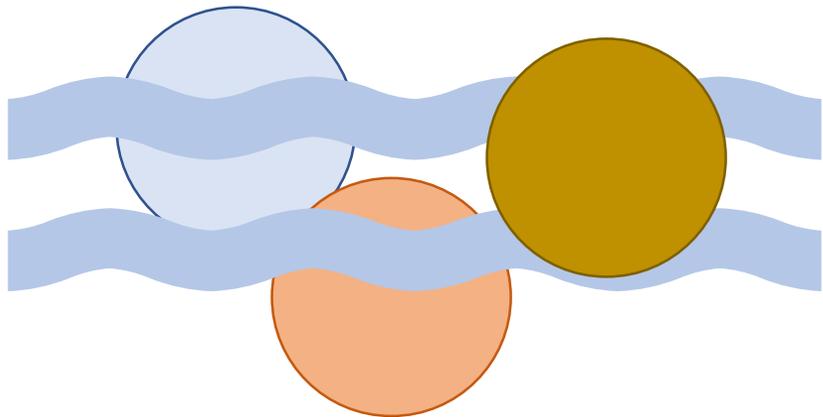
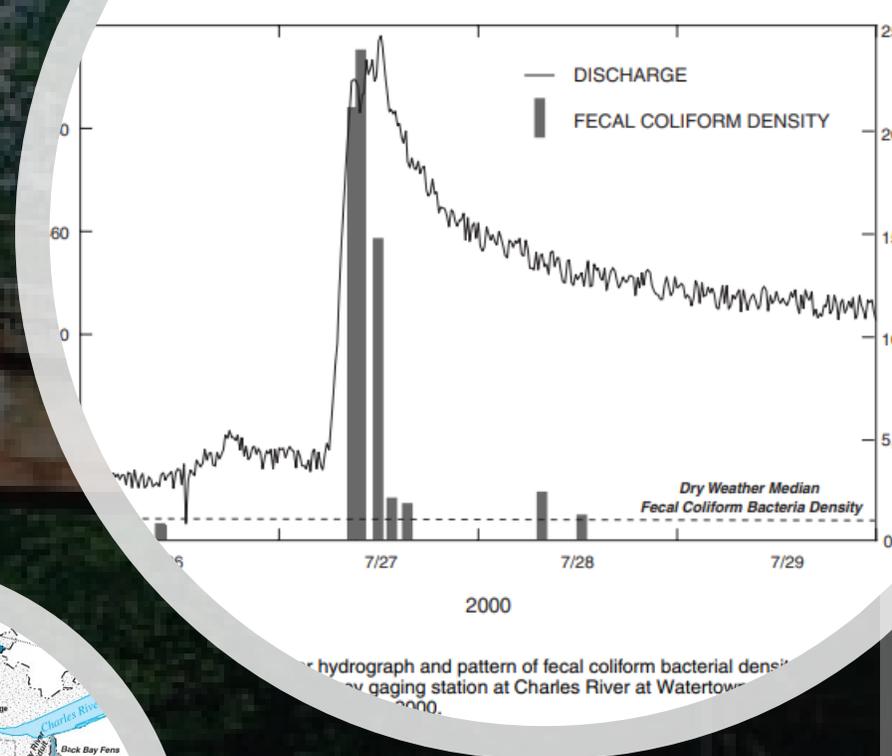
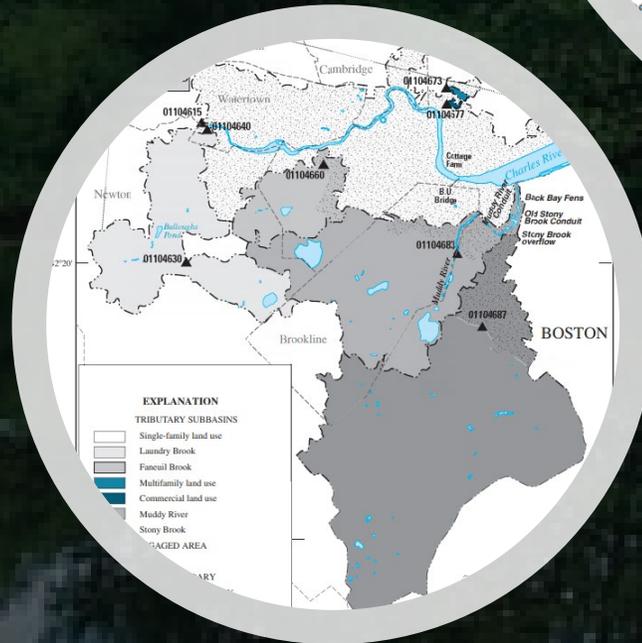


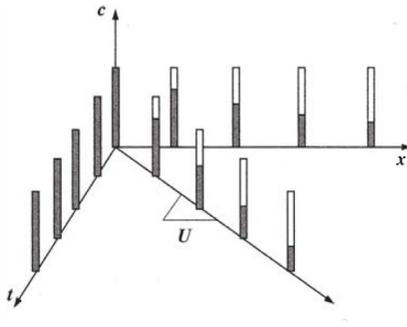
Distributed Systems (Time-Variable)



We continue our discussion of distributed systems by studying the temporal characteristics of plug-flow & mixed-flow systems. A focus will be on instantaneous discharge into a one-dimensional channel (e.g. spills and tracer studies).



Plug Flow



The time-variable mass balance for the plug-flow system can be written as:

$$\frac{\partial c}{\partial t} = -U \frac{\partial c}{\partial x} - kc$$

If a spill causes a concentration c_0 at $t = x = 0$, the solution is:

$$\begin{aligned} c &= c_0 e^{-kt} && \text{for } t = x/U \\ c &= 0 && \text{otherwise} \end{aligned}$$

Plug Flow

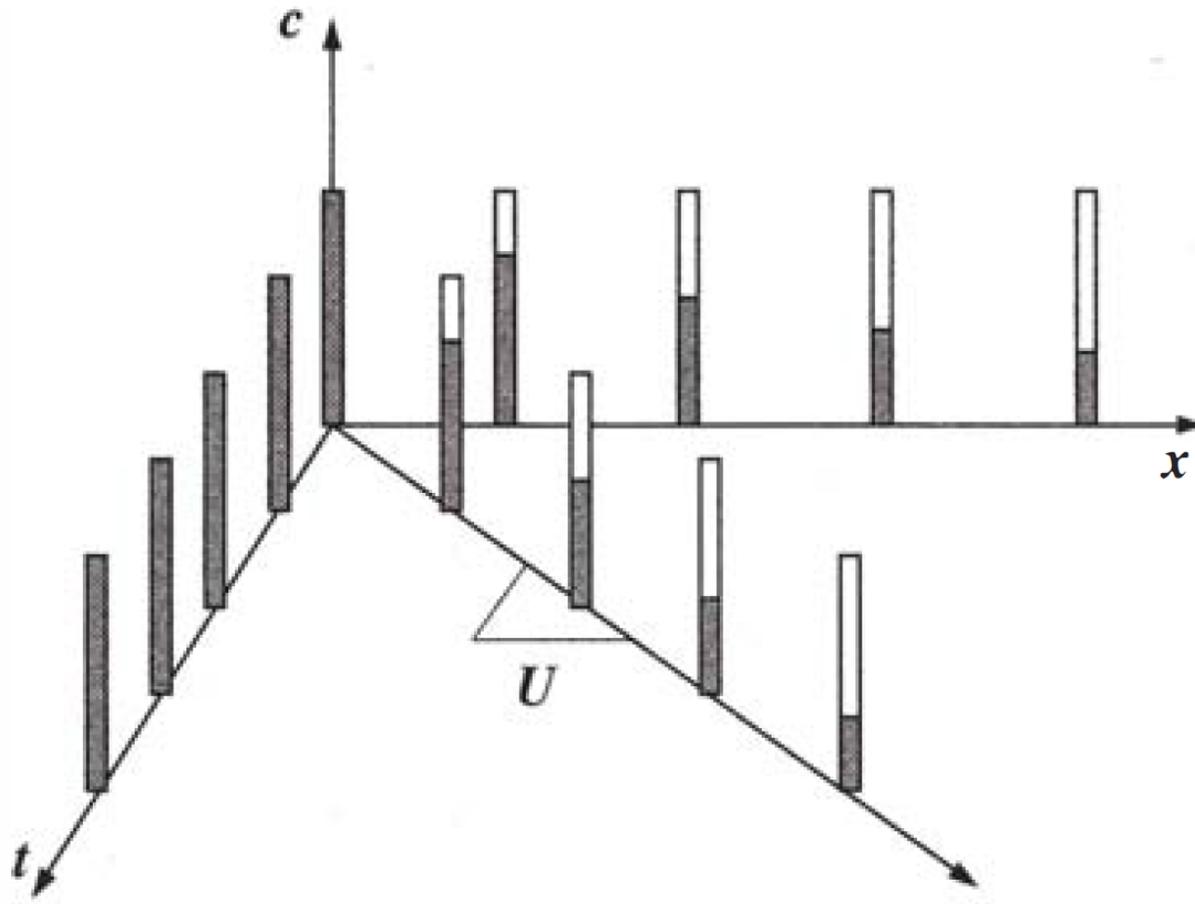
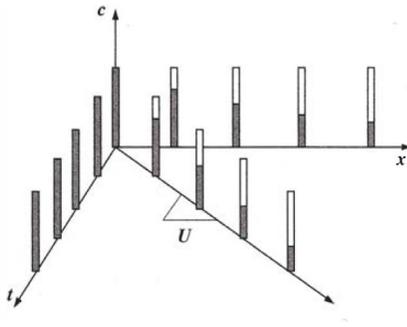


