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1.061 / 1.61 Transport Processes in the Environment

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Answer 4.1 - Describe the concentration field inside the box from $t=0$ to $t=L^{2} / D$.

## Hint 1 - When will the mass be mixed uniformly in the vertical?

From equation 4.24 a mass released mid-way between two parallel boundaries a distance $\mathrm{L}_{Z}$ apart will be mixed to a uniform concentration between those boundaries in time $\mathrm{t}=$ $\mathrm{L}_{\mathrm{Z}}{ }^{2} / 4 \mathrm{D}$, where $\mathrm{L}_{\mathrm{Z}}$ is the distance between the boundaries. The time for the concentration to become well-mixed in the vertical is then, $t=(0.01 \mathrm{~L})^{2} / \mathrm{D}=0.0001 \mathrm{~L}^{2} / \mathrm{D}$.

## Hint 2 - Estimate when the mass will reach each vertical wall in the box.

We estimate the time that the cloud will first touch a boundary based on the standard deviation of the mass distribution. The cloud will touch the top and bottom walls when, $3 \sigma=3 \sqrt{2 \mathrm{Dt}}=\mathrm{L}$, or at the time $\mathrm{t}=\mathrm{L}^{2} / 18 \mathrm{D}$. The cloud will touch the far wall when $3 \sigma=3 \sqrt{2 \mathrm{Dt}}=99 \mathrm{~L}$, or at the time $\mathrm{t} \approx 545 \mathrm{~L}^{2} / \mathrm{D}$.

Hint 3-How will each boundary impact the solution in the time $t=0$ to $L^{2} / D$ ?
Use the time scales determined in hint 1 and 2. Because the concentration field becomes uniform in the vertical very rapidly, within $1 / 10,000^{\text {th }}$ of the time of interest, we will assume that the concentration is instantly uniform in $z$, i.e. $\partial \mathrm{C} / \partial \mathrm{z}=0$ for all time. In the time of interest, the cloud will never reach the far walls ( $545 \mathrm{~L}^{2} / \mathrm{D} \gg \mathrm{L}^{2} / \mathrm{D}$ ), so these boundaries do not impact the solution. The cloud will reach the near walls ( $\mathrm{L}^{2} / 18 \mathrm{D}<$ $L^{2} / D$ ), and a correction must be made to satisfy the no flux condition at these walls.

Hint 4 - Place images sources to satisfy the no-flux boundary condition.
Image sources are needed at the following locations. Image 2 balances the loss of mass from Image 3 across the $x$-axis and the loss of mass from Image 1 across the $y$-axis.

Image 3, ( $x=-L, y=L$ ) $\bigcirc$


Image 2, $(x=-L, y=-L) \bigcirc$ Image $1,(x=L, y=-L)$

Solution - The concentration in the box is described by a superposition of twodimensional, instantaneous, slug releases (equation 3.23) at each of the above sources.

$$
\begin{aligned}
& C(x, y, t)=\frac{M}{L_{z} 4 \pi D t} \cdot \\
& \left(\exp \left(-\frac{(\mathrm{x}-\mathrm{L})^{2}+(\mathrm{y}-\mathrm{L})^{2}}{4 \mathrm{Dt}}\right)+\exp \left(-\frac{(\mathrm{x}-\mathrm{L})^{2}+(\mathrm{y}+\mathrm{L})^{2}}{4 \mathrm{Dt}}\right)+\exp \left(-\frac{(\mathrm{x}+\mathrm{L})^{2}+(\mathrm{y}+\mathrm{L})^{2}}{4 \mathrm{Dt}}\right)+\exp \left(-\frac{(\mathrm{x}+\mathrm{L})^{2}+(\mathrm{y}-\mathrm{L})^{2}}{4 \mathrm{Dt}}\right)\right) \\
& \text { real source }
\end{aligned}
$$

## Solution 4.2

(a) An image source is needed at $x=-150 \mathrm{~m}$ to account for the no-flux boundary at the end of the canal. The concentration of fuel in the canal is described by the superposition of these two instantaneous, 1-D sources.

$$
\begin{gathered}
C(x, t)=\frac{M}{A \sqrt{4 \pi D t}}\left[\exp \left(\frac{-x^{2}}{4 D t}\right)+\exp \left(\frac{-(x+150)^{2}}{4 D t}\right)\right] \\
R E A L \quad I M A G E
\end{gathered}
$$

