Fate & Transport of Chemicals in the Environment

Homework #9 University of South Florida
Due Monday, April 18, 2022 Prof J A Cunningham

For all of the problems on this assignment, consider a long river that has a depth of 0.5 m, a width of 2.0 m, and a volumetric flow rate $Q = 2.5\ \mathrm{m^3/min}$. (From that information, you should be able to calculate the average velocity in the river pretty easily.)

1. (25 pts) A new factory has just started its operation and has just started discharching its waste into the river. The factory's operating permit indicates that it will discharge Chemical Z into the river at an estimated rate of 100 kg/d. Chemical Z does not volatilize into the air, does not adsorb or partition into the sediment of the river, and does not undergo any appreciable chemical reactions in the river.

    a. Assume that the dispersion coefficient for Chemical Z in the river is $D = 60\ \mathrm{m^2/min}$. Make a graph that shows the concentration of Chemical Z in the river as a function of the distance downstream from the factory. Let's use the symbol x to denote downstream distance, and we'll consider $x = 0$ to be the location of the factory discharge pipe. On your graph, draw the concentration profiles you'd expect to see after 1 day, 2 days, and 3 days of factory operation and discharge. Put all three profiles on the same graph. Use km for the units on x and use mg/L for the units on concentration. Make your graph for the stretch of river that extends 16 km downstream of the factory. Label your graph "Problem 1a".

       Hint: use Excel, Matlab, or something similar. I like Matlab, but I think it is do-able in Excel.

    b. Re-draw the graphs from part (a) if the dispersion coefficient for Chemical Z in the river is $300\ \mathrm{m^2/min}$ instead of $60\ \mathrm{m^2/min}$. Label your graph "Problem 1b". Briefly discuss how your graphs changed and why.

    c. A popular fishing spot is located 20 km downstream of the factory. Draw a graph of the concentration of Chemical Z at the fishing spot, as a function of time. Use days for the units of time, and use mg/L as the units of concentration. Use the higher value of dispersion coefficient, i.e., assume $D = 300\ \mathrm{m^2/min}$. Make your graph for the first 10 days of the factory's operation. Label your graph "Problem 1c".

    d. For the scenario described in part (c), let's assume that if/when the concentration of Chemical Z exceeds 20 mg/L, the fish will either start to die or else will look for a new place to live. Based on your graph, once the factory goes on-line, how long can we still fish at our favorite fishing spot?

2. (25 pts) Let's consider a different scenario. Instead of thinking about a factory, let's assume that a truck overturns while driving along the river, and 50 kg of Chemical Z very rapidly spill out of the truck into the river. We'll use x to denote the position in the river downstream of the spill location, so $x = 0$ indicates the point on the river where the chemical was spilled. For this problem, assume that the dispersion coefficient for Chemical Z in the river is $D = 60\ \text{m}^2/\text{min}$ (the smaller of the values from problem 1).

   a. On a single graph, plot the spatial concentration distribution (C vs x) at $t_1 = 500$ min and at $t_2 = 2000$ min. On your graph, make the range of the x-axis go from $x = 0$ to $x = 8000$ m. Use units of g/m^3 for C. Label your graph "Problem 2a".

   b. For both t_1 and t_2, determine the peak concentration, C_{max}, and the value of x where it occurs, $\bar{x}$. How does the value of C_{max} at t_2 compare to the value at t_1? Does that seem to agree with your graph from part (a)?

   c. What about $\bar{x}$? – how does the value of $\bar{x}$ compare at the two times, and does that agree with your graph?

   Let's define plume width as that section of the river where the chemical concentration is at least 1% of it's maximum value, i.e., where $C \geq 0.01\ C_{\text{max}}$.

   d. Estimate/calculate the plume width at both t_1 and t_2. How does the value at t_2 compare to the value at t_1? Does that seem to agree with your graph from part (a)?

   e. Summarize the results from parts (a)–(d). How does the elapsed time affect the peak concentration, C_{max}? How does elapsed time affect the x location of the peak? the spread, $(\Delta x)_{\text{plume}}$, i.e., the range of x over which $C \geq 0.01\ C_{\text{max}}$?

