3450:436/536 Mathematical Models, Kreider, Spring 2014

Homework Set 1

Due date: Monday 27 January

Type your responses to the extent possible. If necessary, leave blank space in the document to write equations by hand.

1. (25 pts) Consider a 2D rectangular domain that contains a concentration C of some chemical. The concentration outside the domain is C_{bulk}. The *transport boundary condition*, given by

$$-D\frac{\partial C}{\partial n} = K(C - C_{bulk})$$

describes the transport of the chemical into (if $C_{bulk} > C$) or out of (if $C_{bulk} < C$) the domain. The normal derivative $\dfrac{\partial C}{\partial n}$ points out of the domain. You've seen this before as Newton's Law of Cooling, which is also known as Fick's Law.

(a) Use dimensional analysis to identify the units on the mass diffusivity D and the mass transfer coefficient K given that each side of the equation has units of flux (area density per time, or [mol]/[L^2]/[T]). To use the standard concentration units [mol]/[L^3], we typically presume the 2D domain is the side of a volume that has thickness 1, and that whatever quantities we consider in that domain are uniform through the thickness.

(b) For the right side of the domain, the normal is in the $+x$ direction, so that $\dfrac{\partial C}{\partial n} = \dfrac{\partial C}{\partial x}$. Identify the specific form of the normal derivatve for the other 3 sides.

(c) Suppose that $C > C_{bulk}$, so that the chemical is leaking out of the domain. Write an argument that justifies the minus sign on the left. Look at the sign of each quantity to show that the left and right sides of the equation have the same sign. Pick one side of the domain to analyze. This is a writing assignment, so focus on making the argument clear and concise.

2. (15 pts) In class, we derived the chemical reactor equation $\beta c' = \beta(1 - c) - c$, where we scaled concentration C by C_{in} and time by V/q. The initial condition is $c(0) = \gamma = C_0/C_{in}$. Consider the case where β is large. Provide a physical explanation of what this means, solve the ODE and write the solution in dimensional form. Draw a qualitative sketch of the solution (by hand is fine) for the cases $C_0 > C_{in}$ and $C_0 < C_{in}$.

3. (15 pts) Consider the dimensional chemical reactor equation $\dfrac{dC}{dt} = \dfrac{q}{V}(C_{in} - C) - kC$. Nondimensionalize this equation by scaling concentration by C_{in} and time by $1/k$. Use the symbol δ for the nondimensional grouping.

4. (15 pts) Consider the chemical reactor equation with the reaction rate changed to $r(C) = RC^2$ instead of $r(C) = kC$. Nondimensionalize the equation by scaling concentration by C_{in} and time by V/q. Show that the parameter grouping you get is dimensionless. Solve the ODE.