Math 486/522 - Homework 3

Fall 2024 **Len Washington III**

1. In class (Lecture 5), we considered a simplified drug path diffusion model. Let $u(x,t)$ (M/L in 1 space dim.) be the concentration of a drug at depth x from the surface of the skin at time t. We found that u satisfies the diffusion equation problem

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2}, \quad x > 0, \quad t > 0$$
$$\text{IC: } u(x,0) = 0, \quad \text{BC: } u(0,t) = u_0, \quad u(\infty,t) = 0.$$

Using the similarity variable $\eta = \frac{x}{\sqrt{Dt}}$, we converted the PDE to an ODE and derived the solution

$$u(x,t) = u_0 \text{erfc}\left(x/2\sqrt{Dt}\right), \quad \text{erfc}(y) = 1 - \frac{2}{\sqrt{\pi}}\int_0^y e^{-r^2}dr. \tag{1}$$

If $u_0 = 10$ and $D = 1/4$ then

(a) Make a graph of $u(2,t)$, i.e. at depth $x = 2$, from $t = 0$ to $t = 100$. Does this make sense? Problem 1a answer here.

(b) Find the first time t when the concentration at depth $x = 2$ is equal to 4. Problem 1b answer here.

(c) On the same set of axes, plot $u(x,t)$ from $x = 0$ to $x = 10$ for the sequence of times $t = 1, 5, 10, 50$. Please label each graph with its appropriate time t. Problem 1c answer here.

2. Consider a drug delivery system in which the drug is delivered with a constant flow or flux $J = -D\frac{\partial u}{\partial x}$ at the surface of the skin, $x = 0$. You can think of it as a drug pump at $x = 0$. We assume $u(x,t)$ (M/L in 1 space dim.) is the concentration satisfying a chemical diffusion problem with a constant flow or flux at the boundary $x = 0$:

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2}, \quad x > 0, \quad t > 0$$
$$\text{IC: } u(x,0) = 0, \quad \text{BC: } D\frac{\partial u}{\partial x}(0,t) = -A, \quad u(\infty,t) = 0.$$

(a) What are the dimensions of D and A? Problem 2a answer here.

(b) Use dimensional reduction to derive a form of $u(x,t)$. Is there a similarity variable, if so call it η. Be sure your similarity variable vanishes at $x = 0$ so $\eta = 0$. Problem 2b answer here.

(c) Use the class notes to transform the diffusion problem into an ODE-BVP. Verify that the boundary conditions are consistent with the IC and BC of the diffusion problem. Problem 2c answer here.

3. A more realistic model of the drug patch has the drug diffusing in the skin with diffusion coefficient D but also degrading according to a first order chemical reaction with rate constant k, lookup a first chemical reaction online. The chemical concentration of the drug is $u(x,t)$ (M/L) in the skin and the patch at $x=0$ provides a concentration $u(0,t) = Ae^{-kt}$. $k>0$, also decaying in time. The PDE problem for the concentration u of the drug is:

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2} - ku, \quad x>0, \quad t>0 \tag{2}$$

$$\text{IC: } u(x,0) = 0 \tag{3}$$

$$\text{BC: } u(0,t) = Ae^{-kt}, \quad u(\infty,t) = 0. \tag{4}$$

(a) Describe the meaning of each term on the right side of equation (2). Problem 3a answer here.

(b) If the concentration is independent of x, i.e. a simple first order chemical reaction, state and solve the ODE for kinetics of the reaction assuming as initial concentration of A. You can look for a solution of (2) that only depends on t. Problem 3b answer here.

(c) Suppose the boundary condition at $x=0$ in (4) is changed to $u(0,t)=A$. Use (2) to find an equation for the long-time or steady-state concentration, i.e. $U(x) = \lim_{t\to\infty} u(x,t)$, i.e. independnt of t. Find $U(x)$. Problem 3c answer here.

(d) In the original problem (2)-(4), find the dimensions of A, D and k. Problem 3d answer here.

(e) Use dimensional analysis to identify three dimensionless quantities that involve the variables and parameters in the problem. Problem 3e answer here.

4. ODE review. Please review Dawkin's ODE notes, if needed. Classify and solve:

(a) Find the general solution $y(t) : \frac{dy}{dt} = 2t - y$. Problem 4a answer here.

(b) Solve the initial value problem $y(t) : \frac{dy}{dt} - 2ty = 2$, $y(0) = 0$ and write your solution in terms of the error function: $\text{erf}(t) = \frac{2}{\sqrt{\pi}}\int_0^t e^{-z^2}dz$. Problem 4b answer here.

(c) Find the general solution $y(t)$ to:

(i) $y'' - 4y = 0$ Problem 4c(i) answer here.

(ii) $y'' + 5y' + 6y = 0$ Problem 4c(ii) answer here.