UNIVERSITY *of* LIMERICK
OLLSCOIL LUIMNIGH

Faculty of Science & Engineering
Department of Mathematics and Statistics

END OF SEMESTER ASSESSMENT PAPER

MODULE CODE: MS4408

SEMESTER: Spring 2007-08

MODULE TITLE: Mathematical modelling

DURATION OF EXAMINATION: 2 hrs 30 mins

LECTURER: Prof. S.O'Brien

PERCENTAGE OF TOTAL MARKS: 90%

EXTERNAL EXAMINER: Prof. J.R. King

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

1 (a) Heat is flowing through a conducting body. The energy density (energy per unit volume) is given by $E(\mathbf{x}, t)$, the heat flux vector by $\mathbf{q}(\mathbf{x}, t)$ and the temperature by $T(\mathbf{x}, t)$. For an arbitrary fixed volume V in the body, use the divergence theorem (Green's theorem) to show that conservation of energy leads to

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

If the energy density is given by $E = \rho c T$, and Fourier's law $\mathbf{q} = -k\nabla T$ applies, where ρ, c, k are constants representing the density, the specific heat capacity and the thermal conductivity, show that the transport of heat is governed by the diffusion equation:

$$\frac{\partial T}{\partial t} = \frac{k}{\rho c}\nabla^2 T.$$

9 %

(b) In the one dimensional case, where $k = k(x)$ is not a constant and $T = T(x, t), q = q(x, t)$ are scalar quantities, show that the one dimensional diffusion of heat reduces to solving an equation of the form $\rho c u_t = \frac{\partial}{\partial x}(k \frac{\partial T}{\partial x})$.

A thin bar ($0 < x < 1$) of heat conducting material is in a **steady state** with the boundary conditions $T(x = 0, t) = T_0,\ T(x = 1, t) = T_1$. **Formulate** and solve the mathematical problem for the steady state temperature if the thermal conductivity is given by $k = \exp(ax)$ where $ax \ll 1, 0 \leq x \leq 1$.

Obtain an approximation to the temperature distribution by using the smallness of a and compare the exact and approximate solutions. 9 %

2 Consider the projectile problem

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

where the parameters are acceleration due to gravity, $g(\approx\ 10\text{ms}^{-2})$, the radius of the earth $R(\approx 6 \times 10^6\text{m})$, the initial velocity $V(= 10\text{ms}^{-1})$ and the variables are $x^*(\text{m}),\ t^*(\text{s})$.

(a) Non-dimensionalise the problem (including the boundary conditions) via $x^* = yR, t^* = \tau R/V$ and show that a dimensionless parameter $\varepsilon \equiv \frac{V^2}{gR}$ arises. Estimate the size of ε and explain why this is not a good scaling of the problem. 5 %

(b) 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:

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

6 %

(c) Use the fact that $\varepsilon \ll 1$ to show that at leading order $x(t) \sim t - t^2/2$. 5 %

(d) How large does V have to be so that the approximate model fails? 2 %

3 (a) Explain what is meant by stable, unstable and neutral equilibrium. In the context of a mathematical system with solution $\mathbf{u}(x, y, z, t)$ and equilibrium solution $\mathbf{u}_s(x, y, z)$, give a precise mathematical definition of asymptotic and neutral stability. 6 %

(b) Consider the dimensionless pendulum problem:

$$\frac{d^2\theta}{dt^2} + 3\frac{d\theta}{dt} + 2\sin\theta = 0.$$

Show that $\theta_s = 0$ is an equilibrium solution. By writing the ODE as a system of two first order ODEs, or otherwise, show that θ_s is asymptotically stable.

Comment on the stability of the other equilibrium point. 6 %

(c) Show that the ODE:

$$\frac{du}{dt} = u(1-u)$$

has one stable and one unstable equilibrium point.

How would you expect solutions to evolve from the initial conditions $u(0) = 0.001, u(0) = 1.001$? 6 %

4 Consider the enzyme catalysis reaction

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

where at $t^* = 0, s^* = \bar{s}, e^* = \bar{e}, c^* = 0, p^* = 0$.