FIGURE 10.1

Depiction of the movement of dye in space and time for a plug-flow system. The whole plugs show the movement of a conservative substance. The shaded portions show a substance that reacts with first-order kinetics.

Plug Flow



If a spill causes a concentration c_0 at $t = x = 0$, the solution is:

$$\begin{aligned} c &= c_0 e^{-kt} && \text{for } t = x/U \\ c &= 0 && \text{otherwise} \end{aligned}$$

Further, the velocity establishes a direct relationship between time and space,

$$t = \frac{x}{U}$$

i.e. the solution can also be:

$$\begin{aligned} c &= c_0 e^{-\frac{k}{U}x} && \text{for } x = U/t \\ c &= 0 && \text{otherwise} \end{aligned}$$

EXAMPLE 10.1. SPILL INTO A PLUG-FLOW SYSTEM. Five kg of a conservative pollutant is spilled into a stream over a period of about 5 min. The stream has the following characteristics: flow = $2 \text{ m}^3 \text{ s}^{-1}$ and cross-sectional area = 10 m^2 . Determine the concentration and the extent of the spill and how long it takes to reach a water intake located 6.48 km downstream.

Plug Flow

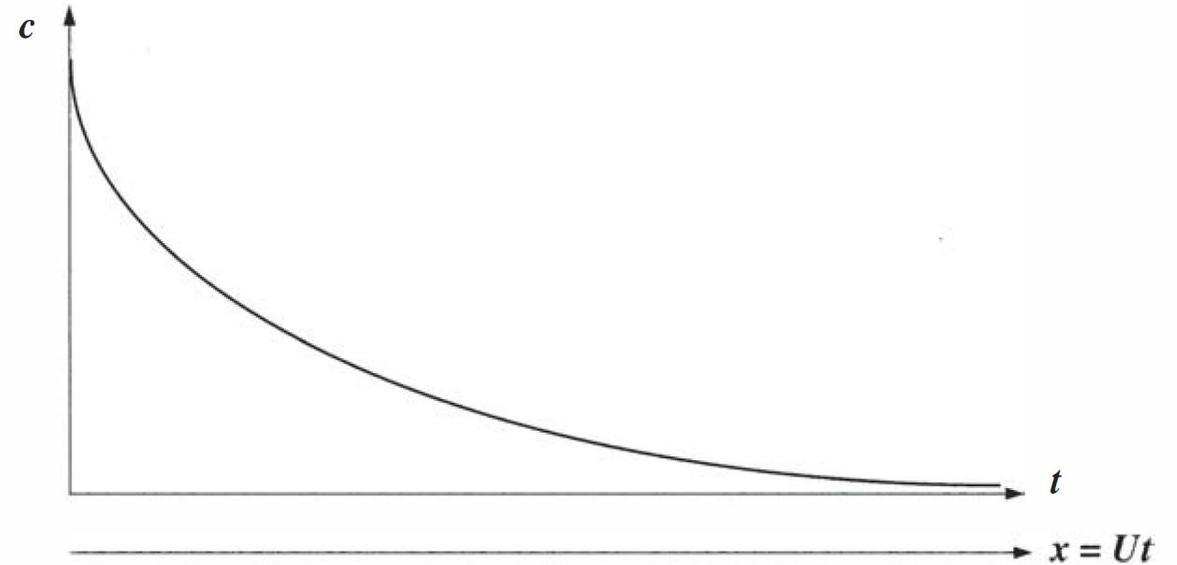
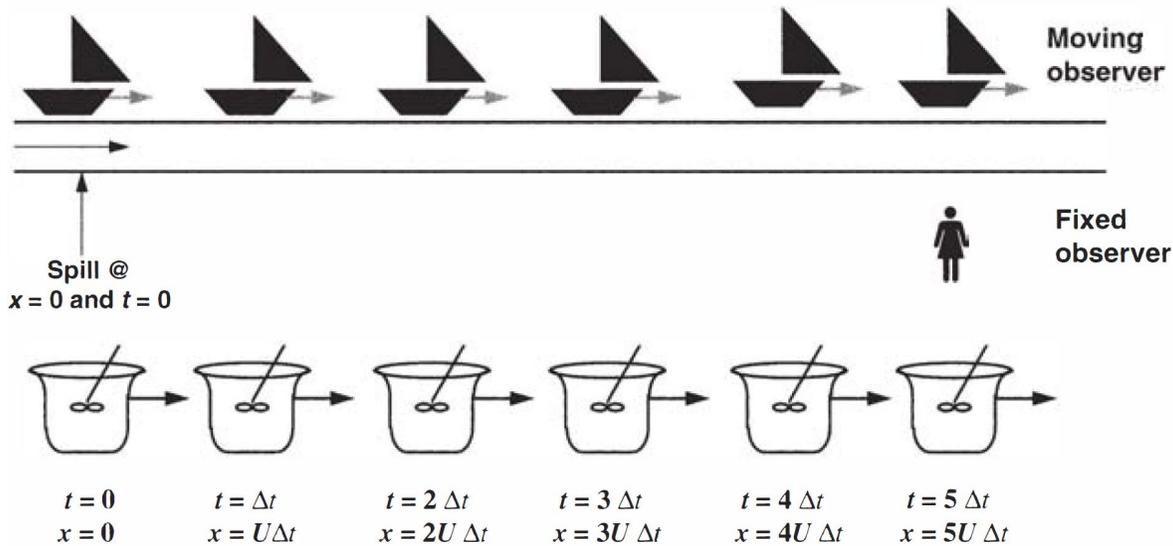


FIGURE 10.2

Two perspectives for viewing temporal and spatial changes in a plug-flow system.

We recognize two perspectives of an observer at a fixed location and a moving observer. The fixed observer sees nothing until $t = x/U$. If the spill is decaying, the concentration will be reduced at this observation period.

Moving observers would watch the concentration decay exponentially as if watching a batch reactor.

Plug Flow

The interrelationship between space and time also applies to steady-state solutions. For example, recall the steady-state solution for a continuous load into a plug-flow system:

$$c = c_0 e^{-\frac{k}{U}x}$$

Now we should recognize again with $t = x/U$:

$$c = c_0 e^{-kt}$$

Where t represents travel time below the point source.



