UNIVERSITY *of* LIMERICK
OLLSCOIL LUIMNIGH

Faculty of Science & Engineering
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END OF SEMESTER ASSESSMENT PAPER

MODULE CODE: MS4408

SEMESTER: Spring 2012-13

MODULE TITLE: Mathematical modelling

DURATION OF EXAMINATION: 2 hrs 30 mins

LECTURER: Prof. S.O'Brien

PERCENTAGE OF TOTAL MARKS: 90%

EXTERNAL EXAMINER: Prof. T. Myers

INSTRUCTIONS TO CANDIDATES: Full marks for **5** questions. Number each question carefully **in the margin provided on your script**.

There are some useful results at the end of the paper.

1 **Porous flow**

(a) Sketch a typical aquifer (underground porous rock) showing the ground-water zone, the water table and a well. 2 %

(b) Consider two dimensional dam seepage as in figure 1.

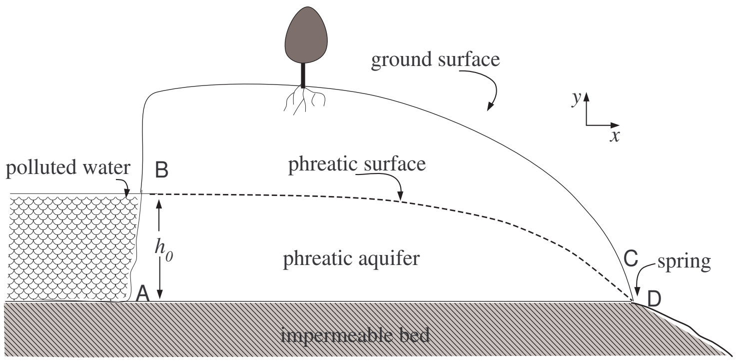

Figure 1: Geometry of the dam seepage problem.

(i) Use conservation of mass to derive the the following conservation law

$$\frac{\partial}{\partial t}(\rho\phi) + \nabla \cdot (\rho \mathbf{u}) = 0,$$

where $\phi, \rho, \mathbf{u}$ are the porosity, liquid density and velocity respectively.

Use Darcy's law

$$u = -\frac{k}{\mu}p_x,\ v = -\frac{k}{\mu}(p_y + \rho g)$$

to obtain:

$$\frac{\partial}{\partial t}(\rho\phi) = \nabla. \left[\frac{k}{\mu}\rho\nabla p\right].$$

If ρ, ϕ, k are constant, deduce that the pressure must satisfy Laplace's equation:

$$\nabla^2 p = 0.$$

8 %

(ii) The full mathematical formulation of the dam seepage problem is:

$$u = -\frac{k}{\mu}p_x,\; v = -\frac{k}{\mu}(p_y + \rho g),$$
$$u_x + v_y = 0,$$

with boundary conditions

$$v = 0 \text{ on } y = 0,$$

$$p = 0,\; v = \phi h_t + u h_x \text{ on } y = h(x,t),$$
$$p = \rho g(h_0 - y) \text{ on } x = 0,$$
$$p = 0 \text{ on } x = l.$$

Explain carefully the significance of each element of this model. Non-dimensionalise this model using the scales:

$$x \sim l,\; y \sim h_0,\; p \sim \rho g h_0,\; u \sim k\rho g h_0/\mu l,$$

$$v \sim k\rho g/\mu,\; t \sim \phi h_0 \mu/k\rho g\delta^2,\; \delta \equiv h_0/l \ll 1,$$

to obtain the scaled version:

$$p_y = -1 \text{ on } y = 0,$$

$$p = 0,\; \delta^2 h_t = -(p_y + 1) + \delta^2 p_x h_x \text{ on } y = h(x,t),$$
$$p = 1 - y \text{ on } x = 0,$$
$$p = 0 \text{ on } x = 1.$$