(a) 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:

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

6 %

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

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

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:

$$\dot{s} = \frac{-\lambda s}{s + \kappa}, s(0) = 1.$$

Explain carefully what is meant by the quasi-steady hypothesis and why it is appropriate for this problem. 8 %

(c) By rescaling the time t appropriately, write down the inner equations, valid for small times. 4 %

5 (a) A semi-infinite block of ice $0 \le x < \infty$ is melting with the ice/water boundary given by $x = s(t)$. Derive the Stefan boundary condition describing the motion of the phase boundary:

$$\rho\lambda\frac{ds}{dt} = \left[-k\frac{\partial u}{\partial x}\right]_{ice}^{water} \qquad (1)$$

in the usual notation where λ is the latent heat of fusion of ice. 5 %

(b) A large (semi-infinite) mass of ice ($0 \le x^* < \infty$) has its left hand boundary $x^* = 0$ raised to $u_m = 20^0$ at $t^* = 0$. The moving water/ice interface is located at $x^* = s^*(t),\ s^*(0) = 0$. **Assume that the temperature in the ice remains identically at zero temperature for all**

time. Assuming that heat flows via diffusion in the water 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 water respectively, formulate a mathematical model (equations and all boundary conditions) for the melting problem. 4 %

(c) 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:

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

where $\mathrm{St} = \lambda/(cu_m)$ is the Stefan number. 4 %

(d) If $\mathrm{St} \gg 1$, explain why a quasi-steady approximation of the diffusion equation is appropriate. Using a rescaling of the time $t = \mathrm{St}\,\tau$, or otherwise, show that the motion of the free boundary is given approximately by:

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

5 %

6 Consider the mechanism by which tissues in the body transport solute (e.g. a salt) into a bathing fluid (water) which has a higher solute concentration. The accepted mechanism is via active transport into a portion of long thin channels in the secreting tissue and advection-diffusion along the channels of length L into the bathing fluid. The active transport is assumed to take place only along a portion of the channel ($0 \le x^* \le \delta$). Water enters the tube via osmosis.

(a) Explain what is meant by active transport and osmosis in the context of this problem. Why cannot diffusion be the dominant mechanism by which the transport of solute takes place? 4 %

(b) Derive the following equations for the conservation of fluid and solute mass in a channel:

$$\frac{dv^*}{dx^*} = Pca^{-1}(C^* - C_0),$$
$$cN^*(x^*) - a\frac{dF^*}{dx^*} = 0,$$
$$F^* = v^*C^* - D\frac{dC^*}{dx^*},$$
$$v^*C^* - D\frac{dC^*}{dx^*} = \begin{cases} a^{-1}cN_0x^* & \text{for } 0 \le x^* \le \delta, \\ a^{-1}cN_0\delta & \text{for } \delta < x^* \le L. \end{cases}$$

assuming that the solute advects and diffuses along the channel. Here P, c, a, D, C_0 are the wall permeability, channel circumference, channel cross section, solute diffusivity constant, ambient solute concentration in the bathing fluid. v^*, C^*, F^* are the fluid velocity, solute concentration and solute flux along the channel. You may assume that $N^* = N_0,\ 0 \le x^* \le \delta;\ N^* = 0,\ \delta < x^* \le L.$ 7 %

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

$$v^*(x^* = 0) = 0,\ \frac{dC^*}{dx^*}(x^* = 0) = 0,\ C^*(x^* = L) = C_0,$$
$$v^*, C^* \text{ continuous at } x^* = \delta.$$

3 %

(d) A dimensionless formulation of the problem is:

$$C - 1 = \nu\frac{dv}{dx},\ \ \nu\kappa^2 vC - \lambda^2\frac{dC}{dx} = \nu\kappa^2\begin{pmatrix} x \\ 1 \end{pmatrix}$$
$$v(0) = 0,\ C(x = \lambda) = 1, C, v \text{ continuous at } x = 1.$$
$$0 < \nu \ll 1,\ \kappa, \lambda = O(1).$$

Expand the equations and boundary conditions (but do NOT solve them) as far as $O(\nu)$ using the perturbation expansions $v = v_0 + \nu v_1,\ C = C_0 + \nu C_1$ and write down the full mathematical problem (equations and boundary conditions) at each order. 4 %

7 Answer any **three** of the following:

(a) Find a similarity solution of the Stefan (melting ice problem):

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

where St is the dimensionless Stefan number. (Hint: take the similarity variable as $\eta = x/(2\sqrt{t})$ and let $u = f(\eta),\ s = 2\gamma\sqrt{t}$, γ a constant to reduce to the ODE problem: $f''(\eta) + 2\eta f'(\eta) = 0$).