Therefore, at $\mathrm{x}=-50 \mathrm{~m}, \mathrm{t}=10 \mathrm{hrs}(=36000 \mathrm{~s})$,

$$
\begin{aligned}
C & =\frac{1000 \mathrm{~g}}{5 \mathrm{~m}^{2} \sqrt{4 \pi\left(0.01 \mathrm{~m}^{2} \mathrm{~s}^{-1}\right)(36000 \mathrm{~s})}}\left[\exp \left(\frac{-(-50 \mathrm{~m})^{2}}{4\left(0.01 \mathrm{~m}^{2} \mathrm{~s}^{-1}\right)(36000 \mathrm{~s})}\right)+\exp \left(\frac{-(100 \mathrm{~m})^{2}}{4\left(0.01 \mathrm{~m}^{2} \mathrm{~s}^{-1}\right)(36000 \mathrm{~s})}\right)\right] \\
& =2.97 \mathrm{gm}^{-3}(0.176+0.001)=\mathbf{0 . 5 3} \mathbf{g m}^{-3}
\end{aligned}
$$

(b) This is best solved graphically. The plot of:
$\mathrm{C}(-50 \mathrm{~m}, t)=\frac{1000 \mathrm{~g}}{5 \mathrm{~m}^{2} \sqrt{4 \pi\left(0.01 \mathrm{~m}^{2} \mathrm{~s}^{-1}\right) t}}\left[\exp \left(\frac{-(-50 \mathrm{~m})^{2}}{4\left(0.01 \mathrm{~m}^{2} \mathrm{~s}^{-1}\right) t}\right)+\exp \left(\frac{-(100 \mathrm{~m})^{2}}{4\left(0.01 \mathrm{~m}^{2} \mathrm{~s}^{-1}\right) t}\right)\right]$
is shown below.


From this plot, we can see that the maximum concentration at the house is approximately $1.3 \mathbf{~ g m}^{-3}$ (when $t \approx 2.4 \times 10^{5} \mathrm{~s}=67 \mathrm{hrs}$ )
(c) The easiest ways to solve the equation in (b) for $\mathrm{C}=0.2 \mathrm{gm}^{-3}$ are graphically, or by trial and error. As the above plot lacks detail in the early stages, we will use trial and error in our spreadsheet to solve
$0.2 \mathrm{gm}^{-3}=\frac{1000 \mathrm{~g}}{5 \mathrm{~m}^{2} \sqrt{4 \pi\left(0.01 \mathrm{~m}^{2} \mathrm{~s}^{-1}\right) t}}\left[\exp \left(\frac{-(-50 \mathrm{~m})^{2}}{4\left(0.01 \mathrm{~m}^{2} \mathrm{~s}^{-1}\right) t}\right)+\exp \left(\frac{-(100 \mathrm{~m})^{2}}{4\left(0.01 \mathrm{~m}^{2} \mathrm{~s}^{-1}\right) t}\right)\right]$
for $t$. This yields a solution of $\boldsymbol{t}=\mathbf{2 1 0 6 0} \mathbf{s}=\mathbf{5 . 8} \mathbf{~ h r s}$.
Compare this solution to that of Problem 1.5 to see the effect that the no-flux boundary has on the concentration of fuel observed at your house.
(d) An image sink is needed at $x=-150 m$ to account for the perfectly absorbing boundary at the end of the canal (see Chapter 4 notes, $p 4$ )

$$
\begin{gathered}
C(x, t)=\frac{M}{A \sqrt{4 \pi D t}}\left[\exp \left(\frac{-x^{2}}{4 D t}\right)-\exp \left(\frac{-(x+150)^{2}}{4 D t}\right)\right] \\
R E A L \\
I M A G E
\end{gathered}
$$

Repeating (a) - (c) is relatively simple, the results being:

- $C(x=-50 \mathrm{~m}, t=36000 \mathrm{~s})=\mathbf{0 . 5 2} \mathbf{~ g m}^{\mathbf{- 3}}$ (i.e. at this short time, the boundary has little/no effect).
- $C_{\text {max }}(x=-50 \mathrm{~m})=\mathbf{0 . 8 2} \mathbf{~ g m}^{-\mathbf{3}}$ (i.e. at $\left.t \approx 83000 \mathrm{~s}=23 \mathrm{hrs}\right)$.

- $C=0.2 \mathrm{gm}^{-3}$ when $\boldsymbol{t}=\mathbf{2 1 0 6 0} \mathbf{~ s}$. This is the same answer as in (c) - before the cloud encounters the boundary (i.e. for $2 \sqrt{2 D t}<75 \mathrm{~m} \Rightarrow t<70300 \mathrm{~s}$ ), the boundary has little/no effect.