Using the fact that $\delta \ll 1$, show that the pressure field is given by:

$$p \approx h(x,t) - y$$

and that

$$h_t = (hh_x)_x, h(x = 0,t) = 0, h(x = 1,t) = 0.$$

Deduce the free surface shape in the steady state situation where $h = h(x)$. Show that h has infinite slope at $x = 1$ and comment on this fact. 8 %

2 **Advection-diffusion of a chemical**

In order to test the transport properties of a particular allergy medicine in an artificial capillary, the transport of the soluble chemical along the tube is examined. A water based solvent flows with uniform constant velocity $v = 10^{-3}$ m s^{-1} along a thin tube of length $L = 10^{-2}$ m. At $t^* = 0$ the concentration is zero. At $t^* > 0$, chemical is introduced at the two ends of the tube in such a way that the boundary conditions are $c^*(x^* = 0, t^*) = c_0$, a known concentration, and at $x^* = L$ the total flux (Q) is zero, where $c^*(x^*, t^*)$ is the chemical concentration. Assuming the chemical advects and diffuses (with diffusion constant $D = 10^{-9}$ m^2 s^{-1}),

(a) show that conservation of chemical leads to the equation:

$$c^*_{t^*} + Q_x = 0; \quad Q(x^*) \equiv -Dc^*_{x^*} + vc^*.$$

Write down the boundary and initial conditions. 5 %

(b) Non-dimensionalise the problem (including the boundary and initial conditions) using an advection time-scale (L/v) to obtain the form:

$$c_t + c_x = \varepsilon c_{xx}; \quad c(x, 0) = 0; \; c(0, t) = 1; \; \varepsilon c_x(1, t) = c(1, t).$$

Show that the Peclet number is related to ε, that it is large, and comment on the significance of this. Contrast the diffusive and advective time-scales. 4 %

(c) For $\varepsilon = 0$, using the method of characteristics or otherwise, show that the solution is $c(x, t) = H(t - x)$ or $1 - H(x - t)$, where $H(\cdot)$ is the Heaviside step function (defined at the end of the paper).

How does one reconcile this approximate solution with the (approximate) boundary condition $c(x = 1, t) = 0$? 5 %

(d) Find either the *exact steady state* solution, or an approximate asymptotic steady solution based on $\varepsilon \ll 1$, governed by $\varepsilon \frac{d^2c}{dx^2} = \frac{dc}{dx}$ and satisfying both boundary conditions. 4 %

3 **Active transport from kidney tissues**

Kidney tissues transport dissolved salts into a bathing fluid which has a higher salt concentration. It is believed that this occurs via active transport into a portion of long thin channels in the kidney tissue and advection-diffusion along the channels of length L into the bathing fluid. The active transport is assumed to take place at a constant rate only along a portion of the channel ($0 \leq x^* \leq \delta$). Water also enters the tube via osmosis.

(a) Explain the terms *active transport, semi-permeable membrane, osmosis* in the context of this problem. Explain why diffusion is not the dominant mechanism by which the transport of solute takes place? 3 %

(b) Write down equations for conservation of fluid and salt, and show that the following model applies in the steady state:

$$\begin{aligned} \frac{d[u^*(x^*)c^*(x^*)]}{dx^*} &= D\frac{d^2c^*(x^*)}{dx^{*2}} + \frac{2}{r}N^*(x^*) \\ \frac{du^*(x^*)}{dx^*} &= P\frac{2}{r}(c^*(x^*) - c_0), \end{aligned}$$

assuming that the solute advects and diffuses along the channel. Here P, r, D, c_0 are the wall permeability, channel radius, solute diffusivity constant, ambient solute concentration in the bathing fluid. u^*, c^* are the fluid velocity and solute concentration. You may assume that the active transport function is defined by $N^* = N_0,\ 0 \leq x^* \leq \delta;\ N^* = 0,\ \delta < x^* \leq L.$ 6 %

(c) Explain the significance of the following boundary conditions:

$$u^*(x^* = 0) = 0,\ \frac{dc^*}{dx^*}(x^* = 0) = 0,\ c^*(x^* = L) = c_0,$$
u^*, c^* continuous at $x^* = \delta$.