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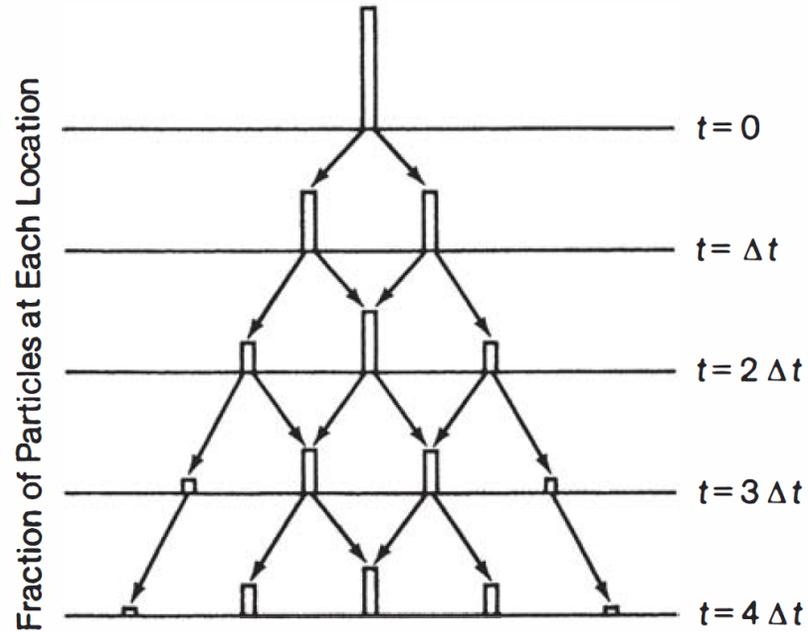
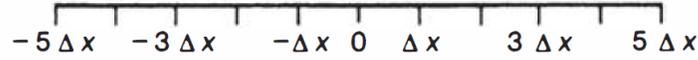


FIGURE 10.3

Graphic representation of a random walk. At time $t = 0$, all particles are grouped at the origin ($x = 0$). During each time step Δt , half the particles at each location move left and half move right. The result is that over time the particles spread out in a bell-shaped pattern.

Random (Or “Drunkard’s”) Walk

The random walk describes the type of random motion found in diffusion processes. The name DW stems from similar pattern.

After each Δt , particles will have equal likelihood of moving small distances to the left ($-\Delta x$) or to the right (Δx). After several Δt intervals, the particles will begin to spread out as at each interval there is a 50-50 chance of moving to the left/right.

Extremes are less likely due to successive moves.

The random walk process can be expressed mathematically as:

$$p(x, t) = \frac{1}{2\sqrt{\pi Dt}} e^{-\frac{x^2}{4Dt}}$$

where $p(x, t)$ = the probability that a particle will be at x after an elapsed time t and D = a diffusion coefficient, defined as:

$$D = \frac{\Delta x^2}{2\Delta t}$$

If the population is grouped at the origin at time zero, the number of individuals at position x at a subsequent time t would be proportional to the probability of an individual particle's being at x . Thus the probability equation can be expressed in terms of mass and concentration.

Random Walk

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$$c(x, t) = \frac{m_p}{2\sqrt{\pi Dt}} e^{-\frac{x^2}{4Dt}}$$

Random Walk

$$c(x, t) = \frac{m_p}{2\sqrt{\pi Dt}} e^{-\frac{x^2}{4Dt}}$$

where m_p = total mass of the particles normalized to the cross-sectional area (ML^{-2}). Thus the distribution of population of particles is described by a series of bell-shaped curves that spread out over time symmetrically about the origin.

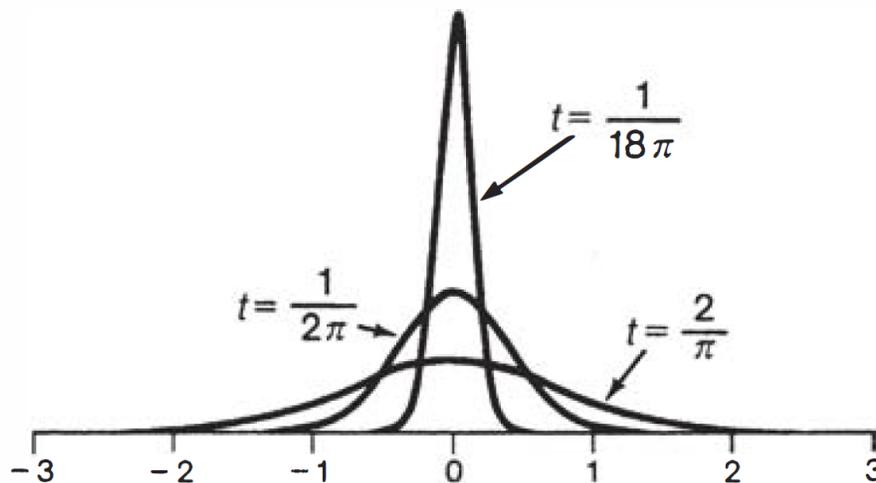


FIGURE 10.4

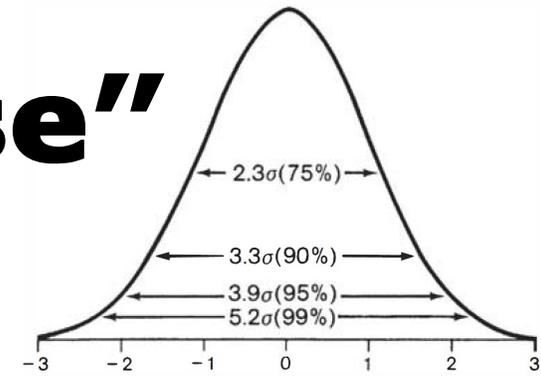
Representation of the random walk by a normal or “bell-shaped” distribution.

An aerial photograph showing a large, irregularly shaped oil spill in a wide river. The spill is a dark, viscous substance that has spread across a significant portion of the water's surface. In the background, there are several modern buildings, including one with a sign that reads "RIVERWALK". A pier or dock structure is also visible on the right side of the image.

Spill Models

Beyond random walk, we can integrate dispersion into models of instantaneous discharges into uniform, one-dimensional channels. We investigate spills occurring instantaneously and then a model for continuous input.

Instantaneous or “Impulse” Spills



We will add mechanisms on a term-by-term basis.

Diffusion/dispersion: A mass balance for a substance that disperses in a one-dimensional channel can be written as (with $k=U=0$):

$$\frac{\partial c}{\partial t} = E \frac{\partial^2 c}{\partial x^2}$$

This relationship is sometimes referred to as Fick’s second law. The solution for the case where the substance is initially concentrated at $x=0$ is:

$$c(x, t) = \frac{m_p}{2\sqrt{\pi Et}} e^{-\frac{x^2}{4Et}}$$

Instantaneous or “Impulse” Spills

For a conservative substance that is discharged in a lump sum to a water body, its tendency to spread outward from its center of mass. This could be represented by the standard deviation:

$$\sigma = \sqrt{2Et}$$

or also as multiples of standard deviation (depicted in the curve). E.g. 95% and 99% spreads are roughly approximated by 4σ and 5σ .

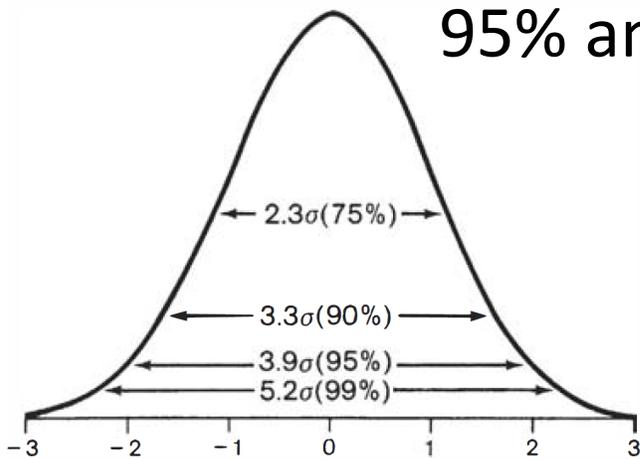


FIGURE 10.5

A standardized normal distribution showing the probability (expressed as percent) encompassed by various multiples of the standard deviation. For example 3.9σ encompasses 95% of the area under the curve.

