1.061 / 1.61 Transport Processes in the Environment
Fall 2008

Answer 3.1

Estimate the coefficient of diffusivity within this region of atmosphere.

Hint 1 - Can you assume uniform concentration in any direction?
The gas is effectively released into an unbounded domain, so that one cannot expect it to mix rapidly to uniform conditions in any direction, i.e. $\partial C/\partial y \neq 0$, $\partial C/\partial z \neq 0$, $\partial C/\partial y \neq 0$. All three dimensions must be retained in the governing equation.

Hint 2 - What assumption can you make about the air currents?
The atmosphere is stagnant, which implies that there are no ambient air currents. You may assume that u=v=w=0. The passage of each plane will create air movement. This movement may locally and temporarily enhance the dilution of the cloud. However, this effect dies out within a few minutes, so that over an hour time frame, the effect is negligible.

Hint 3 - What assumption must you make about the coefficient of diffusion?
Since you are only given one value of concentration, you can solve uniquely for only one value of diffusion. Thus, to make the problem tractable, you must assume that the diffusion is isotropic.

With the above assumptions, the transport equation reduces to,

$$\frac{\partial C}{\partial t} = D\left[\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2}\right].$$

Letting the initial release point be at (x, y, z)=0, the initial condition can be written,

$C(x,y,z,t=0) = M\,\delta(x)\,\delta(y)\,\delta(z)$.

The solution to the above equation and initial condition is Equation 25 in Chapter 3.

$$C(x,y,z,t) = \frac{M}{(4\pi D t)^{3/2}} \exp\left(-\frac{x^2+y^2+z^2}{4Dt}\right).$$

The maximum concentration within the cloud is given in Equation 26 in Chapter 3.

$$C_{MAX} = \frac{M}{(4\pi D t)^{3/2}}.$$

Using the information given in the problem statement, we can find D,

$$D = \left(M/C_{MAX}\right)^{2/3} / 4\pi t = \left(10\text{kg}/3\times10^{-5}\ \text{kgm}^{-3}\right)^{2/3} / (4\ \pi\ 3600\ \text{s}) = 0.1\text{m}^2\text{s}^{-1}$$

Answer 3.2

What governing equation describes the evolution of the gas concentration in the hall?
For isotropic diffusion, the governing equation is:

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} + v\frac{\partial C}{\partial y} + w\frac{\partial C}{\partial z} = D\left[\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2}\right]$$

Align the coordinate x to the length of the hallway and define the y-z plane as the cross-section. Since the gas "mixes rapidly" in the vertical and horizontal, we assume $\partial C/\partial y = \partial C/\partial z = 0$. The problem statement gives no information about air currents in the hallway, so we assume they are negligible, $u = 0$. With these assumptions, the governing equation is reduced to,

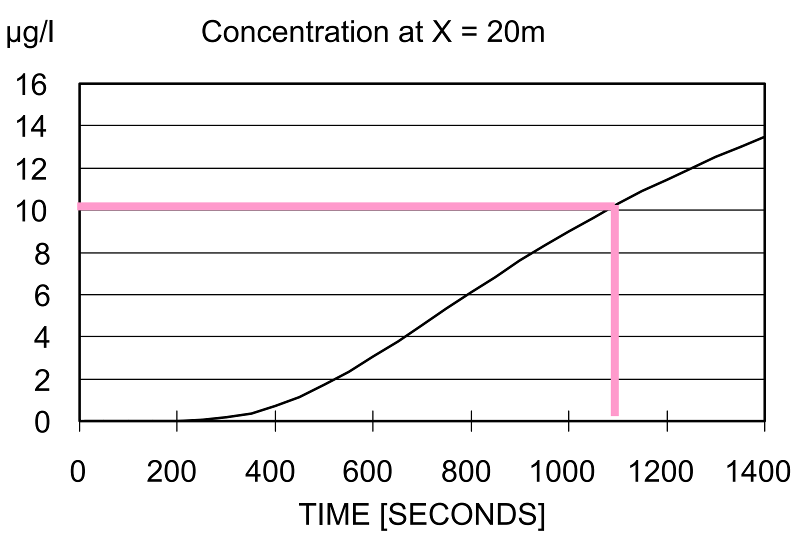
$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} \quad .$$

If the spill location is taken as $x = 0$, the initial condition is then, $M = \delta(x)$

At what time after the spill do you smell the gas?
The governing equation and initial condition above describe an instantaneous, point release diffusing in one-dimension. The concentration field is described by Equation 10 in chapter 3.

$$3.10 \qquad C(x,t) = \frac{M}{A_{yz}\sqrt{4\pi Dt}} \exp\left(-\frac{x^2}{4Dt}\right) = [M/L^3]$$

Use 3.10 to find the time at which the concentration at your door, $C(x=20\text{m}, t)$ is 10 $\mu g l^{-1}$. As time appears in both the exponential and leading terms, it is simpler to use a graphical solution.



