1.061 / 1.61 Transport Processes in the Environment
Fall 2008

3. Diffusion of an Instantaneous, Point Release
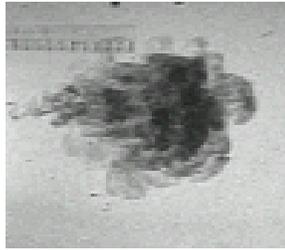
This section follows on from Section 1, exploring the Gaussian concentration profile that develops after an instantaneous, point release. Several important properties of the Gaussian distribution (and their utility) are emphasized. The spread of a point release in all 3 dimensions is discussed, noting that the profile of concentration along any straight line cut through the patch will have a Gaussian distribution. The animation shows the spread of an instantaneous, point release with anisotropic diffusivity, highlighting the dependence of length scales of the Gaussian distribution on the square root of D.

3. Diffusion of an Instantaneous Point Source

The equation of conservation of mass is also known as the transport equation, because it describes the transport of scalar species in a fluid systems. In this and subsequent sections we consider analytical solutions to the transport equation that describe the fate of mass under different boundary and initial conditions. For incompressible flow with isotropic and homogeneous diffusion coefficients, we can begin with the following form of the transport equation. At this point we will also ignore the source/sink term.

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

The first solutions describes the evolution of a slug of mass, M, released instantaneously at time $t = 0$ into a stationary fluid (u,v,w = 0). We consider a one-dimensional system in the x-direction, i.e. the system is uniform in y and z, such that $\partial/\partial y = 0$ and $\partial/\partial z = 0$. A model for such a system is shown below. A slab of mass (gray) is released into a long, narrow tube. The mass is distributed uniformly in the y-z plane and with negligible dimension in x, such that the initial concentration is $C(x) = M\,\delta(x)$, where $\delta()$ is the Dirac delta function. The transport equation for this system is given in (2).
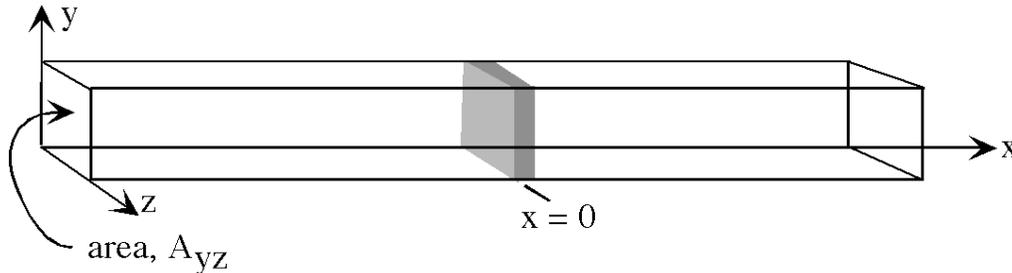
(2) $$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} \quad, \qquad \text{M released at } t = 0, x = 0.$$

The solution, C(x,t), can be found as follows. From (2) we anticipate that the concentration will be a function of M, D [$L^2 T^{-1}$], x[L], and t[T], with dimensions expressed in brackets in terms of mass [M], length [L], and time [T]. In a one-dimensional system, concentration has units of mass per length, C[$M\,L^{-1}$]. From dimensional analysis (e.g. Buckingham Pi Theorem) the above parameter set forms the following dimensionless groups.

(3) $$\frac{C}{M/\sqrt{4\pi Dt}} = f\left(\frac{x}{\sqrt{4Dt}}\right)$$

The factors 4π and 4 are added now for convenience, because they appear in the final solution. Originally, these factors were found through trial and error. Defining $\eta = x/\sqrt{4Dt}$, and then evaluating (2) with (3),

(4) $\dfrac{d}{d\eta}\left(\dfrac{df}{d\eta} + 2f\eta\right) = 0$

Setting the terms within the bracket to zero provides one solution to (4),

(5) $\dfrac{df}{d\eta} + 2f\eta = 0$,

which in turn has the solution

(6) $f = A_0 \exp(-\eta^2)$,

with A_0 an arbitrary constant. (6) gives us a specific form for (3) that is a solution for (2).