2 %

(d) Scale the problem using the following scheme:

$$\begin{aligned} c^*(x^*) &= c_0 + c(x)C_s, \\ u^*(x^*) &= u(x)V_s, \\ x^* &= xL, \\ N^*(x^*) &= N_0N(x), \end{aligned}$$

choosing C_s and V_s suitably and show that the problem can be written in the following dimensionless form:

$$\begin{aligned} \frac{d(u(1+\varepsilon c))}{dx} &= \frac{\varepsilon}{Pe}\frac{d^2c}{dx^2} + N(x) \\ \frac{du}{dx} &= c, \end{aligned}$$

where $Pe \equiv \frac{V_s L}{D} \equiv \frac{2N_0 L^2}{Drc_0}$, $\varepsilon \equiv C_s/c_0 \ll 1$ with boundary conditions:

$$u(x=0)=0,\ \frac{dc}{dx}(x=0)=0,\ c(x=1)=0.$$

(i) Find a leading order solution assuming that the region of active transport is $0 \le x \le \gamma$ with $\gamma = O(1)$.

(ii) Demonstrate that the leading order solutions contain a corner. Outline how you would resolve this corner by inserting interior layers. 7 %

4 **Dimensional analysis, similarity solutions**

Consider the heat flow problem on $0 \le x^* < \infty, t^* \ge 0$:

$$\kappa u^*_{x^*x^*} = u^*_{t^*},\ u^*(0,t^*) = u_0,\ u^*(\infty,t^*) = 0,\ u^*(x^*,0) = 0,\ x^* > 0.$$

The parameters in the problem are u_0, κ (m^2 s^{-1}).

(a) Show that the Buckingham Pi theorem suggests the existence of two dimensionless quantities and deduce these.

(b) Using an artificial parameter L, scale as follows: $x^* = xL,\ t^* = tL^2/\kappa,\ u^* = u_0$, to obtain the dimensionless problem:

$$u_{xx} = u_t,\ u(0,t) = 1,\ u(\infty,t) = 0,\ u(x,0) = 0,\ x > 0.$$

(c) Explain why a similarity solution is expected. Using the similarity variables $u = f(\eta),\ \eta = xt^{-1/2}$, show that the problem reduces to the ordinary differential equation problem:

$$-\frac{1}{2}\eta\frac{df}{d\eta} = \frac{d^2f}{d\eta^2},\ f(\eta = 0) = 1,\ f(\eta = \infty) = 0.$$

(d) Solve the problem to obtain the solution:

$$f(\eta) = 1 - \frac{2}{\sqrt{\pi}}\int_0^{\eta/2} e^{-s^2}ds.$$

5 Dimensional analysis, projectile problem

A ball is thrown vertically into the air and drops back to earth under gravity. The mathematical problem is:

$$\frac{d^2x^*}{dt^{*2}} + k\frac{dx^*}{dt^*} = -\frac{gR^2}{(x^*+R)^2},\ x^*(0) = 0,\ \frac{dx^*}{dt^*}(0) = V,$$

where the parameters are an air resistance parameter k, ($[k] = s^{-1}$), acceleration due to gravity, $g(\approx 10$ m s$^{-2})$, the radius of the earth R ($\approx 6\times10^6$ m), the initial velocity V ($= 10$ m s^{-1}) and the variables are $x^*(\mathrm{m}),\ t^*(\mathrm{s})$.

