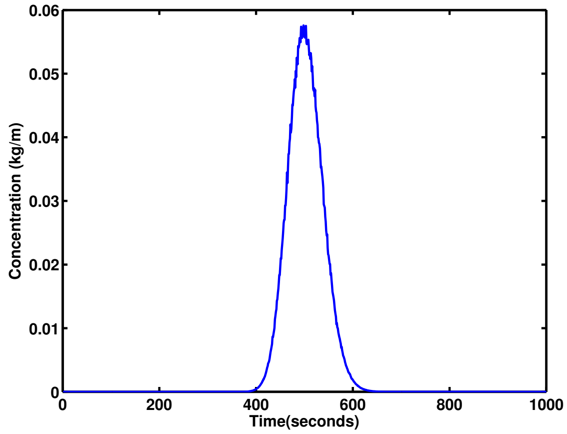

Figure 1: Breakthrough Curve for Problem 1

Problem 1. Steady State Advection Dispersion Reaction

Part 1 You are provided with the following breakthough curve in a stream where you have injected $1kg$ of a conservative solute. The breakthrough curve is measured 100 m downstream of the injection location. To download the data for this curve go to the course webpage and download 'Data for HW4' at the bottom of the page.
Next you conduct an experiment where, at the same injection site, you continually inject a reactive solute in such a way as to maintain the concentration at the injection location as 1kg/m (in one dimensional terms) and run the system until it reaches a steady state. You measure that the concentration of the reactive tracer at $x = 100$ is $0.1kg/m$ (in one dimensional terms). You know that the solute degrades with a first order rate coefficient.

From the information provided here, estimate what this degradation rate is.

Now that you know this degradation rate calculate what the concentration at $x = 100$m would have been if only dispersion occurred, and likewise if only advection occurred.

From your estimates here could you have neglected either advection or dispersion in your calculation. If so, explain why; if not, also explain why.

Part 2 With all the parameters that you have estimated above, consider the following problem. Instead of running a steady state experiment you now run a pulse injection of $1kg$ of the reactive solute and measure the breakthrough curve at $x = 100$. Calculate and plot what will it look like. Also plot the breakthrough curve for a conservative tracer to compare the two.

Problem 2. Instantaneous Reactions

Part 1 Consider the following case. You have an infinite domain. At time zero there is a unit pulse of Copper Sulfate located at $x = -10$ and another unit pulse of EDTA located at $x = 10$. Copper Sulfate and EDTA react together to form Copper-EDTA and the reaction happens so quickly that it can be considered to occur instantaneously. All solutes in this system move simply by diffusion and have a diffusion coefficient $D = 2$.

Write the governing equations with initial conditions for how the concentration of EDTA, Copper Sulfate and Copper EDTA will evolve in this system. Now calculate the concentration distribution of the product CopperEDTA at times t =1, 10, 100, 1000 and 10000. Also calculate the total mass of Copper EDTA produce ($M(t) = \int_{-\infty}^{\infty} C(x, t,)dx$) and plot $M(t)$ against time for each of the times mentioned above.
Note that you may have a hard time doing this entirely analytically (i.e. finding the minimum concentrations) and so you may have to do it by brute force in Matlab by plotting concentrations of conserved species and finding the minima with the computer). You may have to calculate the integral for the total mass numerically too, although you can avoid this if you think carefully about it.

Part 2 Now consider the exact same setup as above except that there is a mean background flow of velocity $v = 10$. Perform the same analysis as above and highlight any differences or similarities and explain why these similarities or differences exist.

Part 3 What happens if the dispersion coefficient is increased to $D = 4$?

Part 4 Finally, discuss what would happen if your domain was finite and had no flux boundaries $\frac{\partial C}{\partial x} = 0$ at $x = -20$ and $x = 20$.