Name:

**Instructions:**

1. **Put your name on every sheet of paper you hand in for grading, including this sheet.** Put your name on every sheet of every file you submit electronically for grading.
2. Read each question carefully and make sure you provide all the requested information.
3. Please provide clear, well-presented solutions. If I cannot understand your solution, you will lose points.
4. Clearly present/explain all assumptions you make in creating a solution. Your solutions will be evaluated on your selection of appropriate assumptions, your model derivation, and the appropriateness of the final model.
5. Please recognize that this is an individual exam so you are not allowed to consult with others. The honesty policy for the course applies for all take home work. Of course you may use any media resources available, and please cite references that are significant to your solutions, as appropriate.
6. You may use appropriate computational resources as needed. Please supply any relevant programs/spreadsheets, etc. as appropriate to your solution.

Your task is to develop a differential equation model for diffusive mass transfer of a drug from a spherical tablet and compute a numerical solution using finite difference methods.

A 2 cm radius spherical tablet composed of an inert carrier (cellulose/clay) initially contains active component X at a uniform concentration of 100 mmol/cm3.

At time=0, the tablet is dropped into a solution of concentration 0 mmol/cm3 and component X diffuses out of the tablet into the surrounding solution.

Assumptions

At the surface of the tablet, the concentration is constant at 0 mmol/cm3 and at the center of the tablet the concentration is constant at 100 mmol/cm3. Since the tablet is mainly inert material, its radius is constant at 2 cm (it does not dissolve).

The rate of diffusion is controlled by Fick's 1st law, which states that the flowrate of mass, F (mmol/time) = *D*\*(area)\*dC/dr,where *D* is the diffusion constant, C is concentration, and r is radial position. The value of D = 0.2 cm2/min.

Part A. (20 points)

Draw a picture and define the system/flows. Derive the differential equation model of the concentration of X (C) as a function of radial position (r) in the tablet and time (t). Make sure you clearly explain/show the steps involved in your derivation, including any assumptions or reasoning in the derivation of your model. You may wish to use the model derivation process (draw picture, etc.), if needed to more clearly explain your solution.

Part B. (15 points)

Using the finite difference numerical method, derive the finite difference equation approximating the differential equation derived in part A. Put your solution in the form used to calculate the concentration at the next time position, ie. Cm p+1 = ...

where m refers to radial position and p refers to time.

Note: Please do not submit the analytical solution to this model, only the finite difference model.

Part C. (15 points)

Using the finite difference equation from part B*,* compute/plot the profiles of concentration of X as a function of radial position (r) and time (t). Calculate the concentration of X at radial increments of 0.2 cm (0<r<2 cm) for time increments of 0.1 min (0<t<1.5 min). Provide appropriate plots of your solutions, clearly indicating concentration, time, and position variables.