(a) Use the Buckingham Pi theorem to show that the problem is governed by an equation of the form:

$$F(\Pi_1, \Pi_2, \Pi_3, \Pi_4) = 0.$$

3 %

(b) Non-dimensionalise the problem (including the boundary conditions) via $x^* = yR, t^* = \tau R/V$ and show that 2 dimensionless parameters appear, $\varepsilon \equiv \frac{V^2}{gR}$ and an air resistance parameter β.
Estimate the size of ε and explain why this is not a good scaling of the problem. 4 %

(c) Non-dimensionalise the problem using the length and time scales $x^* = xV^2/g, t^* = tV/g$ and explain which balances this entails. Show that this reduces the problem to:

$$\frac{d^2x}{dt^2} + \beta\frac{dx}{dt} = -\frac{1}{(1+\varepsilon x)^2},\ x(0) = 0,\ \frac{dx}{dt}(0) = 1.$$

3 %

(d) Assuming that $\beta \equiv 0$ and that $\varepsilon \ll 1$, find a two term approximation for $x(t)$. 5 %

(e) If $\beta = 1, \varepsilon \ll 1$, find the leading order solution. 3 %

6 Michaelis-Menten and chemical kinetics

Consider the following mathematical model for the consumption of an organic substance by a bacterial cell

$$s^* + e^* \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} c^* \overset{k_2}{\rightarrow} p^* + e^*$$

where at $t^* = 0, s^* = \bar{s}, e^* = \bar{e}, c^* = 0, p^* = 0$. Here $s^*(t^*)$ is the concentration of organic molecules, $e^*(t^*)$ is the concentration of unoccupied receptors, $c^*(t^*)$ is the concentration of occupied receptors and $p^*(t^*)$ is the concentration of captured organic molecules. It is assumed that molecular receptors, embedded in the bacterial cell membrane, are responsible for capturing the organic molecules and either releasing them into the interior of the cell or dumping them outside the cell.

(a) Draw a sketch of the mechanism described above and explain the assumptions you will make in modelling the problem as a system of ODEs. 2 %

(b) Write down a system of 4 ODEs (and initial conditions) modelling this system. Hence deduce that:

$$e^*(t^*) + c^*(t^*) = \bar{e};\ s^*(t^*) + c^*(t^*) + p^*(t^*) = \bar{s}.$$

Explain why the problem reduces to solving a system of two ODEs:

$$\begin{aligned}
\frac{ds^*}{dt^*} &= -k_1\bar{e}s^* + (k_1 s^* + k_{-1})c^*, \\
\frac{dc^*}{dt^*} &= k_1\bar{e}s^* - (k_1 s^* + k_{-1} + k_2)c^*, \\
s^*(0) &= \bar{s}, c^*(0) = 0.
\end{aligned}$$

5 %

(c) Show that $e^* + c^* =$ constant is obvious for this problem. 1 %

(d) Using the scaling $s^* = s\bar{s},\ c^* = c\bar{e},\ t^* = t/(k_1\bar{e})$, derive the system in the scaled form:

$$\begin{aligned}
\dot{s} &= -s + (s + \kappa - \lambda)c,\ \kappa = \frac{k_{-1} + k_2}{k_1\bar{s}},\ \lambda = \frac{k_2}{k_1\bar{s}}, \\
\varepsilon\dot{c} &= s - (s + \kappa)c,\ \varepsilon \equiv \frac{\bar{e}}{\bar{s}}, \\
s(0) &= 1, c(0) = 0.
\end{aligned}$$

Assuming $\varepsilon \ll 1$, consider the outer problem at leading order (i.e., solve the problem with $\varepsilon = 0$) and show that $c(t) = s/(s+\kappa)$ and $s(t)$ satisfies:

$$\dot{s} = \frac{-\lambda s}{s+\kappa}. \tag{1}$$

Find $s(t)$ and explain carefully what is meant by the quasi-steady hypothesis in the context of matched asymptotics. Explain carefully why the initial conditions are not appropriate for this approximation.