You will smell the gas at your office approximately 1100 seconds after the spill.

When does the smell, as perceived by humans, disappear from the hallway?
To answer this question we need information on the end conditions of the hallway. Lets first consider that the hallway is open at both ends, so that odor can diffuse beyond the end of the hall. Then, we need only consider the evolution of the maximum concentration, located at the site of the spill, x = 0. We seek the time for which

$$C_{max}(t) = \frac{M}{A_{yz}\sqrt{4\pi Dt}} < 10\mu g l^{-1},$$

or simply

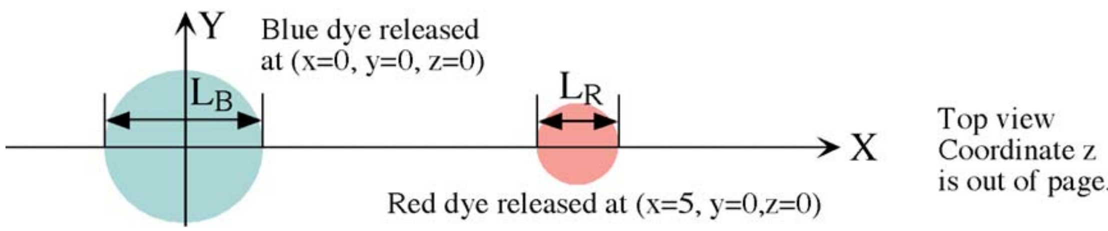
$$t > \left(\frac{10g}{2m \times 3m \times 0.01gm^{-3}}\right)^2 \Big/ \left(4\pi \times 0.05m^2s^{-1}\right) = 44{,}232 \text{ seconds} = 12.3 \text{ hrs}$$

At this time, the length of the cloud will be $4\sigma = 4\sqrt{2Dt} = 266m$, indicating that the cloud has diffused beyond the length of the hallway. The above time scale is correct, only if the hallway is open at both ends. If the hallway is shut off by fire doors at both ends, then in reality the cloud cannot diffuse beyond the length of the hall. Under these conditions, the final concentration in the hallway set the maximum possible dilution, which is determined by distributing the total mass released over the total volume of the hallway (2m x 3m x 100m).

$$C_{final} = 10g \big/ (2m \times 3m \times 100m) = 0.016gm^{-3} = 16\mu g l^{-1}.$$

Since the final concentration is above the detection limit, the smell will not disappear until the fire doors are opened.

Answer 3.3
Hint 1: Make sketch that defines the diameter of each cloud



a. While both clouds are fully visible ($C > 10$-g l^{-1}), which cloud will appear larger, and by how much?

Since the size of the cloud increases in proportion to the diffusion coefficient, the blue cloud will grow more rapidly, and thus appear bigger, than the red cloud. Specifically, the length scale of each cloud, as defined in chapter 3, equation 26, is

$L_B = 4\sigma_B = 4\sqrt{2D_B t}$ and $L_R = 4\sigma_R = 4\sqrt{2D_R t}$.
The ratio of dye cloud diameters is then, $L_B / L_R = \sqrt{D_B / D_R} = 2$.

b. At what time and at what location will the two dye clouds first appear to touch?
Hint 2: Simplify governing equation with assumptions.
Begin with the full transport equation that governs the evolution of both dye drops.

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} + v\frac{\partial C}{\partial y} + w\frac{\partial C}{\partial z} = \frac{\partial}{\partial x} D_x \frac{\partial C}{\partial x} + \frac{\partial}{\partial y} D_y \frac{\partial C}{\partial y} + \frac{\partial}{\partial z} D_z \frac{\partial C}{\partial z} \pm S$$

(1) (2) (3) (4) (5) (6) (7) (8)

Simplifying assumptions:
- The dyes do not interact, so we can drop the source/sink term 8.
- The fluid is stagnant, thus u=v=w=0, and we can drop terms 2,3,4
- Molecular diffusion is homogeneous and isotropic, $D_x=D_y=D_z=D$, and $D \neq f(x,y,z)$.
  This reduces the diffusion terms to: $D\,(\partial^2C/dx^2 + \partial^2C/dy^2 + \partial^2C/dz^2)$.
- The dyes mix rapidly between the plates, such that $\partial C/\partial z = 0$, and we can drop term 7.