## Answer 4.3

a) Estimate the time scale, $T$, at which the dye becomes uniformly distributed in $x$.

The diffusion of dye released at the end wall (top figure) will be similar to the diffusion of dye released mid-way between end walls placed twice as far apart (bottom figure). This is because the diffusion in both systems proceeds as a function of $\exp \left(-x^{2} / 4 \mathrm{Dt}\right)$, which is symmetric about x $=0$. From this similarity we expect that the dye will be well mixed in both systems in the timescale already established for the bottom system. Specifically, from eq. 4.24 applied to the bottom system, $T=(2 \mathrm{~L})^{2} / 4 \mathrm{D}=\mathrm{L}^{2} / \mathrm{D}=10^{7} \mathrm{sec}$.

b) Confirm your estimate by plotting $C(x)$ at the times $t=T / 10, T / 4, T / 2, T$.

Theoretically an infinite number of images is needed to satisfy a no-flux boundary condition at two parallel boundaries. For simplicity we initially consider only one image position for each boundary. The boundary at $\mathrm{x}=0$ requires image I1 at $\mathrm{x}=0$, i.e. co-located with the source. The boundary at $\mathrm{x}=\mathrm{L}$ requires image I 2 at $\mathrm{x}=2 \mathrm{~L}$ for the real source, as well as image I 3 for the image source I1. The concentration field is,

$$
\mathrm{C}(\mathrm{x}, \mathrm{t})=\frac{\mathrm{M}}{\mathrm{~A}_{\mathrm{yz}} \sqrt{4 \pi \mathrm{Dt}}}\left(2 \exp \left(-\mathrm{x}^{2} / 4 \mathrm{Dt}\right)+2 \exp \left(-(\mathrm{x}-2 \mathrm{~L})^{2} / 4 \mathrm{Dt}\right)\right)
$$



The solution indicates that three images are not sufficient, because mass is not conserved in the time of interest. The final concentration should be $1 \mathrm{mg} /\left(10 \mathrm{~cm}^{3}\right)=0.1 \mathrm{mg} \mathrm{cm}^{-3}$, but the above solution yields $0.66 \mathrm{mg} \mathrm{cm}^{-3}$ at $\mathrm{t}=\mathrm{L}^{2} / \mathrm{D}$. In addition, the gradient of concentration should be zero at the boundaries, $\partial \mathrm{C} / \partial \mathrm{x}=0$, to satisfy the no-flux condition. This condition is not met at $\mathrm{x}=$ 10 cm . For comparison, we now consider a solution with seven images, each denoted by I.


I1 balances the real source at boundary $\mathrm{x}=0$.
I2 and I3 balance the real source and I1 at boundary $\mathrm{x}=\mathrm{L}$.
I4 and I5 balance I2 and I3 across the boundary at $\mathrm{x}=0$.
I6 and I7 balance I4 and I5 across the boundary at $\mathrm{x}=\mathrm{L}$.
$C(x, t)=$
$\frac{M}{A_{y z} \sqrt{4 \pi D t}}\left(2 \exp \left(-x^{2} / 4 D t\right)+2 \exp \left(-(x-2 L)^{2} / 4 D t\right)+2 \exp \left(-(x+2 L)^{2} / 4 D t\right)+2 \exp \left(-(x-4 L)^{2} / 4 D t\right)\right)$
$\begin{array}{llll}\text { Real+I1 } & \mathrm{I} 2+\mathrm{I} 3 & \mathrm{I} 4+\mathrm{I} 5 & \mathrm{I} 6+\mathrm{I} 7\end{array}$


With seven images the concentration is correct at $\mathrm{T}=\mathrm{L}^{2} / \mathrm{D}$. At longer times mass will still be lost due to unbalanced images and the concentration will decline. However, longer times hold no interest, because once the system is well mixed in $x(\partial C / \partial x=0$ for all $x)$, the solution may be ended as no further evolution of the true profile will occur. Note, the shape of the concentration profiles are similar with 2 and 6 images, and both solutions indicate a uniform distribution in x is achieved by $\mathrm{T}=\mathrm{L}^{2} / \mathrm{D}$.

Answer 4.4:
a) Estimate the time at which the concentration at $A$ and $A$ ' begin to diverge?

