1.061 / 1.61 Transport Processes in the Environment Fall 2008

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5. Advection and diffusion of an instantaneous release



The diffusion of a cloud in a static fluid was examined in Chapter 3. This chapter takes things one step further and looks at the simultaneous advection and diffusion of an instantaneous release in a uniform flow. The cloud structure studied in Chapter 3 still holds here, as there is a Gaussian concentration distribution about the cloud's center of mass, which now moves at the flow velocity. The distinction between spatial and temporal records of concentration is also examined. The use of the Peclet number in determining the relative importance of advection and diffusion in scalar transport is strongly emphasized. If systems are dominated by either advection or diffusion, it becomes simple to determine the time taken for a chemical to be observed at a given distance from the release.

The example problems test one's ability to simplify analyses based on the Peclet number, and to distinguish between spatial and temporal records of concentration.

5. Advection and Diffusion of an Instantaneous, Point Source

In this chapter consider the combined transport by advection and diffusion for an instantaneous point release. We neglect source and sink terms. For isotropic and homogeneous diffusion the transport equation reduces to,

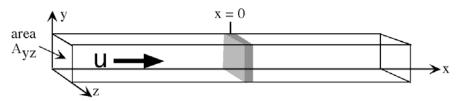
(1)
$$\frac{\partial \mathbf{C}}{\partial t} + \mathbf{u} \frac{\partial \mathbf{C}}{\partial x} + \mathbf{v} \frac{\partial \mathbf{C}}{\partial y} + \mathbf{w} \frac{\partial \mathbf{C}}{\partial z} = \mathbf{D} \left[\frac{\partial^2 \mathbf{C}}{\partial x^2} + \frac{\partial^2 \mathbf{C}}{\partial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

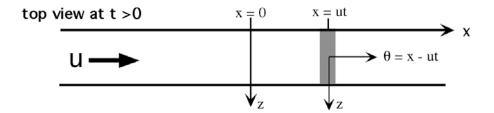
For simplicity we begin with a one-dimensional system in x, *i.e.* all flow parameters are uniform in y and z, such that $\partial/\partial y = 0$ and $\partial/\partial z = 0$. The transport equation reduces to,

(2)
$$\frac{\partial \mathbf{C}}{\partial \mathbf{t}} + \mathbf{u} \frac{\partial \mathbf{C}}{\partial \mathbf{x}} = \mathbf{D} \frac{\partial^2 \mathbf{C}}{\partial \mathbf{x}^2}$$

This equation describes transport in the model system below. Into this system we release an instantaneous, point mass, shown as a gray slab, at x = 0 and t = 0. 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 $\delta(x)$ is the Dirac delta function.

perspective view at t = 0





To solve (2) for $C(x) = M \delta(x)$, it is useful to change the frame of reference from the stationary coordinates (x, t) to the moving coordinates (θ, t) . The longitudinal coordinate $\theta = x - ut$, shown in the top view, moves with the mean flow, u, and $\theta = 0$ remains at the center of mass for all time. We convert (2) from (x, t) to (θ, t) using the chain rule of differentiation and by noting that $\partial\theta/\partial t = -u$.

$$\frac{\partial C(\theta, t)}{\partial t} = \frac{\partial C}{\partial \theta} \frac{\partial \theta}{\partial t} + \frac{\partial C}{\partial t} \frac{\partial t}{\partial t} = -u \frac{\partial C}{\partial \theta} + \frac{\partial C}{\partial t}$$

$$(3) \qquad \frac{\partial C(\theta, t)}{\partial x} = \frac{\partial C}{\partial \theta} \frac{\partial \theta}{\partial x} + \frac{\partial C}{\partial t} \frac{\partial t}{\partial x} = \frac{\partial C}{\partial \theta}$$

$$\frac{\partial^2 C(\theta, t)}{\partial x^2} = \frac{\partial^2 C}{\partial \theta^2}$$

Substituting from (3) for $\partial C/\partial t$, $\partial C/\partial x$, and $\partial^2 C/\partial x^2$, (2) becomes,

(4)
$$\frac{\partial \mathbf{C}}{\partial \mathbf{t}} = \mathbf{D} \frac{\partial^2 \mathbf{C}}{\partial \theta^2}$$
.

