Laura Cox 4/17/2015

I first plugged in all numerical values given to me in the PDE file of the "before tumor." The reaction is homogeneous since the concentration is in nM and the diffusion coefficient units are only cm^2/day.

I chose to use dirichlet boundary conditions due to the homogeneous nature. Convert the concentration from nM to $nmol/cm^3$ to keep units of length consistent with diffusion coefficient.

H (height) = 1 c (concentration) = 100 $nmol/cm^3$

I chose to use the parabolic parameters because we are trying to find the change in concentration over time. Since the time constraint is 2 months, choose to convert to the diffusion coefficient to cm^2/day instead of cm^2/s. D is negative because it's a consumption reaction. The parameters are as followed:

D (diffusion coefficient): -0.0216 cm^2/day Q (RA): ?

After I set up all the parameters given to me, I had to essentially "guess and check" my Q values. The first thing I did to check how well my reaction rate (Q) worked was pick points on the "after file" that I wanted to analyze for different Q values. I assumed these points to be similar on the "before" file and also tried to pick points close to the border/middle of the "after" tumor so I could tell if my RA values were extremely off. The points I chose were as follows:

a. **(0,6) b. (-4, 0) c. (0,2)**

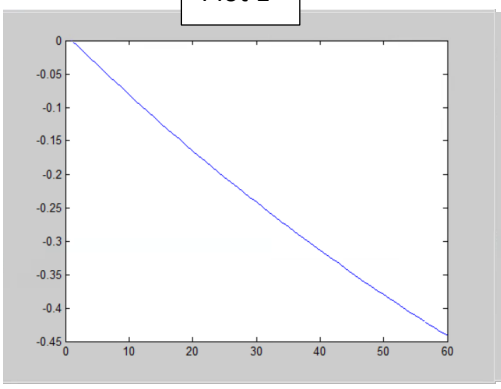
Unfortunately, due to the nature of the shape and the accuracy of refining the mesh I did not model these exact points but locations very similar to it. For my solution file (the "before file"), I refined the mesh two times. The actual x/y values I chose from the extrapolated data from the mesh were as follows: (same points used for all 3 Q value analyzes)

Plot 1: (0.494, 6.037) Plot 2: (-4.28, 0.33) Plot 3: (-0.71, 2.35)

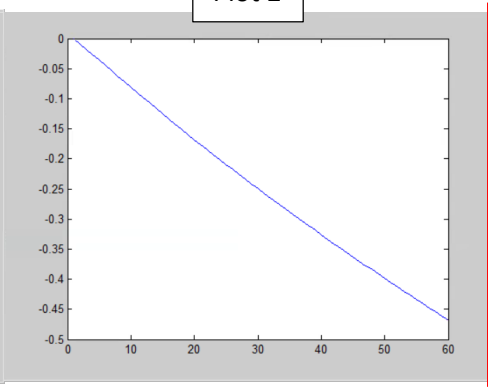
The most informative point was the one I chose near the center, (-0.71, 2.35) highlighted in red. I assumed that beginning concentration near the center should be 0 since the reaction is slow and I also did not want my concentration values to ever be negative. The border points are not accurate due to the shape differences between the "before" and "after" files. The following plots are in c(x,y) vs t to test different Q values:

RA = -9 x 10^{-3} $nmol/cm^3$ day (starting point since in mL or cm^3 so 10^{-3} seems reasonable)

