

Homework assignment for Environmental Fate and Transport
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Solutions

A) (i) After the salt fully mixes throughout the ditch, the salt concentration distribution within the ditch will be uniform. The concentration after it fully mixes will be:

$$C(x,t) = \frac{M}{V} = \frac{M}{AL} = \frac{30 \text{ mg}}{(0.5 \text{ m}^2)(15 \text{ m})} = 4 \text{ mg} / \text{m}^3 \quad (t > T_{\text{mix}})$$

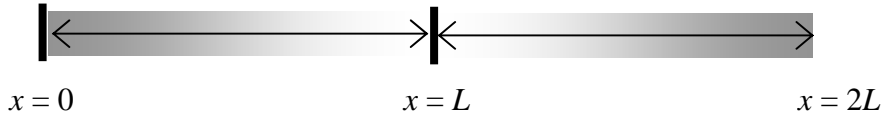
This is less than the concentration that causes biological harm.

(ii) The ditch is expected to fully mix after the mixing timescale $T_{\text{mix}} = L^2/D = 112,500 \text{ s} = 31 \text{ hr}$.

(iii) Because the salt was released across the entire end of the ditch, it will be fully mixed in the cross section at all times. This system is therefore 1-D with diffusion occurring over length only. The solution for how the concentration distribution will evolve within a 1-D system is:

$$C(x,t) = \frac{M}{A\sqrt{4\pi Dt}} \exp\left(-\frac{(x - x_{\text{c.o.m.}})^2}{4Dt}\right)$$

Here, the solution must be adjusted to account for the no-flux boundaries located at $x = 0$ and $x = L$. To account for the boundary at $x = 0$, we add an image source co-located with the real source at $x = 0$. To account for the boundary at $x = L$, we add an image source that is at the mirror image across the boundary, so located at $x = 2L$.



Because the real source and the co-located image source at $x = 0$ will spread to touch the boundary at $x = L$ at the same time, there actually must be two image sources co-located at $x = 2L$. The final equation for diffusion within the ditch until it fully mixes is:

$$C(x,t) = \frac{2M}{A\sqrt{4\pi Dt}} \exp\left(-\frac{x^2}{4Dt}\right) + \frac{2M}{A\sqrt{4\pi Dt}} \exp\left(-\frac{(x - 2L)^2}{4Dt}\right) \quad (t < T_{\text{mix}})$$

(iv) The no-flux boundary at $x = 0$ will be important at all times, since it constrains the concentration distribution and affects the total amount of mass within the ditch as soon as the salt enters. Therefore, the image source co-located with the real source is important from the introduction of the salt up until the ditch fully mixes.

(v) The no-flux boundary at $x = L$ will start to affect the concentration distribution when the salt cloud spreads to touch the far wall. This will be at a time $T_{\text{touch}} = L^2/8D = 14,000 \text{ s} = 3.9 \text{ hr}$. For times between T_{touch} and T_{mix} , the image sources at $x = 2L$ will be important in calculating the concentration distribution.

B) (i) The integral form of the conservation of mass equation states that (for a conservative tracer) the change in mass within each box equals the difference between the rate of transport in and the rate of transport out. Here, the only transport mechanism is diffusion. Therefore, for box j in the middle of the ditch,

$$\frac{\Delta M_j}{\Delta t} = V \frac{\Delta C_j}{\Delta t} = \underbrace{-DA \frac{C_j - C_{j-1}}{\Delta x}}_{\text{In from the left}} + \underbrace{DA \frac{C_{j+1} - C_j}{\Delta x}}_{\text{Out to the right}} = DA \left[\frac{(C_{j+1} - C_j)}{\Delta x} - \frac{(C_j - C_{j-1})}{\Delta x} \right]$$

where $V = A\Delta x$ is the (constant) volume of each box and C_j represents the concentration in the j th box. Dividing through by the volume of each box, we obtain an expression for how the concentration will change over time within each box in the middle of the ditch.

$$\frac{\Delta C_j}{\Delta t} = \frac{D}{\Delta x} \left[\frac{(C_{j+1} - C_j)}{\Delta x} - \frac{(C_j - C_{j-1})}{\Delta x} \right] = \frac{D}{(\Delta x)^2} (C_{j+1} - 2C_j + C_{j-1})$$

(ii) Because the ditch ends are no-flux boundaries, the boxes on each end (box 1 and box 10) will only exhibit transport in one direction, and will not lose or gain mass from outside of the domain. The concentration in the first box (the box adjacent to the near end) will evolve as follows:

$$\frac{\Delta C_1}{\Delta t} = \frac{D}{\Delta x} \left[\frac{(C_2 - C_1)}{\Delta x} \right] = \frac{D}{(\Delta x)^2} (C_2 - C_1)$$

(iii) Similarly, in the box adjacent to the far end:

$$\frac{\Delta C_{10}}{\Delta t} = \frac{D}{\Delta x} \left[-\frac{(C_{10} - C_9)}{\Delta x} \right] = -\frac{D}{(\Delta x)^2} (C_{10} - C_9)$$

C) The full differential form of the conservation of mass equation is:

$$\underbrace{\frac{\partial C}{\partial t}}_A + \underbrace{u \frac{\partial C}{\partial x}}_B + \underbrace{v \frac{\partial C}{\partial y}}_C + \underbrace{w \frac{\partial C}{\partial z}}_D = D \left(\underbrace{\frac{\partial^2 C}{\partial x^2}}_E + \underbrace{\frac{\partial^2 C}{\partial y^2}}_F + \underbrace{\frac{\partial^2 C}{\partial z^2}}_G \right) - \underbrace{kC}_H$$

Because the fluid within the ditch is still, $u = v = w = 0$, and terms B, C, and D will equal zero. If the salt is released uniformly across the cross section, then diffusion can never create cross-sectional gradients, and $\frac{\partial C}{\partial y} = \frac{\partial C}{\partial z} = 0$ at all times. Therefore, terms F and G equal zero and can be neglected.