The concentrations at A and A' diverge when the boundary impacts the solution in System 1. This occurs when the diffusing cloud reaches the boundary. Estimate this time by equating the edge of the cloud with the length scale $3 \sigma$. That is, the cloud will touch the boundary when $3 \sigma=3 \sqrt{2 \mathrm{Dt}}=50 \mathrm{~cm}$, such that $\mathrm{t}=(50 \mathrm{~cm})^{2} / 18 \cdot 2 \mathrm{~cm}^{2} \mathrm{~s}^{-1}=70$ seconds.
b) What is the final concentration at $A\left(A^{\prime}\right)$, and when is this concentration achieved?

The final concentration in System 1 will be $C=(100 \mathrm{~g}) /(1 \mathrm{~m} \times 1 \mathrm{~m} \times 0.1 \mathrm{~m})=1000 \mathrm{ppm}$.
It is achieved when the mass is fully mixed across the domain. Using the largest dimension to estimate this time-scale, $\mathrm{t}=(\mathrm{L})^{2} /(4 \mathrm{D})=1250 \mathrm{~s}$. As noted in the text, this is a conservative estimate, and $t=(\mathrm{L})^{2} /(8 \mathrm{D})=625 \mathrm{~s}$, is also a reasonable estimate. Because System 2 is unbounded, infinite dilution is possible and the final concentration is $\mathrm{C}=0 \mathrm{ppm}$, but theoretically this will take infinite time. Because the probe has a detection limit of 10 ppm , zero concentration will be recorded for any concentration $\mathrm{C}<10 \mathrm{ppm}$, which occurs in a finite time.
c) Describe the evolution of the concentration field in each system, i.e. $\mathbf{C}(\mathbf{x}, \mathrm{y}, \mathrm{z}, \mathrm{t})$. In both systems the concentration is uniform in z by $\mathrm{t}=(10 \mathrm{~cm})^{2} /\left(4 \times 2 \mathrm{~cm}^{2} \mathrm{~s}^{-1}\right)=12.5 \mathrm{~s}$ after release. Because this is short relative to other time scales of interest ( 1250 sec ), we neglect the 3-D phase and use a two-dimensional solution. For System 1, an infinite number of image sources is needed to satisfy the no-flux boundaries.

$$
\mathrm{Cl}(\mathrm{x}, \mathrm{y}, \mathrm{t})=\frac{\mathrm{M}}{\mathrm{~L}_{\mathrm{z}} 4 \pi \mathrm{Dt}}\left[\underset{\text { real source }}{\exp \left(-\frac{\mathrm{x}^{2}+\mathrm{y}^{2}}{4 \mathrm{Dt}}\right)+\sum_{\mathrm{n}=1}^{\infty} \exp \left(-\frac{\mathrm{x}^{2}+(\mathrm{y} \pm 2 \mathrm{~nL})^{2}}{4 \mathrm{Dt}}\right)+\sum_{\mathrm{n}=1}^{\infty} \exp \left(-\frac{(\mathrm{x} \pm 2 \mathrm{~nL})^{2}+\mathrm{y}^{2}}{4 \mathrm{Dt}}\right)} \underset{\text { images along y axis }}{\text { images along } \mathrm{x} \text { axis }}\right.
$$

$$
+\frac{\mathrm{M}}{\mathrm{~L}_{\mathrm{z}} 4 \pi \mathrm{Dt}}\left[\sum_{\mathrm{n}=1}^{\infty} \exp \left(-\frac{(\mathrm{x} \pm 2 \mathrm{~nL})^{2}+(\mathrm{y} \pm 2 \mathrm{~nL})^{2}}{4 \mathrm{Dt}}\right)\right]
$$

corner images


The images in the second line are located at the corners (see sketch), to offset the losses of $y$-axis images across the boundaries at $\mathrm{x} \pm \mathrm{L} / 2$; and the loss of x -axis images across the boundaries at $y= \pm L / 2$. In practice an infinite number of images is not needed. For time less than required to reach a well-mixed condition between the boundaries ( $\mathrm{t}<\mathrm{L}^{2} / 4 \mathrm{D}$ ), three images per boundary is sufficient to approximate the full solution with infinite images. Beyond this time, the concentration is steady and uniform, and the detailed solution above is no longer needed. System 2 is described by a simple twodimensional slug-release,
$\mathrm{C} 2(\mathrm{x}, \mathrm{y}, \mathrm{t})=\frac{\mathrm{M}}{\mathrm{L}_{\mathrm{z}} 4 \pi \mathrm{Dt}} \exp \left(-\frac{\mathrm{x}^{2}+\mathrm{y}^{2}}{4 \mathrm{Dt}}\right)$.