Sketch the right hand side of equation (1) as a function of s and discuss in the context of saturation kinetics. 6 %

(e) By rescaling the time t appropriately write down the inner equations, valid for small times, and find a leading order small time approximation. Match this with the outer solution. 4 %

7 Stefan problems

(a) Define *latent heat, sensible heat*? If heat is being removed at a constant rate from a well mixed finite volume of a liquid, sketch the temperature/time profile in the region of its freezing point, illustrating the change of phase from liquid to solid. 2 %

(b) A mass of water, initially in $0 \leq x < \infty$, is freezing such that at a later time the solid/liquid phase boundary is at $x = s(t)$ with the solid in $0 < x < s(t)$. Derive the Stefan boundary condition describing the motion of the phase boundary:

$$\rho\lambda\frac{ds}{dt} = \left[-k\frac{\partial u}{\partial x}\right]_{solid}^{liquid}$$

in the usual notation where λ is the latent heat of fusion of the solid phase. 3 %

(c) A mass of ice, at its melting temperature of $0°$, initially located in $0 \leq x^* < \infty$ has its left hand boundary $x^* = 0$ in contact with warm water so that its temperature is raised to $u_m = 5°$ at $t^* = 0$. The subsequently moving liquid/solid phase boundary is located at $x^* = s^*(t),\ s^*(0) = 0$. Assume that the temperature in the solid phase remains identically at zero temperature for all time. If heat flows via diffusion in the liquid phase so the Fourier heat law and a diffusion equation hold:

$$q^*(x^*, t^*) = -k\frac{\partial u^*}{\partial x^*};\ \frac{\partial u^*}{\partial t^*} = \kappa\frac{\partial^2 u*}{\partial x^{*2}};\ \kappa \equiv \frac{k}{\rho c},$$

where k, ρ, c, κ are the thermal conductivity, density, specific heat capacity and thermal diffusivity of liquid respectively, formulate a mathematical model (equations and all boundary conditions) for the melting problem. 3 %

(d) Using the scales:

$$u^* = uu_m; x^* = xL; t^* = tL^2/\kappa; s^* = sL$$

where L is an artificial length scale, show that the problem can be written in the dimensionless form:

$$u_t = u_{xx}\ , 0 < x < s(t),\ u(0,t) = 1; u(x = s(t), t) = 0,$$
$$-\frac{\partial u}{\partial x}(x = s(t), t) = \mathrm{S}\frac{ds}{dt},\ s(0) = 0$$

where $\mathrm{S} = \lambda/(cu_m)$ is the Stefan number. 3 %

(e) If S $\gg 1$ use a rescaling of the time $t = \mathrm{S}\tau$ to show that the motion of the free boundary is given approximately by:

$$s(\tau) = \sqrt{2\tau}.$$

3 %

(f) If $S = O(1)$, indicate briefly how you might find an exact solution exploiting the absence of a length scale in the problem. 2 %

(g) Find an approximate solution of the transcendental equation

$$\gamma e^{\gamma^2} = 1/\varepsilon, \;\; \varepsilon \ll 1.$$

2 %

8 Answer any **two** of the following:

(a) Use dimensional analysis (and similar triangles) to prove Pythagoras' theorem. You may assume the area of a right angled triangle is a function of the length of the hypotenuse and the smallest angle. 9 %

(b) Heat is diffusing through a volume of stationary water. The heat energy density at any point is given by $E(\mathbf{x}, t)$, the flux density vector by $\mathbf{q}(\mathbf{x}, t)$. For an arbitrary fixed volume V of the water, use the divergence theorem (Green's theorem) to show that conservation of energy leads to

$$\frac{\partial E}{\partial t} + \nabla \cdot \mathbf{q} = 0.$$

Assuming that heat diffuses via Fick's law $\mathbf{q} = -k\nabla u$, where k is the heat conductivity constant, u is the temperature, show that the transport of heat is governed by the diffusion equation:

$$\frac{\partial u}{\partial t} = \kappa \nabla^2 u, \ \kappa \equiv k/(\rho c).$$

You may assume that $E = \rho c u$ where ρ is the water density and c is the specific heat capacity.