   Now consider the same truck spill, but imagine that you are monitoring the concentration of Chemical Z at the location $x = 5000$ m, i.e., 5 km downstream of where the spill occurred.

   f. Graph the concentration of Chemical Z versus time (C vs t) for the location $x = 5000$ m. Make the time axis go from 0 to 4000 min (which is between 2 and 3 days). Label your graph "Problem 2f".

3. (30 pts) Let’s consider a different scenario. A chemical pipeline that runs along the river suddenly developed a leak, and it started leaking Chemical Z into the river. Luckily, the pipeline is instrumented properly – when the leak developed, the pressure in the pipeline dropped, and that triggered an alarm. The pipeline owner was able to pretty quickly find the leak and shut down that section of the pipeline until it could be repaired properly. Nevertheless, it is estimated that Chemical Z was leaking into the river at a rate of about 10 kg/hr for a period of about 5 hours. We will call $t = 0$ the midpoint of this leaky period, i.e., the leak occurred from $t = -2.5$ hr $= -150$ min until $t = +2.5$ hr $= +150$ min. For this problem, assume the dispersion coefficient $D = 60$ m^2/min, the same as in problem 2.

    a. Plot the tracer’s spatial concentration distribution (C vs x) at $t_1 = 500$ min and at $t_2 = 2000$ min. On your graph, make the range of the x-axis go from $x = 0$ to $x = 8000$ m. Use units of g/m^3 for C. Label your graph “Problem 3a”.

    b. Compare the results of problem 3(a) to the results of problem 2(a). You can “eyeball” it, or you can try to more quantitatively estimate things like peak height and plume spread, perhaps using your graphs. Does the form of the chemical addition (instantaneous versus finite-duration) appear to make a difference once we have reached $t = 500$ min? what about when we have reached 2000 min?

    Imagine that you are monitoring the concentration of Chemical Z at the location $x = 5000$ m, i.e., 5 km downstream of where the leak occurred.

    c. Graph concentration of Chemical Z versus time (C vs t) for the location $x = 5000$ m. Make the time axis go from 0 min to 4000 min (even though, technically speaking, the equation is only valid for $t > 150$ min). Label your graph “Problem 3c”. Compare the graph to that from problem 2(f). Are they pretty similar? Pretty different? Somewhere in between?

    d. Now make a new graph on which you plot C vs x for both types of chemical addition (infinitesimal and short finite) at $t = 300$ min. Let x go from 0 to 2000 m. Label your graph “Problem 3d”. For the case of the leaky pipepline, that is just a little while after the leak is repaired. At this short time, can you discern the differences between the two types of mass addition?

    e. Based on your observations from parts b through d, discuss briefly the effect of the pulse form (infinitesimal vs. short finite) on the distribution of Chemical Z in the river, focusing on the effect of elapsed time.

4. (20 pts) Let’s go back to the truck spill from problem 2. Now, however, assume that Chemical Z undergoes first-order degradation after it is spilled into the river. All other conditions are the same as in problem 2. The rate coefficient for the degradation is $k = 0.001$ min^{-1}.

   a. Again plot the chemical’s spatial concentration distribution at $t_1 = 500$ min and at $t_2 = 2000$ min. For comparison, include both the non-reactive case and the degradable case on this graph (so you will have four pulses on the graph in total). Indicate clearly which curves are for the non-reactive case and which are for the degradable case. Label your graph “Problem 4a”.

   b. Compare the degradable case to the non-reacting case: how does degradation affect the *peak concentration* of Chemical Z? What about the plume width, i.e., the spread of the concentration distribution?

   c. For the degradable case, what fraction of the original spilled mass remains after 500 min? What about after 2000 min?

   Imagine that you are monitoring the concentration of Chemical Z at the location $x = 5000$ m, i.e., 5 km downstream of where the spill occurred.

   d. Graph the concentration of Chemical Z versus time (C vs t) for the location $x = 5000$ m. Make the time axis go from 0 to 4000 min (which is between 2 and 3 days). Label your graph “Problem 4d”. Compare the results to those from problem 2(f). What is the same in the two cases? What is different? Explain why.