With the initial condition C ($\theta = 0$, t = 0) = M $\delta(\theta)$, the solution to (4) is (eq. 10, ch. 3),

(5)
$$C(\theta,t) = \frac{M}{A_{yz}\sqrt{4\pi Dt}} \exp(-\theta^2/4Dt).$$

Converting back to the stationary frame of reference, we arrive at

(6)
$$C(x,t) = \frac{M}{A_{yz} \sqrt{4\pi Dt}} \exp(-(x-ut)^2/4Dt)$$

Instantaneous, Point Release in One Dimension

Transport equation:
$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} = D \frac{\partial^2 C}{\partial x^2}$$

Initial Condition:
$$C = M \delta(x)$$
 at $t = 0$.

$$C(x,t) = \frac{M}{A_{yz}\sqrt{4\pi Dt}} \exp(-(x-ut)^2/4Dt).$$

The concentration field described by (6) is depicted in the Figure 1. An important feature of this solution is that the argument of the exponential is zero at the center of mass, *i.e.* at x = ut, and the maximum concentration, $C_{max} = M/\sqrt{4\pi Dt}$, always occurs at the center of the mass. As seen previously, the length-scale of the diffusing cloud is set by $\sigma = \sqrt{2Dt}$. Since the spatial position of the cloud, x, is coupled to its temporal evolution through the steady advection, *i.e.* t = x/u, both C_{max} and σ grow predictably downstream. Specifically, $\sigma = \sqrt{2Dx/u}$ and $C_{max} \sim x^{-1/2}$.

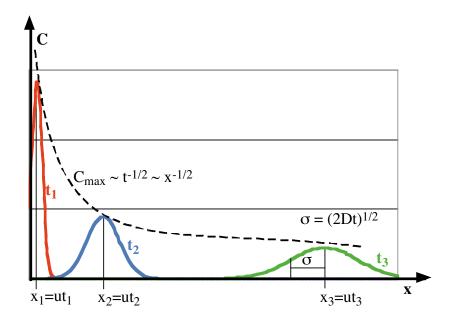


Figure 1. Evolution of concentration field after an instantaneous release of point-mass in a one-dimensional system with steady advection, u, and diffusion, D. Profiles in red, blue, and green represent C(x,t), at $t=t_1$, t_2 , and t_3 , respectively. The peak concentration decays at $t^{-1/2}$ and $x^{-1/2}$, as indicated by the dashed line.

Instantaneous, Point Release in Two and Three Dimensions:

That the argument of the exponential term is zero at the center of mass can be used to quickly devise a solution for any system with multiple components of velocity, anisotropic diffusion, and mass released at an arbitrary position (x_0, y_0, z_0) . In this system, the center of mass traces the trajectory $(x = x_0 + ut, y = y_0 + vt, z = z_0 + wt)$. The concentration field follows from the solution for an instantaneous, point-mass release in a stagnant system, derived in chapter 3, with the arguments of the exponential term adjusted to zero along the above trajectory.

Instantaneous, Point Release in Two Dimensions L_z = length-scale of neglected dimension

Transport Equation:
$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} + v \frac{\partial C}{\partial y} = D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2}$$

Initial Condition:
$$C = M \delta(x-x_0) \delta(y-y_0)$$
 at $t = 0$.

$$C(x,y,t) = \frac{M}{L_z 4\pi t \sqrt{D_x D_y}} exp \left(-\frac{(x - x_0 - ut)^2}{4D_x t} - \frac{(y - y_0 - vt)^2}{4D_y t} \right)$$

Instantaneous, Point Release in Three Dimensions

Transport equation:
$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} + v \frac{\partial C}{\partial y} + w \frac{\partial C}{\partial z} = D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} + D_z \frac{\partial^2 C}{\partial z^2}$$

Initial Condition:
$$C = M \delta(x-x_0) \delta(y-y_0) \delta(z-z_0)$$
 at $t = 0$.

$$C(x,y,z,t) = \frac{M}{(4\pi t)^{3/2} \sqrt{D_x D_y D_z}} exp \left(-\frac{(x-x_0-ut)^2}{4D_x t} - \frac{(y-y_0-vt)^2}{4D_y t} - \frac{(z-z_0-wt)^2}{4D_z t} \right)$$

Example Problem: Mass, M, is injected at x = 0 cm, y = 50 cm, and t = 0 s into a two-dimensional system with constant, uniform velocity, $u = 1 \text{cms}^{-1}$ and isotropic diffusivity, $D = 2 \text{ cm}^2 \text{s}^{-1}$. The center of mass follows the trajectory (x = ut, y = 50 cm). The resulting concentration field follows from the two-dimensional solution given above,

Concentration field:
$$C(x,y,t) = \frac{M}{L_x 4\pi Dt} exp\left(-\frac{(x-ut)^2 + (y-50)^2}{4Dt}\right)$$
.