(b) Consider the case where a river flowing with velocity $\mathbf{u}(x, y, z, t)$, measured in m s^{-1}, contains a pollutant with concentration $c(x, y, z, t)$ (Kg m^{-3}) which is diffusing and advecting. Starting from the conservation law $c_t + \nabla \cdot \mathbf{q} = 0$, assuming Fick's law of diffusion for the diffusive flux: $\mathbf{q} = -D\nabla c$, D constant, and that the flow is incompressible ($\nabla \cdot \mathbf{u} = \mathbf{0}$), show that the transport of pollutant is modelled by the advection-diffusion equation

$$c_t + \mathbf{u} \cdot \nabla c = D\nabla^2 c.$$

In the special one dimensional case where, $c = c(x, t), u \equiv U$ (constant), and assuming the existence of suitable length, time and concentration scales $L, L^2/D, C_0$, non-dimensionalise the equation and show that a Peclet number occurs. (You may use the vector identity: $\nabla \cdot (\mathbf{u}c) \equiv c\nabla \cdot \mathbf{u} + \mathbf{u} \cdot \nabla c$).

(c) With regard to cooking a piece of spherical homogeneous meat, assume that the relevant dimensional quantities are t(s), L(m) and κ(m^{2}s^{-1}), time for cooking, the radius and the thermal diffusivity. Show that dimensional analysis suggests that there is precisely one dimensionless Π. Deduce that $t \propto$ weight$^{2/3}$. How would this change for a thin flat circular piece of meat?

(d) Consider the problem of the two dimensional flow of an incompressible liquid past a circular cylinder of radius a, where the fluid velocity field $\mathbf{u}(x, y, t)$ is assumed known. The advection-diffusion dimensional model is:

$$\rho c(\frac{\partial T^*}{\partial t^*} + \mathbf{u}^* \cdot \nabla^* T^*) = k\nabla^{*2} T^*,\ T^*(x, y, 0) = T_0,$$
$$T^* \to T_\infty \text{ as } x^{*2} + y^{*2} \to \infty,\ T^* = T_0 \text{ on } x^{*2} + y^{*2} = a^2$$

where $T^*(x^*, y^*, t)$ is the temperature. Non dimensionalise this problem (equation and boundary conditions) assuming that U is a given known velocity scale and show that the dimensionless problem contains a dimensionless Peclet number

$$Pe = \frac{\rho c U a}{k} = \frac{Ua}{\kappa},\ \kappa = \frac{k}{\rho c}$$

Explain the physical significance of the Peclet number and explain how the problem can be approximated if Pe $\ll 1$ or Pe $\gg 1$. In particular, if Pe $\gg 1$, explain why eventually the temperature must be everywhere equal (approximately) to its upstream value. Comment on the temperature field near the cylinder in this case.

(e) A thin film of liquid (of thickness $h(x,t)$) on the underside of a ceiling is modelled by the dimensionless equation:

$$h_t = -\alpha \frac{\partial}{\partial x}(h^3 h_x) - \beta \frac{\partial}{\partial x}(h^3 h_{xxx}),\ h_0(x,t) = 1,$$

where $\alpha \equiv 1$ models gravity effects and $\beta = \frac{\gamma}{\rho g L^2} > 0$ models surface tension. Show that $h = 1$ is an equilibrium solution of this equation. If the ceiling is infinite in extent, use a linear stability analysis $h = 1 + \varepsilon \hat{h}(x,t) = 1 + \varepsilon \exp(st)\exp(ikx),\ \varepsilon \ll 1$ to demonstrate that the equilibrium state is unstable. Find the cut-off wave number k_c i.e., find the range of unstable values of $k \in [0, k_c]$.

(f) Using the equations in question 5, write down a mathematical model for the consumption of an organic substance by a bacterial cell. Assume 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. Define all quantities carefully and explain under what circumstances the steady state hypothesis is appropriate for this process.

$3\times 6\%$