

Figure 1: Breakthrough Curve for Problem 1

Problem 1. Advection Dispersion and Moments

This problem is actually based on a real problem I worked on as a consultant and you have all the same information I was given to make these estimates - so good luck consulting!

Part 1 - You are provided with the breakthrough curve shown in figure 1, which was obtained from a contaminant spill that occured. The data is available for download from the course webpage and has been emailed to you. It consists of concentration measurements every second over a period of 22500 seconds. You know that the measurement station is located 1000 meters downstream from the spill site and can assume it was a a pulse of mass M that was released. Unfortunately you are unsure of how much mass was released, but know it was in the range of $1 - 25$ kg.

Assuming that transport can be described with a one dimension ADE, can you use this data to estimate the velocity and dispersion, v and D , in the stream as well as the total mass M that was released (note you have three unknowns, which is one more than we had in the sample problem in class so you will need more than the first two temporal moments, namely the first three, if that is the method you choose to use - note if you can figure out another way that is fine by me).

In particular you are concerned about this concentration reaching a downstream village located 10 km from the spill site, where the contaminant may pose a threat if the concentration arriving there is greater than 0.1 kg/m. Based on your estimates of M , v and D will it exceed this in the village at any time?

Part 2 - A geophysicist has also provided you with spatial moments of the plume (the zeroth, first and second one - normalized appropriately), but they are much less confident in the measurements as they are a good bit noisier. They are shown in figure 2 and also available for download. If you interpret these to calculate v and D are the results consistent with what you got from Part 1(take M as what you obtained from part 1)? Try to be clever in estimating these as noise could particularly make estimating D difficult. If the results are not consistent, what values do you get and what would the maximum concentration arriving at the village 10 km downstream be in this situation?

Figure 2: Spatial Moments for Problem 1

Figure 3: Geometry and Velocity Profile for Problem 2

Problem 2. Taylor Dispersion Between Two Parallel Walls - Poiseuille Flow

Laminar pressure driven flow between two parallel walls is well known to follow the following governing equation (see figure 3 for geometry and velocity profile)

$$
v(y) = \frac{3}{2}\overline{v}\left(1 - \frac{y^2}{h^2}\right) \qquad -h < y < h \tag{1}
$$

where \bar{v} is the average velocity in the channel of width 2h with its bottom boundary at $y = -h$ and top boundary at $y = h$ (i.e. its center at $y = 0$). The average here is defined as

$$
\overline{v} = \frac{1}{2h} \int_{-h}^{h} v(y) dy \qquad -h < y < h \tag{2}
$$

and the advection diffusion equation in 2d in this case is given by

$$
\frac{\partial C(x,y,t)}{\partial t} + v(y)\frac{\partial C(x,y,t)}{\partial x} = D\frac{\partial^2 C(x,y,t)}{\partial x^2} + D\frac{\partial^2 C(x,y,t)}{\partial y^2}
$$
(3)

Follow Taylor's example and decompose concentration into $C(x, y, t) = \overline{C}(x, t) + C'(x, y, t)$. Exactly as we did in class for the radial case write an equation for the average concentration (slide 7 from class ppt) and one for the perturbation concentration(slide 8 from class ppt).

Then, using the same assumptions as Taylor did discard terms in the perturbation equation (slide 10) as unimportant and solve the resulting differential equation for $C'(x, y, t)$. Put this solution back into the equation for $\overline{C}(x,t)$ (in the term looks like $v'(y)C'$ and calculate the effective Taylor dispersion coefficient for this case. Note that to solve the problem you will likely have to use the boundary condition $\frac{\partial C}{\partial y} = 0$ at $y = \pm h$ (i.e. no flux boundaries).

Once you can crack this problem you will be able to do it for absolutely any parallel flow (e.g. streams etc.).

Problem 3. Random Walks With Advection and Taylor Dispersion Between Two Parallel Walls

Write a random walk code corresponding to the flow in problem 2. Set $h = 1$ and $\overline{v} = 1$ and set $D = 0.01$. What is the characteristic time scale for this after which you expect Taylor dispersion to kick in? The Langevin equation for the particle positions will be

$$
x(t + \Delta t) = x(t) + v(y)\Delta t + \sqrt{2D\Delta t}\xi
$$

$$
x(t + \Delta t) = x(t) + \frac{3}{2}\left(1 - y(t)^2\right)\Delta t + \sqrt{2D\Delta t}\xi
$$
(4)

$$
y(t + \Delta t) = y(t) + \sqrt{2D\Delta t}\eta
$$
\n(5)

Note that the velocity of the particle depends on its y position - i.e. $3/2/(1-y^2)$ (hence the two equivalent expressions in (4)), information you must use to solve this problem. Use the same method as you did for the last homework to reflect particles back into the domain to impose to no flux boundary at the lower and upper edges.

Now set the initial condition as all particles uniformly distributed in the y direction (i.e. $x = \text{zeros}(1, N)$ and $y = \text{linspace}(-1, 1, N)$ where N is the number of particles you use - start with $10⁴$) and let the system evolve in time at least up to 10 times the Taylor dispersion time scale, if not more.

During each timestep calculate the spatial moments of the plume. To do this, the first and second moments in terms of particle positions are given by

$$
m_1(t) = \frac{1}{N} \sum_{i=1}^{N} x_i(t) \qquad m_2(t) = \frac{1}{N} \sum_{i=1}^{N} x_i^2(t) \tag{6}
$$

Now measure the dispersion coefficient from these (using perhaps the second centered moment; recall $m2 - m1^2 = 2Dt$). Make sure to measure after the Taylor time scale and check if you indeed get the same dispersion coefficient as what you calculated in problem 2.