To what does this reduce in the one dimensional steady case when $u = u(x)$? 9 %

(c) A model linear problem with a similar structure to the problem in question three is

$$\varepsilon c_{xx} - c_x = -H(1-x), \ c(0) = 0, \ c_x(2) = 0, \ \varepsilon \ll 1, \ 0 < x < 2,$$

where $H(\cdot)$ is the Heaviside step function as defined at the end of the paper (i.e., $-H(1-x) = -1, \ 0 \le x < 1; = 0, \ 1 < x \le 2$).

(i) Show that the leading order solution ($\varepsilon = 0$) is

$$\begin{aligned} c(x) &= x, \ 0 \le x \le 1 \\ &= 1, \ 1 < x \le 2. \end{aligned}$$

Sketch this solution and demonstrate the existence of a corner.

(ii) To smooth this corner, the asymptotic solution consists of a left outer, left interior layer, right interior layer and right outer solution. Use the rescaling $x = 1 + \varepsilon \bar{x}$, $c(x) = \bar{c}(\bar{x})$ to demonstrate the appropriate scaled equation in each region. Solve these equations, satisfying the boundary conditions. Explain how the asymptotic matching would proceed (but it is **not** necessary to carry out this matching). 9 %

(d) Find the exact solution of the problem in part (c) (for $0 \leq x < 1$ and $1 < x \leq 2$) and complete the solution by requiring continuity of $c(x)$ and dc/dx at $x = 1$. 9 %

(e) A chemical reaction proceeds as follows:

$$\begin{array}{ccc} & k_1 & k_2 \\ A \rightarrow & B \rightarrow & C, \end{array}$$

where $k_2 \gg k_1$ and the initial concentrations $a(0) = a_0, b(0) = b_0, c(0) = c_0$ are assumed to be $O(1)$.

Write down a system of differential equations representing this sequence. Non-dimensionalise the problem, define a small parameter $k_1/k_2 \equiv \varepsilon \ll 1$ and hence obtain an approximate solution of the problem. 9 %

Useful results

$$\begin{aligned}
\nabla &\equiv (\frac{\partial}{\partial x},\frac{\partial}{\partial y},\frac{\partial}{\partial z});\quad \nabla T \equiv (\frac{\partial T}{\partial x},\frac{\partial T}{\partial y},\frac{\partial T}{\partial z}), T = T(x,y,z,t).\\
\nabla\cdot\mathbf{u} &\equiv \frac{\partial u_1}{\partial x}+\frac{\partial u_2}{\partial y}+\frac{\partial u_3}{\partial z}, \mathbf{u}=\mathbf{u}(x,y,z,t) = (u_1(x,y,z,t),u_2(x,y,z,t),u_3(x,y,z,t)).\\
\nabla^2 &\equiv \nabla\cdot\nabla \equiv \frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2};\quad \nabla^2 T \equiv \frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 T}{\partial y^2}+\frac{\partial^2 T}{\partial z^2}, T = T(x,y,z,t).\\
\iiint_S \mathbf{q}\cdot d\mathbf{S} &= \iiint_V \nabla\cdot\mathbf{q}\, dV (\text{Divergence Theorem}).\\
\sin x &= x - x^3/3! + x^5/5! + O(x^7).
\end{aligned}$$

Heaviside step function

$$\begin{aligned}
H(x) &= 0,\ x<0,\\
&= 1,\ x>0.
\end{aligned}$$

Leibniz' rule

$$\frac{dI}{dt} \equiv \frac{d}{dt}\int_{\alpha(t)}^{\beta(t)} f(x,t)dx = \int_{\alpha(t)}^{\beta(t)} \frac{\partial f(x,t)}{\partial t}dx - f(\alpha,t)\frac{d\alpha}{dt} + f(\beta,t)\frac{d\beta}{dt}.$$