## 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

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

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

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

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 tp 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 drup 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:

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

- (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  $\eta$ . 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:

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

IC: 
$$u(x,0) = 0$$
 (3)

BC: 
$$u(0,t) = Ae^{-kt}, \quad u(\infty,t) = 0.$$
 (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:  $\operatorname{erf}(t) = \frac{2}{\sqrt{\pi}} \int_0^t e^{-z^2} dz$ . 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.