EXAMPLE 10.2. CONSERVATIVE SPILL IN A CHANNEL WITH NO FLOW.

A barge releases a large quantity of a highly persistent contaminant in the center of a canal that is not flowing. If the dispersion coefficient is approximately $10^5 \text{ m}^2 \text{ d}^{-1}$, how far will the contaminant spread in 1 d? In 2 d? Assume that a 95% band adequately approximates the extent of the spill.

Instantaneous or “Impulse” Spills

Dispersion/advection: Now we can add advection to the model terms developed so far ($\frac{\partial c}{\partial t} = E \frac{\partial^2 c}{\partial x^2}$). This relationship is sometimes referred to as the *advection-diffusion* (or *advection-dispersion*) equation.:

$$\frac{\partial c}{\partial t} = -U \frac{\partial c}{\partial x} + E \frac{\partial^2 c}{\partial x^2}$$

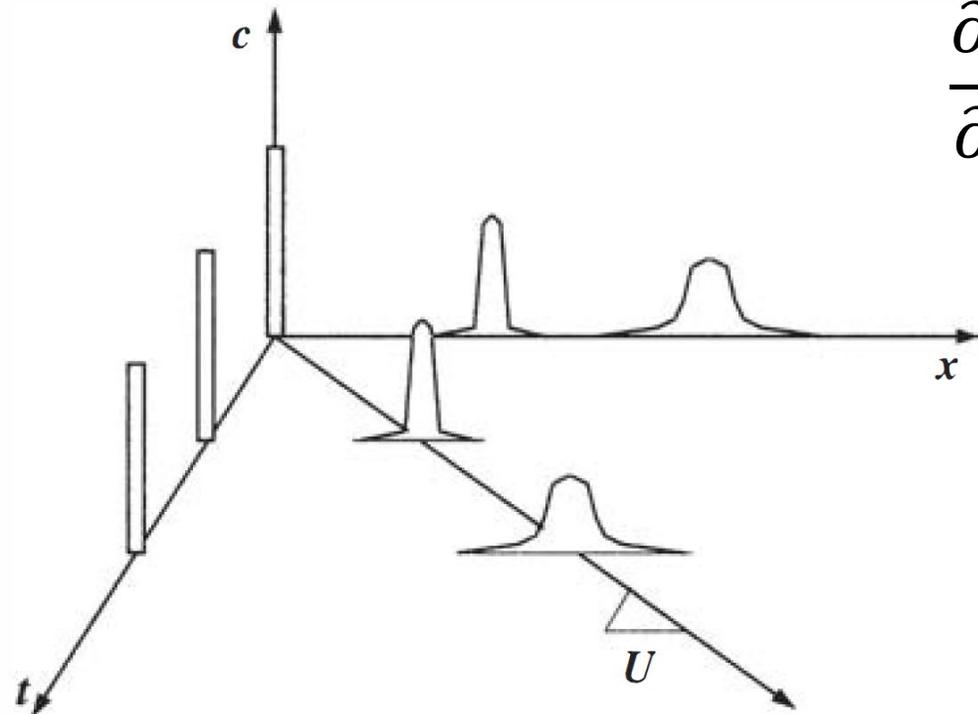


FIGURE 10.6

The movement of conservative dye in space and time for a mixed-flow system.

Instantaneous or “Impulse” Spills

The solution for the case where the substance is initially concentrated at $x = 0$ is:

$$c(x, t) = \frac{m_p}{2\sqrt{\pi Et}} e^{-\frac{(x-Ut)^2}{4Et}}$$

Note that in comparison to $(c(x, t) = \frac{m_p}{2\sqrt{\pi Et}} e^{-\frac{x^2}{4Et}})$, the effect of advection is to “move” the dispersion solution intact downstream at velocity U .

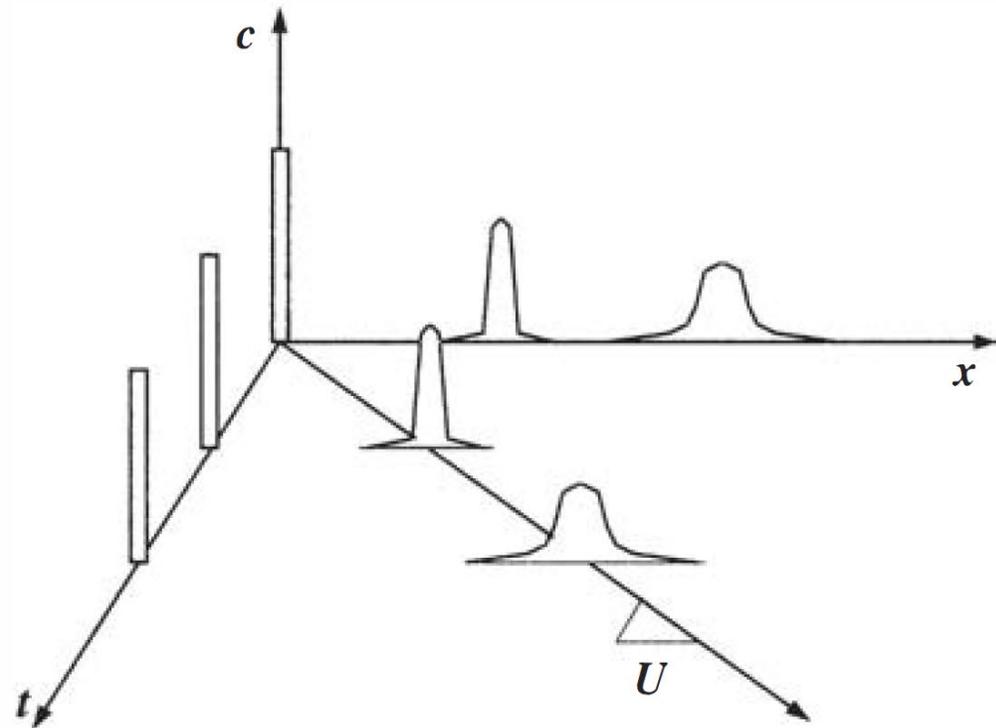


FIGURE 10.6

The movement of conservative dye in space and time for a mixed-flow system.

EXAMPLE 10.3. SPILL INTO A MIXED-FLOW SYSTEM. Evaluate the spill from Example 10.1, but include the effect of dispersion. Assume that a dispersion coefficient of $0.1 \text{ m}^2 \text{ s}^{-1}$ holds for the entire stretch. Also assume that the spill occurs instantaneously as a plane source.

Instantaneous or “Impulse” Spills

Dispersion/advection: Now a first-order reaction can be added to the model:

$$\frac{\partial c}{\partial t} = -U \frac{\partial c}{\partial x} + E \frac{\partial^2 c}{\partial x^2} - kc$$

The solution where the substance is initially concentrated at $x = 0$ is:

$$c(x, t) = \frac{m_p}{2\sqrt{\pi Et}} e^{-\frac{(x-Ut)^2}{4Et} - kt}$$

In comparison with the previous

$$(c(x, t) = \frac{m_p}{2\sqrt{\pi Et}} e^{-\frac{(x-Ut)^2}{4Et}}), \text{ the effect of}$$

decay is to reduce the area under the curve.

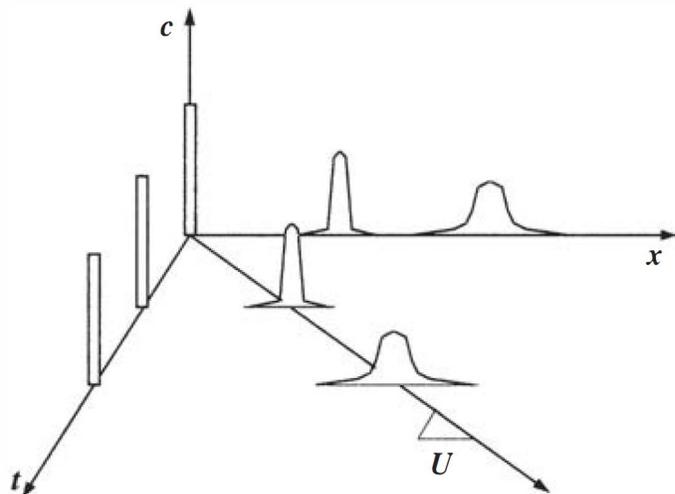


FIGURE 10.6

The movement of conservative dye in space and time for a mixed-flow system.

