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# Assignment: Transient MATLAB-Based FEM Modelling

ME40064: System Modelling & Simulation

## Part 1: Software Verification & Code Quality [55%]

You must extend your finite element code to be able to solve the transient form of the diffusion-reaction equation given in Eq. 1:

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} + \lambda c + f \qquad \text{Eq. 1}$$

Use and document a range of strategies described in the course to demonstrate that your code for solving Eq. 1 is correct at both a unit and overall level. You should consider a variety of input & boundary conditions. You should follow good programming practice such as: using functions & structures/object orientation, meaningful variable names, code comments, separation of data and code.

**At a minimum** you should solve the transient diffusion equation, Eq. 2, for the domain x = 0 to 1, subject to the following initial and Dirichlet boundary conditions, and compare to the analytical solution in Eq. 3:

$$\frac{\partial c}{\partial t} = \frac{\partial^2 c}{\partial x^2} \qquad \text{Eq. 2}$$

$$x = [0,1], \qquad c(x,0) = 0, \qquad c(0,t) = 0, \qquad c(1,t) = 1, \qquad t > 0$$

You should use a range of element sizes and time step values to demonstrate spatial and temporal convergence, using the analytical solution in Eq. 3 as a reference. A MATLAB function to compute Eq. 3, `TransientAnalyticSoln.m`, is provided on Moodle:

$$c(x,t) = x + \frac{2}{\pi}\sum_{n=1}^{\infty}\frac{(-1)^n}{n}e^{-n^2\pi^2 t}\sin(n\pi x) \qquad \text{Eq. 3}$$

**At a minimum** you should include the following two figures in your report to demonstrate that your code is correct:

a. Plot your solution c(x) vs. x, showing the solutions at t = 0.05, 0.1, 0.3, 1.0, in the format shown in Lecture 13, comparing it to the analytical solution.
b. Plot both the analytical solution and your numerical solution at x=0.8, for t = 0 to 1.0.

Higher marks are available for implementing, verifying, and testing:

- The differences between forward Euler, backward Euler, and Crank-Nicolson methods
- Capability to handle time varying source terms and Neumann BCs
- Gaussian quadrature for evaluating integrals
- Quadratic basis functions
- Using the L2 norm to test convergence rate of your finite element method

## Part 2: Modelling & Simulation Results [40%]

Now use and extend your code to solve the drug delivery problem introduced in Lecture 14. The drug concentration distribution in tissue is modelled by Eq. 4:

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} - \beta c - \gamma c \qquad \text{Eq. 4}$$

Your finite element mesh and material parameters must represent the three-layered structure of skin, as shown in Figure 1.

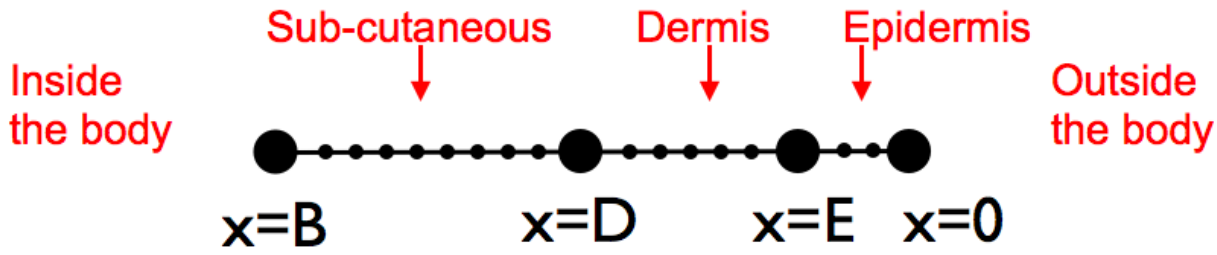


**Figure 1: Schematic of finite element mesh required to represent skin tissue layers. Note: mesh node positions are purely illustrative and not a recommendation.**

Parameter values for each layer are provided in Table 1. The layers of the tissue are defined at the following x coordinates: **E=0.00166667, D=0.005, B=0.01.**

Throughout you should discuss the meaning and accuracy of your results in terms of the physics, initial conditions, boundary conditions, numerical methods, and modelling assumptions. You should consider whether your results are converged in both space and time, and therefore the validity of your conclusions. You may wish to explore differing mesh densities for each layer, and you should explain how you represent the layers in your code.