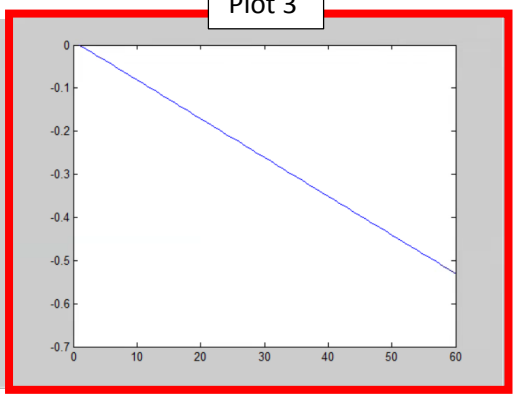
Plot 1



Plot 2

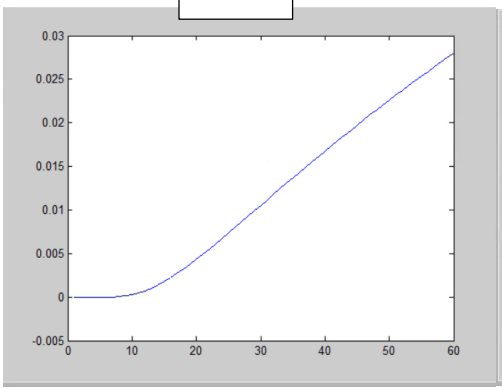


Plot 3

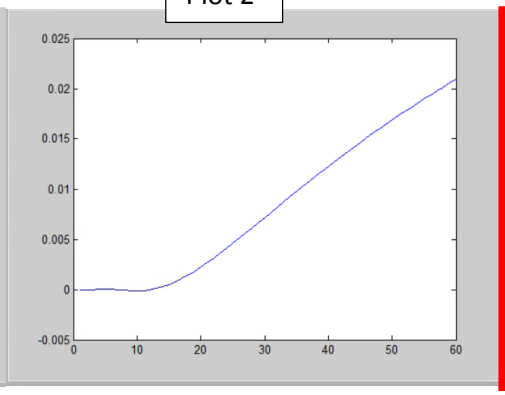


RA = -9 x 10^{-7} nmol/cm^3 day

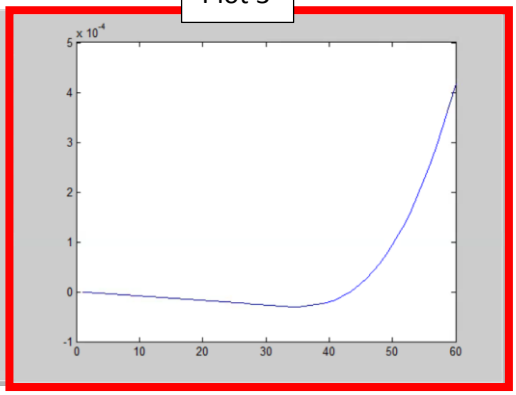
Plot 1



Plot 2

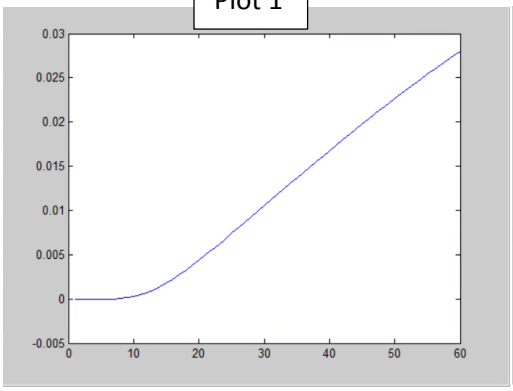


Plot 3

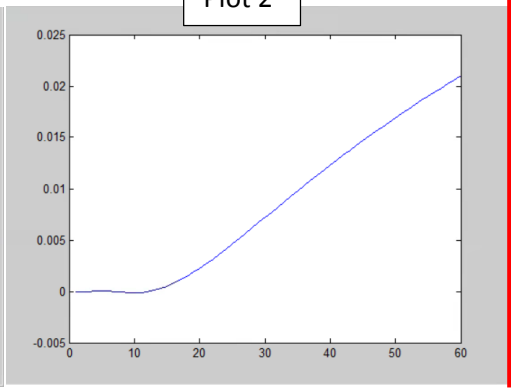


RA = -9 x 10^{-9} nmol/cm^3day

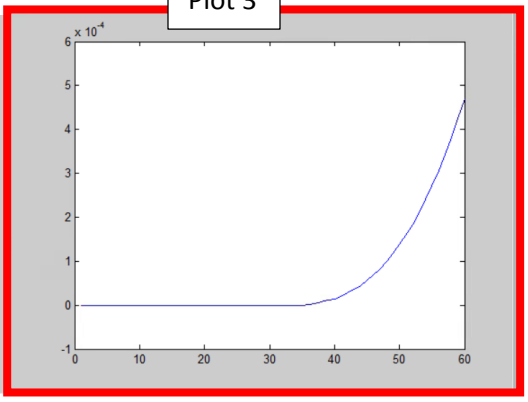
Plot 1



Plot 2



Plot 3



For the first RA value, the concentration was negative in the center and the concentration was decreasing rather than increasing over time so it was eliminated. For the second RA value, the concentration is bordering on the threshold value (converted to 5 x 10^{-3} nmol/cm^3) and also it slightly dipped below zero which doesn't make much sense. I decided to try an even smaller number which gave me a smooth transition into increasing concentration. The last RA value correlates to a number similar to what I would have expected since I am working in nmol and the exponent is -9.

Overlay plot with final RA value **-9 x 10^{-9} nmol/cm^3day** of alive cells from solution and mesh points from the "after file."

Due to the size differences as well as refining the mesh, I had to compromise the final shapes of my solution/after file solution being exactly the same. However, my solution (the red points) is similar in size. Also, arbitrarily picking points to analyze different Q's was inaccurate and a logical compromise I made since the axis's were scaled almost the same in both files.