Instantaneous or “Impulse” Spills

Fixed versus global observer:

This previous equation ($c(x, t) = \frac{m_p}{2\sqrt{\pi Et}} e^{-\frac{(x-Ut)^2}{4Et} - kt}$), is a function of two independent variables x and t . Thus it can be viewed from two perspectives.

We can compute the spatial distribution at a fixed time (see figure) showing global perspective.

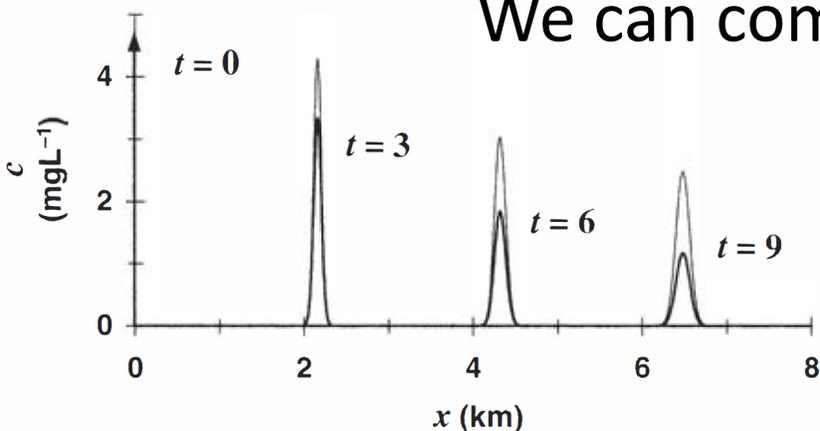


FIGURE 10.7
The effect of decay on the spill model. The thin lines are the same as calculated in Example 10.3. The heavy lines are for the same case but with $k = 2 \text{ d}^{-1}$.

We can also compute the temporal distribution at a fixed point in space. This case is for a static observer.

Instantaneous or “Impulse” Spills

Fixed versus global observer:

We can also compute the temporal distribution at a fixed point in space. This case is for a static observer.

For this case, the view can be skewed because the curve continues to spread out as it is being observed.

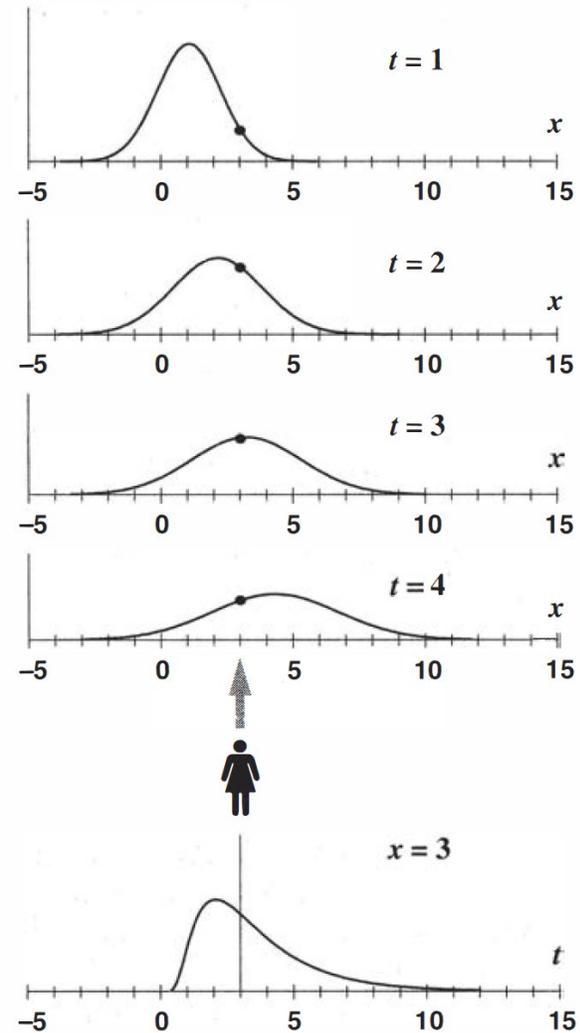


FIGURE 10.8

Although the distribution of a pollutant spill is bell-shaped in space, a fixed observer would “see” a skewed shape in time because the bell-shaped curve continues to spread out as it is being observed.

Continuous Spills

For some tracer studies, the input jumps to a constant level. Two ideal cases are depicted below:

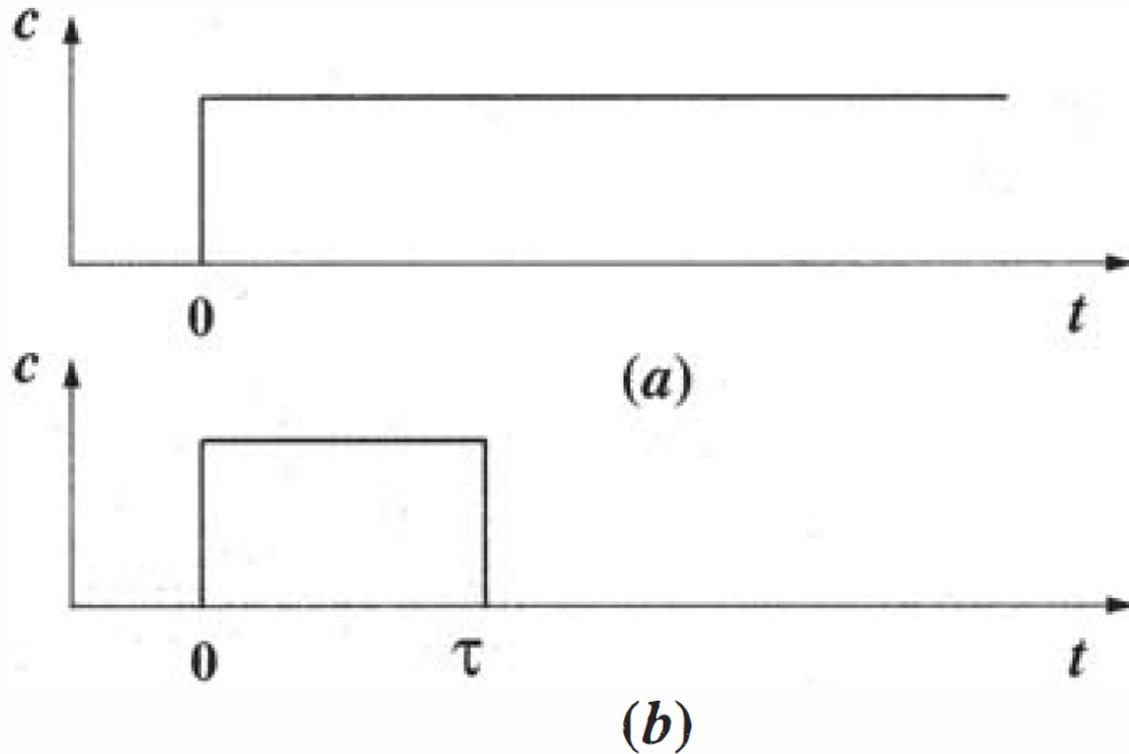


FIGURE 10.9

Continuous inputs are characterized in two ways: (a) infinite and (b) finite durations.

Continuous Spill

First the concentration increase can be maintained for an infinite duration. For this case, the solution of $(\frac{\partial c}{\partial t} = -U \frac{\partial c}{\partial x} + E \frac{\partial^2 c}{\partial x^2} - kc)$, with constant coefficients can be expressed as:

$$c(x, t) = \frac{c_0}{2} \left[e^{\frac{Ux}{2E}(1-\Gamma)} \operatorname{erfc} \left(\frac{x - Ut\Gamma}{2\sqrt{Et}} \right) + e^{\frac{Ux}{2E}(1-\Gamma)} \operatorname{erfc} \left(\frac{x + Ut\Gamma}{2\sqrt{Et}} \right) \right]$$

where

$$\Gamma = \sqrt{1 + 4\eta}$$

$$\text{and } \eta = \frac{kE}{U^2}$$



FIGURE 10.9

Continuous inputs are characterized in two ways: (a) infinite and (b) finite durations.