Here z is the neglected dimension with length-scale, L_z . Concentration is measured at three points in the system. Probe A is located at $x_A = 100$ cm, $y_A = 50$ cm. Probe B is located at $x_B = 250$ cm, $y_B = 50$ cm. Probe C is located at $x_C = 250$ cm, $y_C = 0$ cm.

- 1. Estimate the time at which the peak concentration will be observed at each probe.
- 2. Estimate the physical length of the cloud at the time the peak arrives at each probe.
- 3. Estimate the duration of time that the cloud is observed at station.
- 4. Compare the maximum concentration observed at each probe by estimating the ratios C_{Amax}/C_{Bmax} and C_{Bmax}/C_{Cmax} .

Answer.

- 1. The peak concentration will be observed when the center of mass passes each probe. The center of mass advects at $u = 1 \text{ cms}^{-1}$. Thus, for Probe A, located at $x_A = 100 \text{ cm}$, the peak concentration will arrive at $t_A = x_A/u = 100 \text{ cm}/1 \text{ cms}^{-1} = 100 \text{ s}$. The peak concentration arrives at probes B ($x_B = 250 \text{ cm}$) and C ($x_C = 250 \text{ cm}$) at $t_B = t_C = 250 \text{ s}$.
- 2. The length-scale of the cloud is estimated as $L \approx 4\sigma$ (Ch. 3, eq. 14). At probe A the cloud will be $L_A \approx 4\sigma_A = 4\sqrt{2Dt_A} = 4\sqrt{2\times2cm^2s^{-1}\times100s} = 80$ cm. At probes B and C the cloud will be $L_B = L_C \approx 4\sigma_B = 4\sqrt{2Dt_B} = 4\sqrt{2\times2m^2s^{-1}\times250s} = 126$ cm
- 3. Assuming that the cloud does not grow in the time that it takes to pass the probe, we estimate the duration the cloud is observed, Δt , using the cloud length and the velocity. At Probe A, $\Delta t = L_A/u = 80$ s. At B and C, $\Delta t = L_B/u = 126$ s. Remember that these estimates define the cloud by a fixed fraction of total initial mass. The actual duration that the cloud is observed will also depend on the detection limit of the probe.

4. The peak concentration at each probe location is readily found by evaluating the full solution above at the position of each probe and the time of peak arrival.

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Probe A: C_A(x = 100 \text{ cm}, y = 50 \text{ cm}, t = t_A = 100 \text{ s}) = M/(L_Z 4\pi D t_A)

Probe B: C_B(x = 250 \text{ cm}, y = 50 \text{ cm}, t = t_B = 250 \text{ s}) = M/(L_Z 4\pi D t_B)

Probe C: C_C(x = 250 \text{ cm}, y = 0 \text{ cm}, t = t_B = 250 \text{ s}) = [M/(L_Z 4\pi D t_C)] \exp(-50^2/4D t)

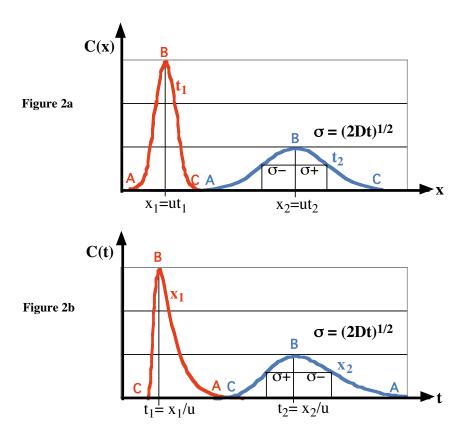
Thus, C_{Amax}/C_{Bmax} = t_B/t_A = x_B/x_A = 2.5; and C_{Cmax}/C_{Bmax} = \exp(-50^2/4D t_C) = 0.29
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Now view the animation on the chapter 5 homepage and confirm that the time- and length-scales derived above are consistent with the full spatial evolution of the cloud, as described by the above equation and depicted in the animation. Note that each probe records a Gaussian-shaped profile, including the probe positioned off-center, i.e. Probe C. The peak concentration decays at $C_{max} \sim x^{-1} \sim t^{-1}$.