Simplified governing equation: $$\frac{\partial C}{\partial t} = D\left[\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2}\right].$$

Initial conditions:
Blue Dye: $C_B(x,y,t=0) = M\,\delta(x)\,\delta(y)$
Red Dye: $C_R(x,y,t=0) = M\,\delta(x-5)\,\delta(y)$

The diffusion of each dye is thus described by the two-dimensional, instantaneous, point release solution. See equation 23 in Chapter 3, with $D_x=D_y=D$. Note, here L_Z is the plate gap, 5mm.

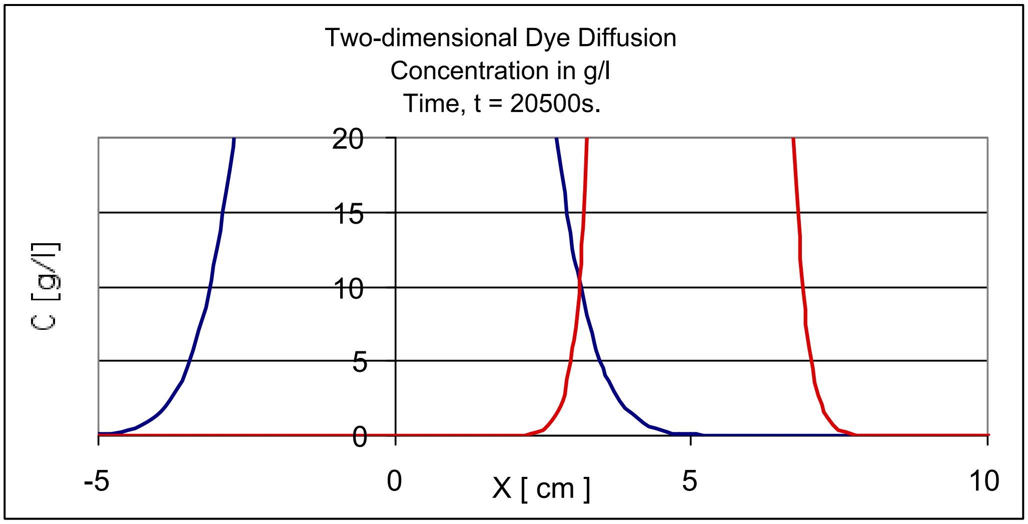
$$C_B(x,y,t) = \frac{M}{L_z\, 4\pi\, D_B\, t} \exp\left(-\frac{x^2 + y^2}{4D_B t}\right)$$

$$C_R(x,y,t) = \frac{M}{L_z\, 4\pi\, D_R\, t} \exp\left(-\frac{(x-5)^2 + y^2}{4D_R t}\right)$$

Note that the exponential is written to be one at the center of the red cloud, i.e. at (x=10,y=0), with the position given in units of centimeters.

Hint 3: Write mathematical criteria for condition when clouds first touch
From geometry, the two clouds will first touch along the line y = 0. We wish to find the time, t, and location, x, for which C_B(x, y=0, t) = C_R(x, y=0, t) = 10 g/l. This could be tackled analyticaly by first finding the position $x_{BR}(t)$ at which C_B=C_R. Then solve for t using this position to constrain x, e.g. solve C_B(x = x_{BR}, y=0, t). However, a simpler approach is to graph C_B and C_R in an interactive graphing package, such as Excel, and then vary time until the intersection of the two concentration curves lies at C = 10 g/l

Solution: - At t = 20500s, the intersection of the blue and red concentration curves corresponds to C = 10 g/l and is located at x = 3.1 cm. The clouds will first appear to touch and x = 3.1 cm.



Make a rough estimate of the location using your result from part a?
Based on the definition used in a. and the definition sketch shown above, the two clouds first appear to touch when, $(L_B/2)+(L_R/2) = 5$. Additionally, $L_R = (L_B/2)$, so the edge of the blue cloud will be at $x = (L_B/2) = 5/1.5=3.3$cm, when it first touches the red cloud.

c. At what time will the line connecting the release points be completely purple?
Hint 4: - Define a mathematical criteria for this to occur?
This condition requires that C_B and $C_R > 10$ g/l in the region x = 0 to 10 cm. Use the spreadsheet created in part b to interrogate the concentration field over a range of time.

Solution - Graph C_B and C_R in an interactive graphing package, such as Excel and vary time until the above criteria is met. You will find that the criteria is never met. Between 0<x<5 cm, when $C_R \geq 10$g/l then $C_B < 10$ g/l, and when $C_B \geq 10$g/l, $C_R < 10$ g/l.