Continuous Spill

$$c(x, t) = \frac{c_0}{2} \left[e^{\frac{Ux}{2E}(1-\Gamma)} \operatorname{erfc} \left(\frac{x - Ut\Gamma}{2\sqrt{Et}} \right) + e^{\frac{Ux}{2E}(1-\Gamma)} \operatorname{erfc} \left(\frac{x + Ut\Gamma}{2\sqrt{Et}} \right) \right]$$

the error function complement, erfc, is equal to one minus the error function: $1 - \operatorname{erf}$. Also, $\operatorname{erf}(-x) = -\operatorname{erf}(x)$. The error function is the evaluation of the following definite integral:

$$\operatorname{erf}(b) = \frac{2}{\sqrt{\pi}} \int_0^b e^{-\beta^2} d\beta \quad \text{with } \beta = \text{dummy variable}$$

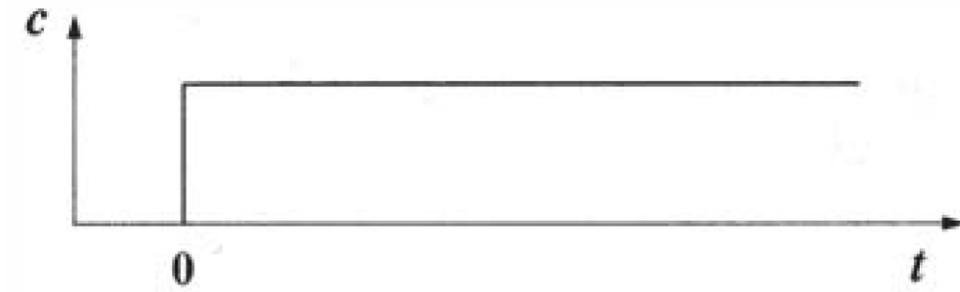


FIGURE 10.9

Continuous inputs are characterized in two ways: (a) infinite and (b) finite durations.

Continuous Spill

$$c(x, t) = \frac{c_0}{2} \left[e^{\frac{Ux}{2E}(1-\Gamma)} \operatorname{erfc} \left(\frac{x - Ut\Gamma}{2\sqrt{Et}} \right) + e^{\frac{Ux}{2E}(1-\Gamma)} \operatorname{erfc} \left(\frac{x + Ut\Gamma}{2\sqrt{Et}} \right) \right]$$

The concentration based on these error functions plot as curves. The curves shown here are referred to as “breakthrough” curves, used extensively in surface and groundwater problem contexts.

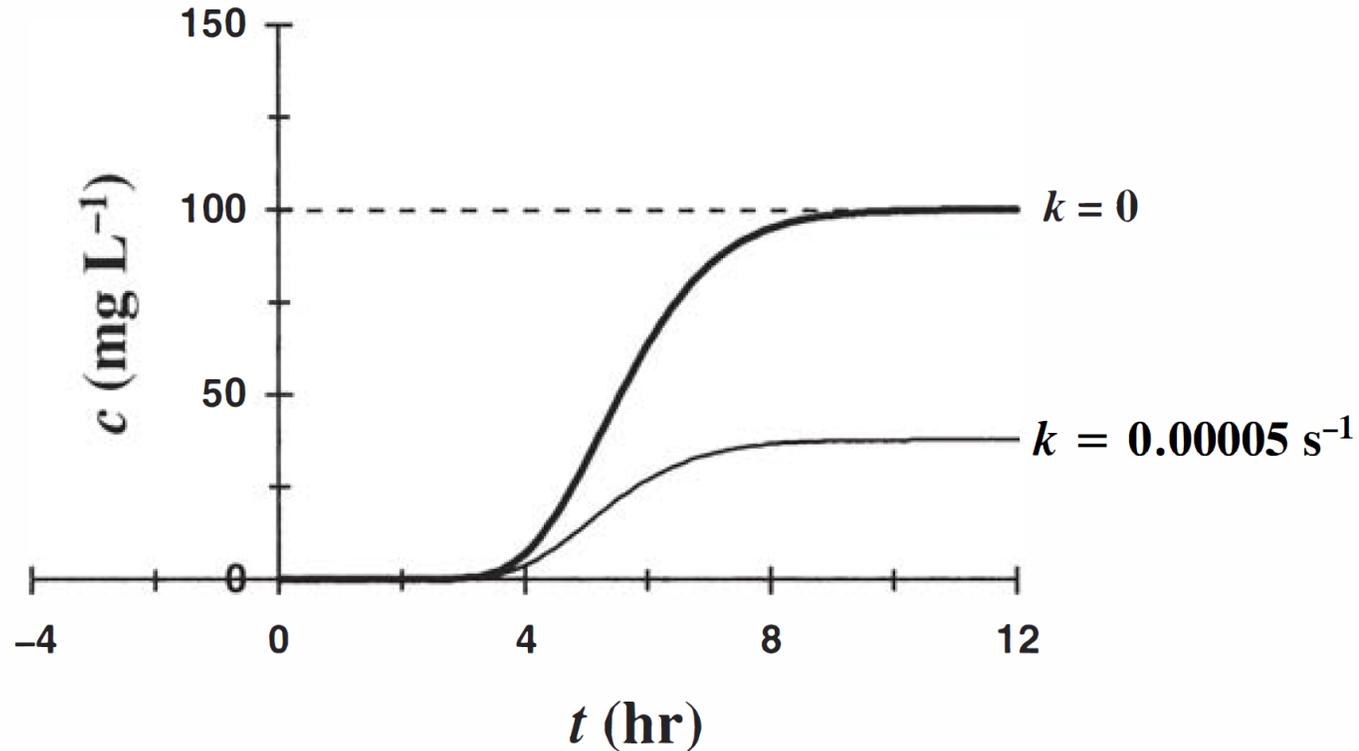
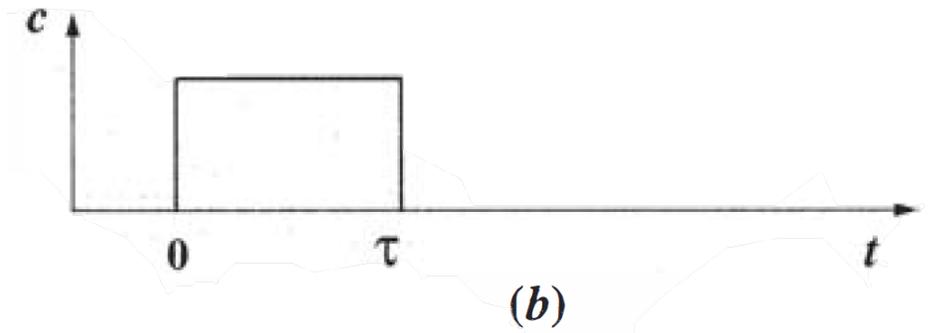


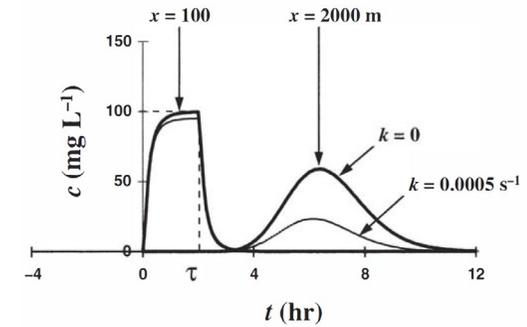
FIGURE 10.10

A simulation of a “breakthrough” curve. A step increase to a concentration of 100 mg L^{-1} is initiated at $x = 0$ at $t = 0$. Shown is the change in concentration at a sampling point 2000 m downstream for a conservative and a nonconservative release. This example used $U = 0.1 \text{ m s}^{-1}$ and $E = 5 \text{ m}^2 \text{ s}^{-1}$.