Spatial and Temporal Records of Concentration:

In practice there are two ways to observe a distribution of concentration. First, one can measure the concentration everywhere in the flow at the same time. From this type of observation one can recreate the full spatial concentration field. While this is feasible in a laboratory where spatial scales are small, it is nearly impossible in the field. In the field it is more common to sample at a single or limited number of fixed positions and record the concentration at each position over time. For the purpose of interpreting field data, it is necessary to relate spatial and temporal observations. Consider an instantaneous, point-mass released in a one-dimensional system, for which the concentration field is described by (6). Figure 2a depicts the spatial distribution, C(x), at two points in time. To directly measure C(x) requires many simultaneous measurements along the x-axis. For comparison, consider observations made by two probes located at fixed positions, x_1 and x_2 , which record continuously over time. These records are shown in Figure 2b.

The curves in 2a and 2b represent the same cloud at different times and spatial positions. First, note that on each set of curves (red and blue) B marks an identical measurement at (x_1, t_1) and (x_2, t_2) , respectively. Second, the spatial distribution, C(x), visually preserves the orientation of leading (C) and trailing (A) edge of the cloud. In the temporal distribution these are visually reversed, such that the leading edge (C) appears to the left of the trailing edge (A), as the leading edge is encountered first. Third, the temporal record C(t) appears skewed to the right (positive time), but the spatial distribution, C(x), is symmetric. Specifically, in Figure 2a the length scale of the cloud downstream of the peak, σ -, is identical to its length scale upstream of the peak, σ +. In C(x), σ – and σ + have dimensions of length. In C(t), σ – and σ + have dimensions of time, and σ + is distinctly less than σ - (Fig. 2b). The skew in C(t) arises because the cloud continues to grow, $\sigma \sim t^{1/2}$, even as it passes position x_2 , such that the trailing edge of the cloud is longer as it passes x_2 at $t > t_2$ than the leading edge of the same cloud was as it passed x_2 at $t < t_2$. The distinction between an apparent skew, as seen here in C(t), and a real skew in mass distribution recorded in C(x) is important because skewness in C(x) indicates a non-Fickian diffusion processes. If the spread of mass follows Fick's Law, the mass distribution will be symmetric. Chapter 8 will introduce several mechanisms that contribute to the spread of mass but which can be non-Fickian and can produce skew in the mass distribution.



Peclet Number

The Peclet Number is a dimensionless parameter that indicates the relative importance of advection and diffusion to the transport of scalars in a given system. If we describe the advection and diffusion in terms of characteristic time scales, the Peclet number is the ratio of these time scales. The time scales are defined by dimensional constraints, *i.e.* the only combination of length scale, L, and flow speed, U, that yields a unit of time is

Advection Time Scale = $T_U \sim L/U$.

The only combination of length, L, and diffusion rate, D, that yields a unit of time is

Diffusion Time Scale = $T_D \sim L^2/D$.

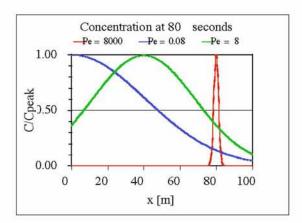
The Peclet Number is then the ratio of these two scales.

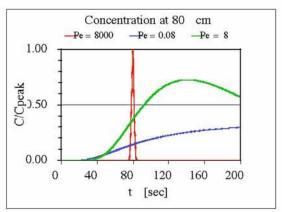
Peclet Number,
$$Pe = \frac{T_D}{T_U} = \frac{UL}{D}$$
.

When $T_U \ll T_D$ transport by advection is faster than transport by diffusion, and we say that the system is advection dominated. This corresponds to Pe >> 1. If Pe << 1,

diffusion dominates. The advection time scale T_U is, in fact, more than just a dimensional construction. Physically, it is exactly the time required to travel distance L at speed U. This is not true of the diffusion time scale T_D . To define a more exact diffusion time scale, we must consider a specific model for the diffusion process. If we assume Fickian diffusion, then we can define the edge of the cloud as being 2σ from the center of mass. Mass originating at x = 0 is estimated to reach x = L by diffusion when $2\sigma = 2\sqrt{2Dt} = L$. This occurs at $T_{2\sigma} = L^2/8D$. Using this revised time scale, we estimate that transport by diffusion will be faster than advection when $T_{2\sigma} << T_U$, or Pe = UL/D << 8. Thus, we refine the scaling estimate by applying a physical model for diffusion. The refinement indicates that for Pe >> 8 advection dominates and for Pe << 8 diffusion dominates.

