Homework assignment for Environmental Fate and Transport
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Consider a small drainage ditch with cross sectional area $A = 0.5$ m^2 and length $L = 15$ m. The ditch is full of clean still water. At time $t = 0$, a farmer spills mass $M = 30$ mg of a toxic salt into the ditch. The salt washes in uniformly across one end of the ditch. The isotropic, homogeneous turbulent diffusion constant within the ditch is $D = 0.002$ m^2/s. Assume that the salt is conservative and too dilute to change the density of the water within the ditch, and also that it results in biological impairment in concentrations above 0.01 mg/L = 10 mg/m^3. An endangered salamander has been observed to lay eggs in the ditch, and a local environmental group asks you to evaluate the potential harm of the spill. Because you want to be very sure of your answer, you decide to tackle the problem in two completely different ways and then compare your predictions to each other.

A)   (i) What will be the concentration of salt in the ditch after it fully mixes and is diluted by the entire volume of the ditch? Will there be a danger to eggs at this point?
        (ii) When do you expect that the ditch will fully mix?
        (iii) Write an analytical expression for the concentration distribution within the ditch before the salt fully mixes within it. Include at least two image sources in your answer to account for no-flux boundaries at either end of the ditch.
        (iv) When do you expect that interaction with the near end of the ditch will start to affect the concentration distribution?
        (v) When do you expect that interaction with the far end of the ditch will start to affect the concentration distribution?

B) The integral form of the conservation of mass equation for a control volume with fixed volume is:

$$V \frac{dC}{dt} = \sum \dot{m}_{in} - \sum \dot{m}_{out} \pm S$$

where V is the volume of the control volume, C is concentration, t is time, $\dot{m}_{in}$ is mass fluxes into the control volume, $\dot{m}_{out}$ is mass fluxes out of the control volume, and S indicates sources and sinks. Apply the conservation of mass equation to the ditch by breaking up the domain into ten boxes, each with length $\Delta x = 1.5$ m, and using the above equation to write an expression for the rate of change of the concentration of salt, $\frac{dC}{dt}$, in:
        (i) each box in the middle of the ditch
        (ii) the box adjacent to the near end of the ditch
        (iii) the box adjacent to the far end of the ditch

C) The differential form of the conservation of mass equation in a system with a first-order reaction is:

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} + v \frac{\partial C}{\partial y} + w \frac{\partial C}{\partial z} = D \left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2} \right) - kC$$

where D is the homogeneous and isotropic diffusivity, k is the first-order removal constant, and u, v, and w indicate velocities in the directions x, y, and z, respectively. Starting from this equation, show how you can obtain the same equations that you wrote above for the rate of change in concentration for each box.

D) USE EXCEL OR MATLAB and the equations that you wrote for the rate of change in salt concentration dC/dt in Parts B and C to create a <u>numerical model</u> that predicts how the concentration within each of the ten boxes will change over time. In addition, calculate the total amount of mass within the ditch during each timestep. Make your timestep Δt small enough to obtain smooth concentration distributions.

E) Add three sections (e.g., groups of columns) to your spreadsheet that show the expected concentration along the ditch during each timestep as predicted by your <u>analytical expression</u> in Part A:
      (i) not accounting for the no-flux boundary at $x = L$.
      (ii) only including image source(s) that account for the no-flux boundary at $x = L$.
      (iii) the expected concentration within the ditch [= the sum of (i) and (ii)].
In addition, calculate the total amount of mass within the ditch during each timestep.

F) Plot the concentration distribution $C(x)$ within the ditch from your numerical integration (Part D) at the x position corresponding to the middle of each box. On the same graphs, plot the real portion of your analytical solution [Part E(i)], the image portion of your analytical solution [Part E(ii)], and your full analytical solution [Part E(iii)]. In total, each plot should have 4 data series. Make your plots at the following times, and use them to answer the following questions:

      (i) $t = 30$ min. Your numerical and full analytical solutions should match. Do they?

      (ii) At the time calculated in Part A at which you expect that the boundary at $x = L$ starts to affect the concentration distribution. How does the presence of the image source that accounts for the boundary at $x = L$ affect the predicted distribution at this time?

      (iii) At the time when you would have lost 1% of system mass across the boundary at $x = L$ if you had not used an image source in your analytical expression. (You'll need to find this time from looking at your spreadsheets.) How does this time compare to the touch time you calculated in Part A?

      (iv) At the time when the ditch is expected to be fully mixed as calculated above in Part A. Compare the total amount of mass accounted for by the analytical solution with the amount that was originally released. What fraction has been lost? How could the analytical solution be modified to address this problem of missing mass?

      (v) At the time when the ditch is actually fully mixed to a precision of 0.1 mg/m³. (You'll need to find this time from looking at your spreadsheets.) How does this time compare to the mixing time you calculated in Part A? Compare the total amount of mass accounted for by the analytical solution with the amount that was originally released. What fraction has been lost?

G) Use your spreadsheets and plots to determine regions of potential salamander egg destruction within the ditch. If the eggs need to be exposed to the toxic contaminant for a certain duration of time (for example, at least 30 minutes, or at least 24 hours), how would your estimates change? How realistic are these estimates for the ditch? How would you recommend that the potential exposure problem be mitigated or addressed?