Continuous Spill



The second idealized application applies to cases in which the step input terminates after a finite time. There are two parts for this solution. For $t < \tau$, $c(x, t) = \frac{c_0}{2} \left[e^{\frac{Ux}{2E}(1-\Gamma)} \operatorname{erfc} \left(\frac{x-Ut\Gamma}{2\sqrt{Et}} \right) + e^{\frac{Ux}{2E}(1-\Gamma)} \operatorname{erfc} \left(\frac{x+Ut\Gamma}{2\sqrt{Et}} \right) \right]$ holds.



Thereafter, the following formula applies:

$$c(x, t) = \frac{c_0}{2} \left\{ e^{\frac{Ux}{2E}(1-\Gamma)} \left[\operatorname{erfc} \left(\frac{x - Ut\Gamma}{2\sqrt{Et}} \right) - \operatorname{erfc} \left(\frac{x - U(t - \tau)\Gamma}{2\sqrt{E(t - \tau)}} \right) \right] + e^{\frac{Ux}{2E}(1+\Gamma)} \left[\operatorname{erfc} \left(\frac{x + Ut\Gamma}{2\sqrt{Et}} \right) - \operatorname{erfc} \left(\frac{x + U(t - \tau)\Gamma}{2\sqrt{E(t - \tau)}} \right) \right] \right\}$$

Continuous Spill

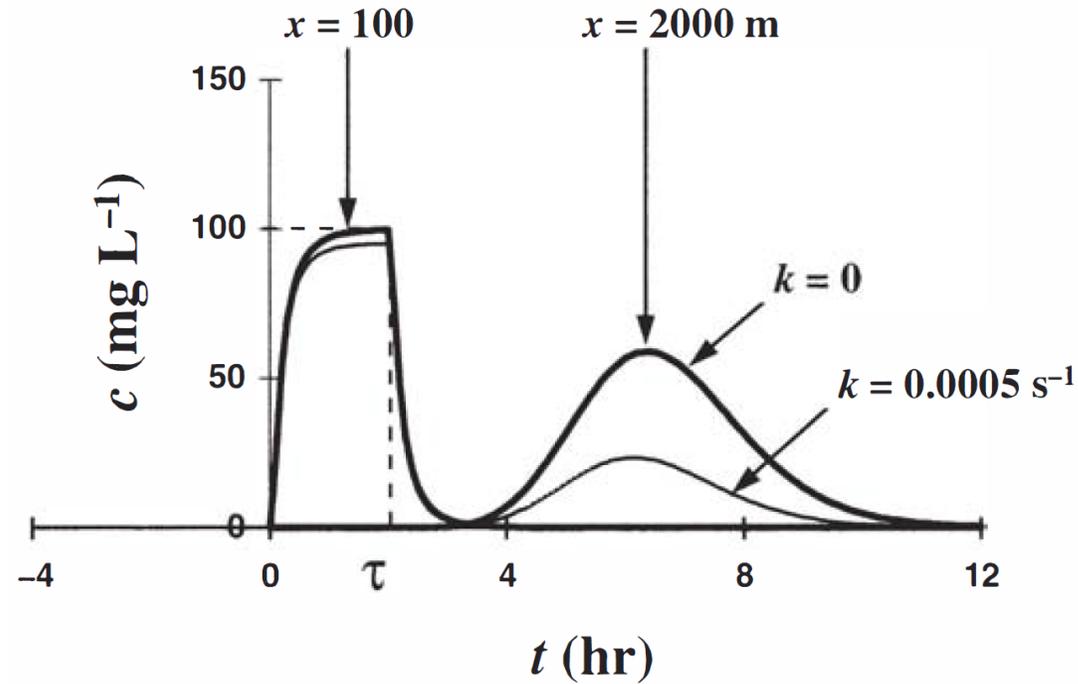


FIGURE 10.11

A simulation of a dye release or spill of finite duration—a “breakthrough” curve. A step increase to a concentration of 100 mg L^{-1} is initiated at $x = 0$ at $t = 0$ and lasts for $\tau = 2$ hr. Shown is the distribution at $x = 0$ (dashed line) along with curves at $x = 100$ and 2000 m for a conservative (bold line) and a nonconservative release (light line). This example used $U = 0.1 \text{ m s}^{-1}$ and $E = 5 \text{ m}^2 \text{ s}^{-1}$.

Tracer Studies

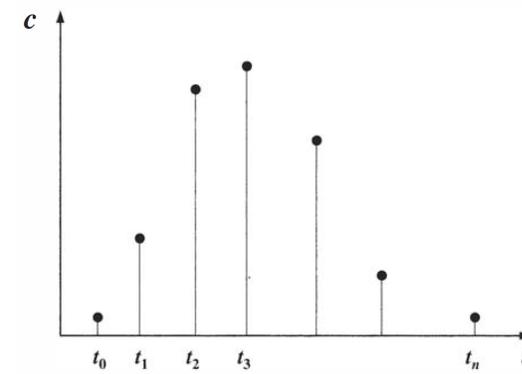


FIGURE 10.12
Concentration data sampled
at a point in space to
characterize the distribution of
a tracer.

The models derived thus far also have utility when trying to account for compounds that are deliberately discharged as tracers. In these cases, the distribution downstream from the injection point can be used to determine key characteristics (e.g. velocity, dispersion coefficient, and decay rate).

It is necessary to estimate some quantities from concentration data. (measured in discrete points in time).

Mean concentration:

$$\bar{c} = \frac{\sum_{i=0}^{n-1} (c_i + c_{i+1})(t_{i+1} - t_i)}{2(t_n - t_0)}$$