Figure 3 compares the concentration records observed in three different systems with Pe = 8000, 8, and 0.08. The upper graph shows the spatial distribution of concentration 80 seconds after an instantaneous injection of mass at x = 0. The lower graph shows the temporal observation of concentration at the fixed point x = 80-cm.





	U [cm s ⁻¹]	D [cm ² s ⁻¹]	L [cm]	$T_U = L/U[s]$	$T_{2\sigma} = L^2/8D [s]$
Pe = 8000	1	0.01	80	80	80,000
Pe = 8	0.5	5	80	160	160
Pe = 0.08	0.01	10	80	8000	80

Figure 3. Concentration observed for Pe = 0.8, 8, 8000, normalized by the peak concentration in each system at t = 80 seconds. System characteristics are summarized in the table above.

Consider C(t) shown in the lower graph of Figure 3. These curves show the arrival of mass at x = L = 80 cm from the point of release. When Pe = 8000, advection controls transport, and mass arrives at the advection time scale, $T_U = 80$ s. When Pe = 0.08, diffusion controls transport, and the mass arrives at the measurement station in the diffusion time scale, $T_{2\sigma} = 80$ s, rather than the advection time scale, $T_U = 8000$ s. Finally, for Pe = 8, the diffusion and advection time scales are identical, $T_U = T_{2\sigma} = 160$ s, but neither is a good estimator of the arrival of mass.

Scaling the Transport Equation

The Peclet number also emerges through scaling the governing equation. For simplicity, consider a one-dimensional system in x with mean velocity, U, and a constant diffusion coefficient, D. We consider the concentration observed over a test section of length L observed for time scale t_0 . The governing transport equation for this system is

(7)
$$\frac{\partial \mathbf{C}}{\partial t} + \mathbf{u} \frac{\partial \mathbf{C}}{\partial x} = \mathbf{D} \frac{\partial^2 \mathbf{C}}{\partial x^2}$$

To determine what processes are most important, we compare the magnitudes of each term. To do this we must recast each variable into a dimensionless form of O(1). For example, we use the test section length, L, to scale the distance x, such that the dimensionless distance $x^* = x/L$ will be O(1) within the test section. Similarly we define $C^* = C / C_{max}$; $u^* = u/U$; $t^* = t/t_0$. We use the new variables to replace C, u, x, and t in (7), and note that $\partial x^2 = \partial x \partial x$ to find

(8)
$$\frac{C}{t_0} \frac{\partial C^*}{\partial t^*} + \frac{UC}{L} u^* \frac{\partial C^*}{\partial x^*} = \frac{DC}{L^2} \frac{\partial^2 C^*}{\partial x^{*2}}.$$

We then divide each term by DC/L² to arrive at the dimensionless equation

(9)
$$\frac{L^{2}/D}{t_{o}} \frac{\partial C^{*}}{\partial t^{*}} + \frac{UL}{D} u^{*} \frac{\partial C^{*}}{\partial x^{*}} = \frac{\partial^{2}C^{*}}{\partial x^{*2}}.$$

$$O(1) \qquad \text{Pe} \quad O(1) \qquad O(1)$$

unsteadiness advection diffusion

Since each starred variable is O(1) by construction, we can compare the unsteadiness, the advection, and the diffusion terms simply by comparing the dimensionless prefactor of each term. For example, the diffusion term has no pre-factor, and so the magnitude of this term is simply O(1). The advection term has the pre-factor UL/D, which defines the Peclet number. If Pe >> 1, then the advection term is larger than the diffusion term, which is O(1). To first order then, the diffusion term can be neglected. Similarly, if Pe << 1, the advection term can be neglected. One can determine the scale of the unsteady term by the magnitude of the prefactor, L^2/Dt_o . For example, if Pe << 1 [diffusion dominates] and L^2/Dt_o >> 1, then unsteadiness in concentration will be observed over the time-scale of interest, t_o . If, L^2/Dt_o << 1, then no unsteadiness in concentration will be observed (to first order) over time t_o .