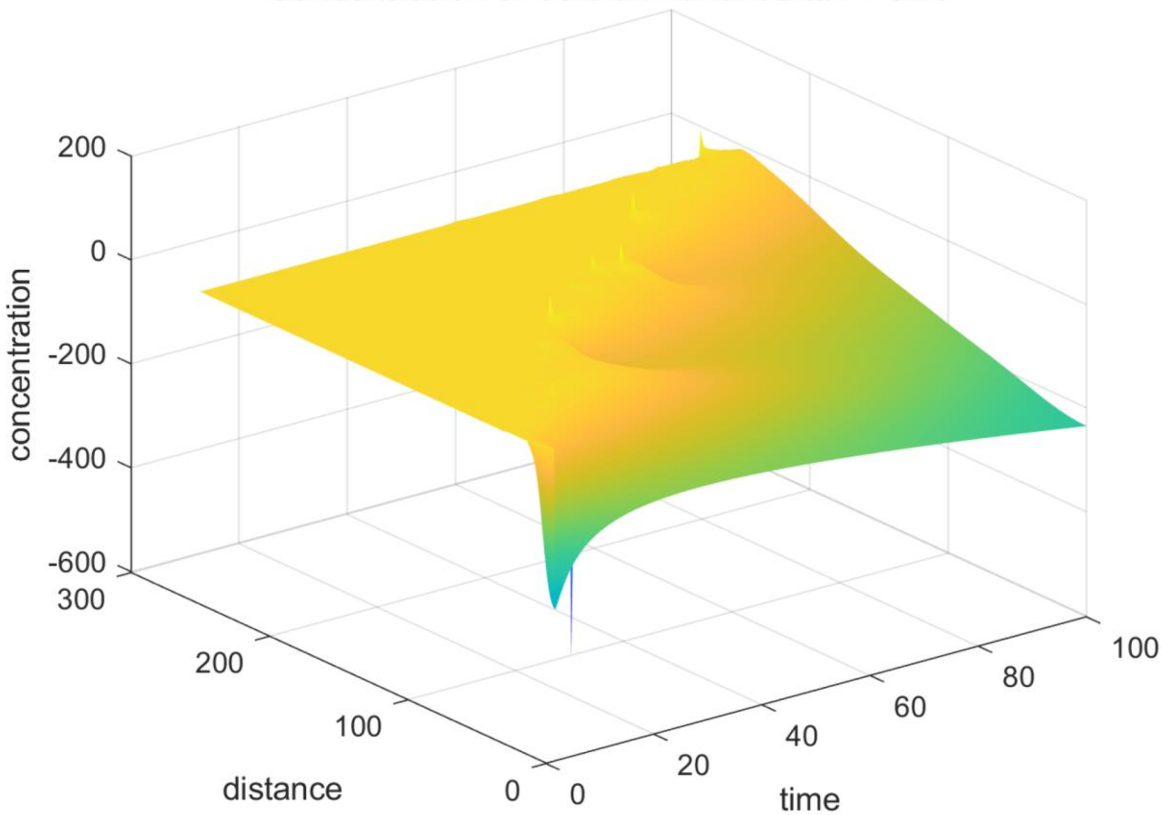

Concentration of Calcium ions: deltaT = 0.05
2
1.5
1
0.5
0
concentration
300
200
100
0
distance
0
20
40
60
80
100
time


Concentration of Calcium ions: deltaT = 0.1
2
1.5
1
0.5
0
-0.5
concentration
300
200
100
0
distance
0
20
40
60
80
100
time

Concentration of Calcium ions: deltaT = 0.2



Concentration of Calcium ions: deltaT = 0.25



```
%% Q3 PART C

%Q: What large a time step can you take and still get
qualitatively the same behavior seen in c and d of part 1?
%A: I tested time steps of 0.05, 0.1, 0.2, and 0.25. From these
plots, the first three qualitatively resemble the plots from
part 1. However when deltaT is 0.25, the graph “explodes” and
doesn’t produce a similar graph.
```