(7) $C(x,t) = \dfrac{A_0}{\sqrt{4\pi Dt}} \exp\left(-\dfrac{x^2}{4Dt}\right)$

Since the total mass must be conserved over time, for all time

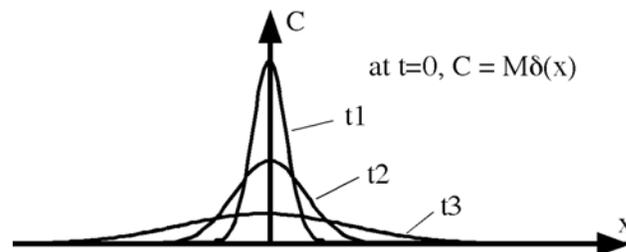(8) $M = \displaystyle\int_{x=-\infty}^{\infty} C dx$,

so that $A_0 = M$.   In summary we have the following solution.

One-dimensional, Instantaneous Point Source
M released at $t = 0$ and $x = 0$.
Initial condition, $C(x) = M\,\delta(x)$.

(9) $C(x,t) = \dfrac{M}{\sqrt{4\pi Dt}} \exp\left(-\dfrac{x^2}{4Dt}\right) = [M/L]$

Note that the above solution is correct for a one-dimensional mathematical system, in which C[M/L]. In real (three-dimensional) systems concentration must have units of M/L^3. To convert the mathematical solution given in (9) to real space, divide by the neglected dimensions, here the cross-sectional area of the system in the y-z plane, A_{yz}.

$$(10) \quad C(x,t) = \frac{M}{A_{yz}\sqrt{4\pi Dt}} \exp\left(-\frac{x^2}{4Dt}\right) = [M/L^3]$$

Recall that the same solution was derived from a statistical model of diffusion, as described in Conceptual Model of Diffusion.

Moments of the Concentration Distribution.
It is useful to characterize the geometry of the evolving distribution of mass based on its moments. The zeroth moment gives the total mass, M, within the cloud,

$$\text{zeroth moment} = M_0 = M = \int_{-\infty}^{\infty} C(x,t)dx.$$

Higher moments indicate the centroid and variance of the mass distribution.

$$\text{first moment} = M_1 = \int_{-\infty}^{\infty} xC(x,t)dx$$

$$\text{second moment} = M_2 = \int_{-\infty}^{\infty} x^2 C(x,t)dx$$

The mean indicates the centroid of mass for the cloud,

$$\text{Mean} = \mu = \frac{M_1}{M_0}.$$

The variance indicates the width of the distribution.

$$\sigma^2 = \frac{\int_{-\infty}^{\infty}(x-\mu)^2 C(x,t)dx}{\int_{-\infty}^{\infty} C(x,t)dx} = \frac{M_2}{M_0} - \mu^2.$$

Evaluating the mean and variance for the distribution given in (10), we find that the mean, $\mu = 0$, i.e. the centroid of the patch remains at x = 0 for all time. The variance is

$$(11) \quad \sigma^2 = 2Dt.$$

If the coefficient of diffusion, D, is constant, the variance of the mass distribution grows linearly in time. Taking the derivative of (11),

$$(12) \quad D = \frac{1}{2}\frac{d\sigma^2}{dt} = \frac{1}{2}\frac{\sigma_2^2 - \sigma_1^2}{t_2 - t_1}.$$

This provides a useful tool for estimating the diffusion coefficient by tracking the variance of a diffusing tracer over time. It is useful to note that for a Gaussian distribution, the concentration at one standard deviation from the center of mass is,

$$(13) \quad C(x = \sigma = \sqrt{2Dt}) = \left[\frac{M}{A_{yz}\sqrt{4\pi Dt}}\right]\exp\left(-\frac{2Dt}{4Dt}\right) = C_{max}(t)\exp(-1/2) = 0.61C_{max},$$

where C_{max} is the maximum concentration in the patch at time t, and is given by the bracketed coefficient to the exponential term in (13), $C_{max} = M / (A_{yz}(4\pi Dt)^{1/2}))$.

