Mass diffusion

I. READING

This week you should read

- Chapter 5.

II. PROBLEMS

1. Write a short MATLAB (or python or whatever) program to simulate the 1D random walk of a set of particles. Locate 10,000 particles at the origin $x = 0$. At each time step move the particles a distance proportional to a normally distributed random number (use the `randn` command). Use the MATLAB vector notation to keep this simple. For example to update the particle position at each time step you can simply do `x = x + dt*randn(size(x));` where dt is a time step size that doesn't matter - just a scaling factor. Use the `hist` command to plot the distribution of particles. Compare the result to the analytical solution based on the diffusion equation which is
$$c(x,t) = \frac{C}{\sqrt{4\pi Dt}} \exp\left(-\frac{x^2}{4Dt}\right)$$
where $C = \int_{-\infty}^{\infty} c(x,t)dx$ is the total amount of stuff. While a one to one comparison is possible, you can just confirm the result qualitatively. If your program is more than a few lines long, see me for some MATLAB help.

2. Write a short MATLAB (or whatever) program to simulate a 2D random walk of a set of particles. Locate 10,000 particles at he origin, $x = 0, y = 0$. Take the same procedure above for stepping the x and y coordinate. Step the two dimensions separately, i.e. a random step in x and y. At each time step compute the total distance each particle has traveled from the origin $r = \sqrt{x^2 + y^2}$. Plot the average distance from origin as a function of time and confirm that $r_{ave} \sim \sqrt{t}$.

3. These are estimates to get a sense for some orders of magnitude.
   - The diffusivity of dissolved oxygen in blood is about $2 \times 10^{-9}\mathrm{m}^2/\mathrm{s}$. How long does it take oxygen to diffuse over a distance of 5 microns (the scale of capillaries) ? 1 micron (the barrier between oxygen and blood in the lungs)?
   - Typical diffusion constants for sugar in water are $5 \times 10^{-10}\mathrm{m}^2/\mathrm{s}$. How long would it take for diffusion to mix sugar in a cup of water.
   - Typical diffusion constants for acetone in air are around $1.2 \times 10^{-5}\mathrm{m}^2/\mathrm{s}$. How long would it take you to smell a bottle after opening if there were only molecular diffusion.

4. Imagine a 1D problem where a stationary fluid is bounded by two walls seperated by a distance L. On the left wall, there is a chemical reaction at the wall that produces chemical i at a rate of J $\mathrm{mol}/(\mathrm{s}\cdot\mathrm{m}^2)$. On the right there is a chemical reaction that consumes chemical species i. The diffusivity of the chemical species in the fluid is $\mathcal{D}$. At steady state the consumption rate must equal the production rate. At steady state, what is the difference in concentration across the two walls in terms of the parameters provided?

5. The solution to the problem presented in section 5.3 was given as
$$c(x,t) = \frac{1}{2} + \sum_{n=1}^{\infty} \frac{2\sin\left(\frac{n\pi}{2}\right)}{n\pi} \mathrm{e}^{-n^2\pi^2 t} \cos(n\pi x).$$
This solution was used to generate Figure 5.6. Simply plot the solution and see that you can recreate something that looks like 5.6.

6. A 1D box is uniformly filled with a trace chemical species to initial concentration, c_0. The width of the box is L. The diffusivity is $\mathcal{D}$. The boundary condition is such that there is a chemical reaction at both ends that consumes the species so quickly that the concentration at the walls is effectively 0 for $t > 0$. Over time, the reaction will consume all the chemical in the box - though it takes time as the chemical originally near the center takes time to diffuse to wall in order to be consumed.

- How would you estimate how long it takes for the reaction to consume the contents of the box?
- State the problem, in 1D, mathematically in dimensionless terms. See section 5.3 for guidance. State the equation, initial condition, and boundary conditions.
- Follow the procedure in section 5.3.3 to solve the equation for these new boundary conditions. Show that the solution has a form $c(x,t) = \mathrm{e}^{\lambda^2 t} f(\lambda x)$. For these boundary conditions, the function f turns out to be either sine or cosine, which is it? What is the value of λ that satisfies the boundary condition?
- See if you can follow 5.3.3 and figure out the whole solution? It will have a form similar to that in the book, only the details and constants will be all different. Note that in the section where the integral properties of cosine are presented - those relations also hold for sine. If you can't figure this out, don't spend too much time - but give an honest effort. The only way you will know if you are correct is if you try to plot the solution at select instances in time.