Tracer Studies

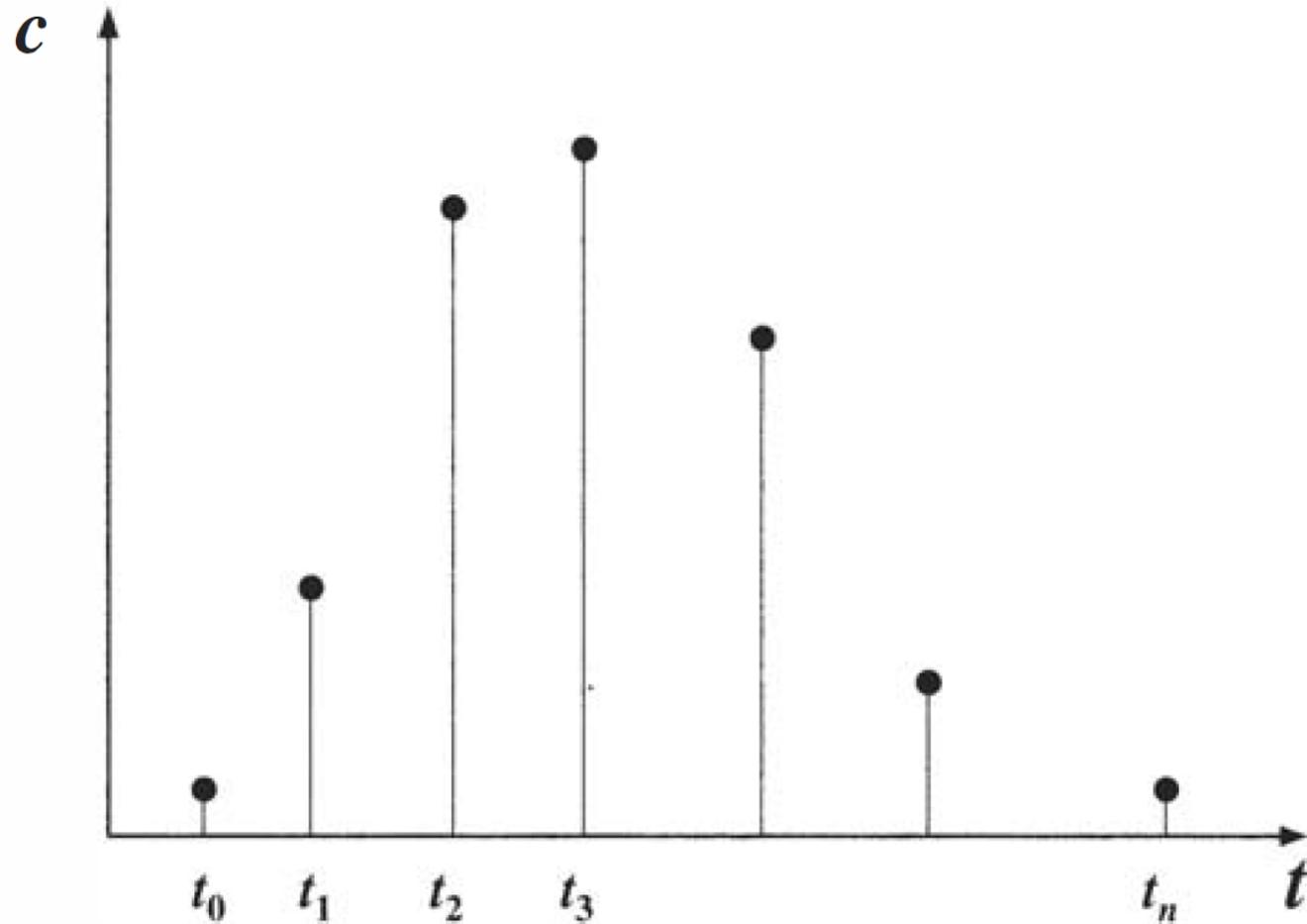


FIGURE 10.12

Concentration data sampled at a point in space to characterize the distribution of a tracer.

Tracer Studies

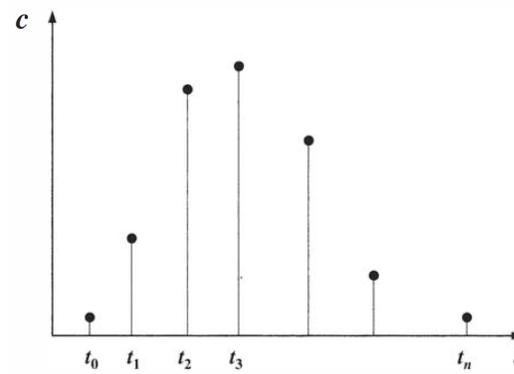


FIGURE 10.12
Concentration data sampled
at a point in space to
characterize the distribution of
a tracer.

Mass:

$$M = Q\bar{c}(t_n - t_0)$$

Travel Time:

$$\bar{t} = \frac{\sum_{i=0}^{n-1} (c_i t_i + c_{i+1} t_{i+1})(t_{i+1} - t_i)}{\sum_{i=0}^{n-1} (c_i + c_{i+1})(t_{i+1} - t_i)}$$

Temporal Variance:

$$s_t^2 = \frac{\sum_{i=0}^{n-1} (c_i t_i^2 + c_{i+1} t_{i+1}^2)(t_{i+1} - t_i)}{\sum_{i=0}^{n-1} (c_i + c_{i+1})(t_{i+1} - t_i)} - (\bar{t})^2$$

Tracer Studies

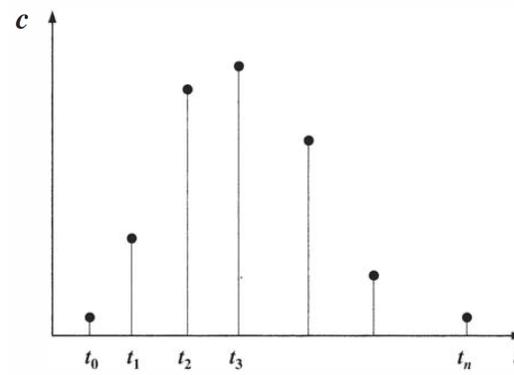


FIGURE 10.12
Concentration data sampled
at a point in space to
characterize the distribution of
a tracer.

If the data are available from two stations, located at x_1 and x_2 , the mean velocity can be estimated by:

$$U = \frac{x_2 - x_1}{\bar{t}_2 - \bar{t}_1}$$

The velocity estimate can, in turn, be used to calculate the dispersion coefficient by:

$$E = \frac{U^2 (s_{t_2}^2 - s_{t_1}^2)}{2(\bar{t}_2 - \bar{t}_1)}$$

EXAMPLE 10.4. EVALUATION OF A TRACER STUDY. A tracer study is conducted in a stream with a flow of $3 \times 10^5 \text{ m}^3 \text{ d}^{-1}$ and a width of 45 m. At $t = 0$, 5 kg of a conservative substance, lithium, is instantaneously injected at $x = 0$. Concentrations are measured at two downstream stations:

$x = 1 \text{ km}$

$t \text{ (min)}$	30	40	50	60	70	80	90	100	110	120
Lithium ($\mu\text{g L}^{-1}$)	0	100	580	840	560	230	70	15	3	0

$x = 8 \text{ km}$

$t \text{ (min)}$	370	400	430	460	490	520	550	580	610
Lithium ($\mu\text{g L}^{-1}$)	0	10	80	250	280	140	35	5	0

Determine (a) the velocity (m d^{-1}) and (b) the dispersion coefficient ($\text{cm}^2 \text{ s}^{-1}$).

Tracer Studies

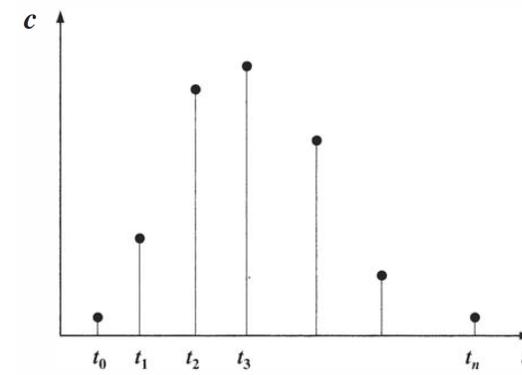


FIGURE 10.12
Concentration data sampled
at a point in space to
characterize the distribution of
a tracer.

Dye studies can also be used to determine first-order reaction rates. For this case, the mass under the concentration-time curve is determined at two positions. The rate is estimated as:

$$k = \frac{1}{\bar{t}_2 - \bar{t}_1} \ln \frac{M_1}{M_2}$$

Estuary Number

The relative importance of advection and dispersion can be assessed by a dimensionless analysis

$$\frac{\partial c}{\partial t} = -U \frac{\partial c}{\partial x} + E \frac{\partial^2 c}{\partial x^2} - kc$$

Three dimensionless parameter groups can be defined as:

$$c^* = \frac{c}{c_0}$$

$$x^* = \frac{kx}{U}$$

$$t^* = kt$$

Estuary Number

These equations can be solved for c , x and t , respectively, and the results substituted into $(\frac{\partial c}{\partial t} = -U \frac{\partial c}{\partial x} + E \frac{\partial^2 c}{\partial x^2} - kc)$ to yield:

$$\frac{\partial c^*}{\partial t^*} = -\frac{\partial c^*}{\partial x^*} + \eta \frac{\partial^2 c^*}{\partial x^{*2}} - c^*$$

where η is called the estuary number:

$$\eta = \frac{kE}{U^2}$$

This term defines whether the second derivative is important.

Estuary Number

where η is called the estuary number:

$$\eta = \frac{kE}{U^2}$$

This term defines whether the second derivative is important.

		<u>Suggested ranges</u>
$\eta \gg 1$	Diffusion predominates	$\eta > 10$
$\eta \approx 1$	Advection/diffusion important	$0.1 < \eta < 10$
$\eta \ll 1$	Advection predominates	$\eta < 0.1$

$$\frac{\partial c^*}{\partial t^*} = -\frac{\partial c^*}{\partial x^*} + \eta \frac{\partial^2 c^*}{\partial x^{*2}} - c^*$$

EXAMPLE 10.5. ESTUARY NUMBER. Evaluate the estuary number for the stream from Example 10.4 for a nonconservative tracer with a half-life of 1 d.