Finally, as described in Chapter 1, the standard deviation, σ, provides a useful length-scale for the diffusing patch. Noting that 95% of the total mass is contained within $\pm 2\sigma$ of the centroid, a conventional length-scale for a patch is

$$(14) \quad L = 4\sigma.$$

With this definition for patch size, the edges of the patch are defined by the concentration $C(x = \pm 2\sigma) = 0.14 C_{max}$.

Instantaneous Point Source in Two-Dimensions
A slug of mass, M, is released at x = y = z = 0 in a stationary fluid (u = v = w = 0). The flow conditions are uniform in z ($\partial/\partial z = 0$). The mass slug is initially distributed uniformly in z and with negligible dimension in y and x, such that the initial concentration is C(x, y, t=0) = M $\delta(x)\delta(y)$, where $\delta()$ is the Dirac delta function.
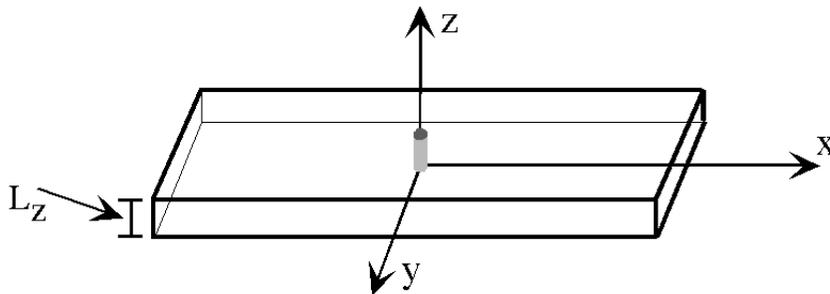
For generality we will assume anisotropic diffusion, $D_x \neq D_y$. The transport equation for this system is then,

$$(15) \qquad \frac{\partial C}{\partial t} = D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2}.$$

From Fick's Law and by inspection of (15), the diffusion in x (1st term on right hand side) depends only on the distribution in x and the diffusion in y (2nd term on right hand side) depends only on the distribution in y. This leads us to propose that the solution to (15) may be the product of two uncoupled solutions describing the distribution in x and y.

$$(16) \qquad C(x,y,t) = MC_1(x,t)C_2(y,t),$$

where, explicitly, C_1 is not a function of y and C_2 is not a function of x. Inserting the proposed solution form into (15),

$$(17) \qquad \frac{\partial}{\partial t}\left(C_1 C_2\right) = C_1 \frac{\partial C_2}{\partial t} + C_2 \frac{\partial C_1}{\partial t} = D_x C_2 \frac{\partial^2 C_1}{\partial x^2} + D_y C_1 \frac{\partial^2 C_2}{\partial y^2}$$

The above equation can be rewritten to isolate the functions C_1 and C_2.

$$(18) \qquad C_2\left[\frac{\partial C_1}{\partial t} - D_x \frac{\partial^2 C_1}{\partial x^2}\right] + C_1\left[\frac{\partial C_2}{\partial t} - D_y \frac{\partial^2 C_2}{\partial x^2}\right] = 0.$$

The trivial, but useless, solution is $C_1 = C_2 = 0$. Alternatively each bracketed set of terms could be zero. For example, setting the first bracketed set to zero yields,

$$(19) \qquad \frac{\partial C_1}{\partial t} = D_x \frac{\partial^2 C_1}{\partial x^2},$$

which is the 1-D, diffusion equation (2). From (7), we can write the solution to (19).

$$(20) \qquad C_1(x,t) = \frac{A_1}{\sqrt{4\pi D_x t}} \exp\left(-\frac{x^2}{4D_x t}\right)$$

A similar form is found for C_2 by setting the second bracketed term in (18) to be zero. The full solution will then have the form,

$$(21) \qquad C(x,y,t) = C_1(x,t)C_2(y,t) = \frac{A_1 A_2}{4\pi t\sqrt{D_x D_y}} \exp\left(-\frac{x^2}{4D_x t} - \frac{y^2}{4D_y t}\right),$$

with A_1 and A_2 constants. The product $A_1 A_2 = M$ is found by applying the condition

(22) $\quad M = \int\limits_{y=-\infty}^{\infty} \int\limits_{x=-\infty}^{\infty} C dx dy$.