1. Run your code for the following initial conditions and Dirichlet boundary conditions, for a maximum of 30 seconds:

   $$c(x,0) = 0, \qquad c(x = B, t) = 0, \qquad c_{DOSE}(x = 0, t) = 30$$

   Plot the concentration distribution through the tissue for a range of time-points between 0-30 seconds and discuss the results.

2. Use your code to determine the minimum effective dose, $c_{DOSE}$ at $x=0$ that will have the desired pharmaceutical effect. This is modelled by evaluating the integral in Eq. 5, **at *x=D***, with effectiveness defined to occur when K>1000:

   $$\mathrm{K} = \int_{t_{eff}}^{t=30} c\, dt \qquad \text{Eq. 5}$$

   Integrate between the time points, $t_{eff}$, (at which the concentration $c$ becomes greater than 40), and t=30. Note that the MATLAB function, `trapz(x)`, assumes an interval of 1, therefore multiply the output by timestep, **Δ**t, to obtain the final value of the integral.

Explain how you used your code, and any other calculations, to estimate this value. Include any data or figures that you feel are relevant to demonstrate your approach to estimating this.

3. Investigate and discuss the influence and suitability of the stated boundary conditions (at both boundaries). For example, what is the influence of setting a zero Neumann condition at $x=B$. Explain which conditions you believe are most suitable and why.

4. Explore the sensitivity of the effective delivered dose (as indicated by K), to diffusion coefficient, $D$, extra-vascular diffusivity, $\beta$, and degradation rate, $\gamma$. Which is the most relevant for controlling this aspect of the drug delivery?

| Parameter | Effect | Epidermis | Dermis | Sub-cutaneous |
|---|---|---|---|---|
| D | Diffusion coefficient | 4e-06 | 5e-06 | 2e-06 |
| beta | Extra-vascular diffusivity | 0 | 0.01 | 0.01 |
| gamma | Drug degradation rate | 0.02 | 0.02 | 0.02 |

**Table 1: Parameter values for Part 2. Note that some are realistic and others are not, having been altered to allow you to solve your model in a reasonable time frame.**

## Presentation Quality [5%]

In addition to the marks for the technical work, marks will also be given based on the quality of presentation of the work, including the following criteria:

- Clear graphical presentation of equations, text, diagrams, and plots
- Standard of written English
- Proper use of references, figure numbering & captions, and table headings
- Clear, logical layout of report

## SUBMISSION GUIDELINES

You may structure your report as a set of answers to these questions – there is no requirement to write this in a lab report format. You do not need to re-explain the entirety of the finite element method, however, your report must be self-contained and therefore must not assume that the reader knows the content in this document, i.e., you should explain what problem you are solving and what each result is.

- **You must** include all your MATLAB source code as **text** in the Appendices such that it could be pasted back into MATLAB and executed. Failure to do this will cause you to lose marks i.e.
  - **Do not** paste your code into the document as an OLE item or as an image.
  - **Do not** upload archived/zipped/compressed folders of these source files.
- **Do not** use MATLAB's symbolic algebra toolbox – you will lose marks.
- Word limit of **3000** words (not including source code).
- Both PDF and MS Word file formats are acceptable, but PDF is recommended.
- You are reminded of the university's policies regarding academic plagiarism: your code and your report must be your own work.
- You are reminded that submitting the output of GenAI software as your own work would also constitute academic plagiarism.

Submit your work via the online submission link on the unit Moodle page.

**Deadline: 4pm on Friday, 8th December 2023.**