Chemistry 545
Spring 2004
Problem Set 3
Due Wednesday, February 25

Reading assignment: Finish reading through Section 8.1

1. Do problem 5.2 Note that in part (b) there is a typographical error: The left hand side of each of the equations is a *time derivative* of the deviation from equilibrium. You should feel free to use Mathematica to solve part (d).

2. Use Mathematica to solve the differential equations in the previous problem.

A. Use the four sets of rate constants given in the table in Problem 5.3 to solve for X, Y, and Z, with A held constant. Assume initial conditions X[0] = 340, Y[0] = 50, and take A = 800. Let t range from 0 to 20. Plot your results for X vs t, Y vs t, and Y vs X. For the last plot you should use ParametricPlot. Do your results make sense, in light of problem 5.2(d)?

B. Add another reaction

$$Z \rightarrow \text{products},$$

with rate constant k_4. Solve the differential equations, with $k_1 = 0.003$, $k_2 = 0.0045$, $k_3 = 0.85$, $k_{1m} = 0.0$, $k_{2m} = 0.0$, $k_{3m} = 0.0$, $k_4 = 1$. Prepare the same plots for this set as in the previous part.

C. Treat A[t] as a variable, with A[0]=800, and modify the last reaction to give $Z \rightarrow A$. You may think of this last reactions as foxes becoming fertilizer for the cabbage. Solve the differential equations, using all the rate constants of part B, and prepare the same plots.

3. In class we claimed that the function $n(x,t) = (4pDt)^{-1/2} e^{-x^2/4Dt}$ satisfies the one-dimensional diffusion equation.

A. Show that n(x,t) does indeed satisfy the one-dimensional diffusion equation.

B. Demonstrate that n(x,t) is normalized. That is, $\int_{-\infty}^{\infty} n(x,t)dx = 1$.

C. Show that $\langle x^2 \rangle = 2Dt$.

4. A. Assuming a fixed value for D and t, write down an expression (in integral form) for the probability that a particle diffuses a distance less than or equal to x_0 in either direction. In other words, what is the probability $p(x_0)$ that $-x_0 \le x \le x_0$ after a time t?

B. Next, write a Mathematica program to calculate $p(x_0)$ for D = 10 and t = 5. Plot your results for $0 \le x_0 < 50$. (I did it with two lines of code – actually just one line after the DD = 10 and t = 5.)

5. In the autocatalysis problem we found that the product concentration has the general form $B(t) = \dfrac{C}{a + be^{-lt}}$. Derive a general expression for the inflection point in terms of the constants in the problem.