Finally, the two-dimensional solution (21) has units [M L^{-2}], because the third dimension has been neglected. To recover the correct concentration in real, three-dimensional space, divide the two-dimensional solution by the length of the missing dimension, e.g. L$_z$ in the figure given above. In summary we have the following solution.

Instantaneous Point Source in Two-Dimensions
M released at t = 0 and x = y = 0.
Initial condition, C = M δ(x) δ(y)

(23) $\quad C(x,y,t) = \dfrac{M}{L_z \, 4\pi t \sqrt{D_x D_y}} \exp\left(-\dfrac{x^2}{4D_x t} - \dfrac{y^2}{4D_y t} \right) = [ML^{-3}]$.

From (23) the profile of concentration, C(x,y) along any straight line cut through the patch will have a Gaussian distribution. Obvious examples are the profiles C(x, y = 0) and C(x = 0, y). This is the direct result of Fick's Law, which requires that the flux in any direction be proportional only to the gradients in that direction.   If the diffusion coefficients are anisotropic, the cloud will grow anisotripically, increasing in length more quickly along the axis of maximum diffusion rate. The length scale of the cloud along any axes will be proportional to the diffusion coefficient along that axes.

(24)
$$L_x = 4\sigma_x = 4\sqrt{2D_x t}$$
$$L_y = 4\sigma_y = 4\sqrt{2D_y t}$$

With this length scale definition, the edge of the patch is located 2σ from the centroid along a concentration contour C = 0.14 C$_{max}$, similar to the one-dimensional case described above. The basic characteristics of a two-dimensional slug release are depicted in the following animation.

Animation - Anisotropic Diffusion in Two-Dimensions - see chapter homepage
This animation depicts the diffusion of a discrete mass released at (x=0, y=0, t=0). The diffusion is anisotropic, D$_x$ = 4 D$_y$. As indicated in (24), the length scales grow in proportion to the square root of the diffusion, such that the dimensions of the cloud are anisotropic, with L$_x$/L$_y$ = $\sqrt{D_x/D_y}$.   In this system, L$_x$ = 2L$_y$. Note that the profiles of concentration along the x- and y-axes are Gaussian in shape. Finally, noting that the 2σ contour reaches x = ±L at t = 600s provides an estimate for the diffusion coefficient, D$_x$. Specifically, use the constraint L$_x$ = 2L at t = 600s in (24) to estimate D$_x$.

The above analyses are easily extended to three dimensions.

Instantaneous, Point Release in Three Dimensions
M released at t = 0 and x = y = z = 0.
Initial Condition, $C = M\, \delta(x)\delta(y)\delta(z)$.

$$(25) \quad C(x,y,z,t) = \frac{M}{(4\pi t)^{3/2}\sqrt{D_x D_y D_z}} \exp\left(-\frac{x^2}{4D_x t} - \frac{y^2}{4D_y t} - \frac{z^2}{4D_z t}\right) = [ML^{-3}]$$

Dilution Rate:
The dilution rate of a patch may be described by the rate of change in the maximum concentration within the patch. For a slug release the maximum concentration, $C_{max}(t)$, occurs at the centroid and corresponds to the coefficient leading the exponential in (10), (23), and (25).

$$1\text{-}D: \quad C_{max} = \frac{M}{A_{yz}(4\pi D\, t)^{1/2}}$$

$$(26) \quad 2\text{-}D: \quad C_{max} = \frac{M}{L_z\, 4\pi t \sqrt{D_x D_y}}$$

$$3\text{-}D: \quad C_{max} = \frac{M}{(4\pi t)^{3/2}\sqrt{D_x D_y D_z}}$$

The three-dimensional system provides the greatest dilution rate, $C_{max} \sim t^{-3/2}$, because diffusion can occur in all directions. In the 1-D and 2-D systems, diffusive flux can only occur in 1 or 2 directions, respectively, such that the rate of dilution is diminished to $t^{-1/2}$ and t^{-1}, respectively. The difference in dilution rate is depicted below. A slug of mass is released into a 1-D, 2-D, and 3-D system, such that at some small time the maximum concentration in each cloud is the same. Subsequently, the maximum concentration decays most rapidly in the least constrained system, i.e. the 3-D system.