Finally, salt is assumed to be conservative, so term H equals zero. The remaining equation is:

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} = D \frac{\partial}{\partial x} \left(\frac{\partial C}{\partial x} \right)$$

This is a continuous equation. If we apply it to a system with discrete boxes, for each box j in the interior of the domain (boxes 2 through 9), we obtain:

$$\frac{\Delta C_j}{\Delta t} = D \frac{\Delta}{\Delta x} \left(\frac{\Delta C_j}{\Delta x} \right) = \frac{D}{\Delta x} \left[\frac{(C_{j+1} - C_j)}{\Delta x} - \frac{(C_j - C_{j-1})}{\Delta x} \right] = \frac{D}{(\Delta x)^2} (C_{j+1} - 2C_j + C_{j-1})$$

The ends of the ditch are no-flux boundaries, so $\frac{\Delta C}{\Delta x} = 0$ across the wall bounding the first box. The expression for the first box will therefore be:

$$\frac{\Delta C_1}{\Delta t} = D \frac{\Delta}{\Delta x} \left(\frac{\Delta C_1}{\Delta x} \right) = \frac{D}{\Delta x} \left[\frac{(C_2 - C_1)}{\Delta x} \right] = \frac{D}{(\Delta x)^2} (C_2 - C_1)$$

Similarly, there will be no concentration gradient between the last box and the other end of the ditch. So:

$$\frac{\Delta C_{10}}{\Delta t} = D \frac{\Delta}{\Delta x} \left(\frac{\Delta C_{10}}{\Delta x} \right) = \frac{D}{\Delta x} \left[-\frac{(C_{10} - C_9)}{\Delta x} \right] = -\frac{D}{(\Delta x)^2} (C_{10} - C_9)$$

All three of these equations are exactly what we wrote above in Part B.

D & E) See attached. I'm showing key rows of a very long spreadsheet; thick black lines indicate where I've hidden rows. In the titles, I use j to refer to the box number and i to the timestep number. I used a time step $\Delta t = 135$ s; values up to approximately 500 s are stable.

F) See attached plots.

(i) The numerical and analytical solutions should match. Note that the numerical solution corresponds to the spatially averaged concentration within each box, which is best plotted in the middle of each box (e.g., $x = 0.75$ m, 2.25 m, . . .).

(ii) At $T_{\text{touch}} = 14,000$ s, the spatial integral/summation of the analytical solution without the image source contains 28.6 mg of salt, or 95% of the mass within the system. At this time, the concentration at the far boundary in the absence of the image source is 0.9 mg/m^3 , which is (as expected) 14% of the peak concentration (6.4 mg/m^3) at that time. Including the image source in the calculation doubles the concentration at the far boundary (as it always does) and also makes the gradient equal zero at the boundary, which properly reflects the lack of diffusion out of the system. In addition, including the image source improves the match between the analytic and the numerical predictions.

(iii) 1% of system mass will have been lost after $t = 7440$ s, which is about half of the calculated T_{touch} . At the time, the concentration at the far boundary would be 0.3 mg/m^3 without the image source or 0.6 mg/m^3 with it. (As always, the concentration at the far boundary doubles when the image source is added.) Therefore, if you require a precise estimate of the concentration near the far boundary, or of the total mass within the system, then you would need to include the image source earlier than $t = L^2/8D$.

(iv) From Part A, $T_{\text{mix}} = 112,500$ s = 31 hr. At this time, the integral of the analytical solution only provides 25.3 mg of salt, so 16% has been lost from the system. To prevent mass from being predicted to leave the system, additional image sources would need to be added.

(v) According to the numerical solution, the ditch is mixed to a precision of 0.1 mg/m^3 at $t = 49,815 \text{ s}$, which is 44% of the value of T_{mix} calculated in Part A. At this time, there is a 5% difference between the maximum and minimum concentrations for the ten-box model. Note that at this time the analytical model accounts for 29 mg, so 3% of the originally released mass has been lost. (This analysis suggests that $T_{\text{mix}} = 0.44 L^2/D$ is a more precise estimator of the mixing time scale than the value we have been using, which is L^2/D , although L^2/D is still useful for quick order-of-magnitude calculations.)

G) As noted above, the salt is safe once it fully mixes throughout the ditch, and the spreadsheets suggest that it rapidly spreads throughout it. Regions within approximately 3 m of the end of the ditch nearest to the spill experience concentrations above the 10 mg/L biological standard, and even in those regions the concentration has dropped to safe levels by 2 hr after the release. If the eggs need to be exposed for 24 hours, they should be safe, but if the exposure threshold is only 30 minutes then there may be localized mortality or harm. The easiest way to prevent egg damage may be to use a baffle to contain the salt in the near end of the ditch before it mixes, or to add an artificial source of turbulence (e.g., a submersible pump, or an aerator) to induce more rapid dilution. Another option would be to move the eggs out of harm's way, although this may possibly be more disruptive. Note that this analysis assumes that the salt is rapidly dissolved into the pond water and that it spreads rapidly and uniformly; non-uniform spreading (due to wind currents, or the isolation of some grains of salt within cattail stands) could create locally higher and potentially toxic concentrations.

