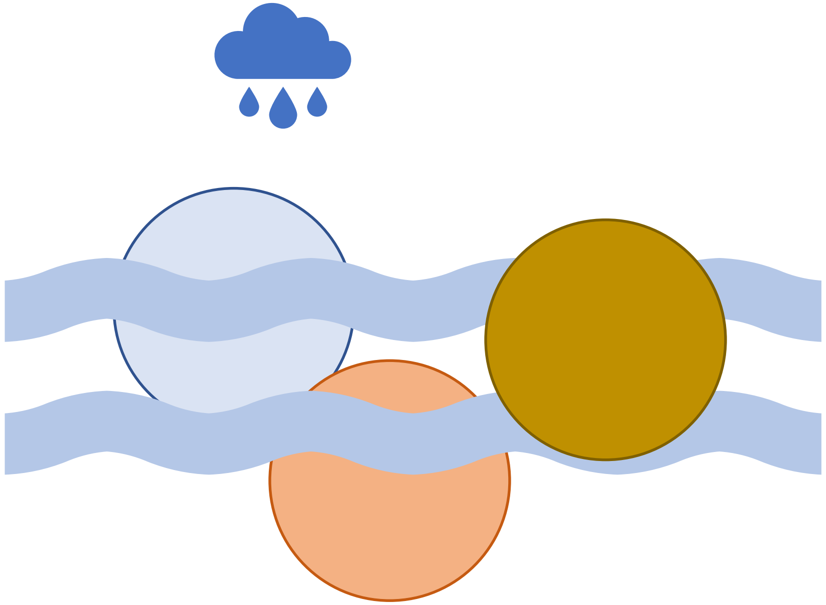
Surface Water Quality Modeling

CEE-EGIN 577



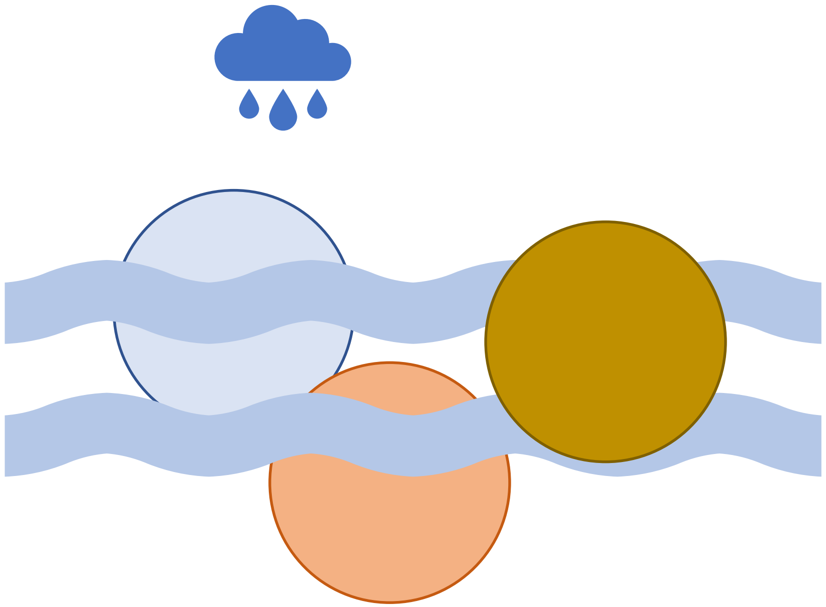
C. D. Guzman, PhD

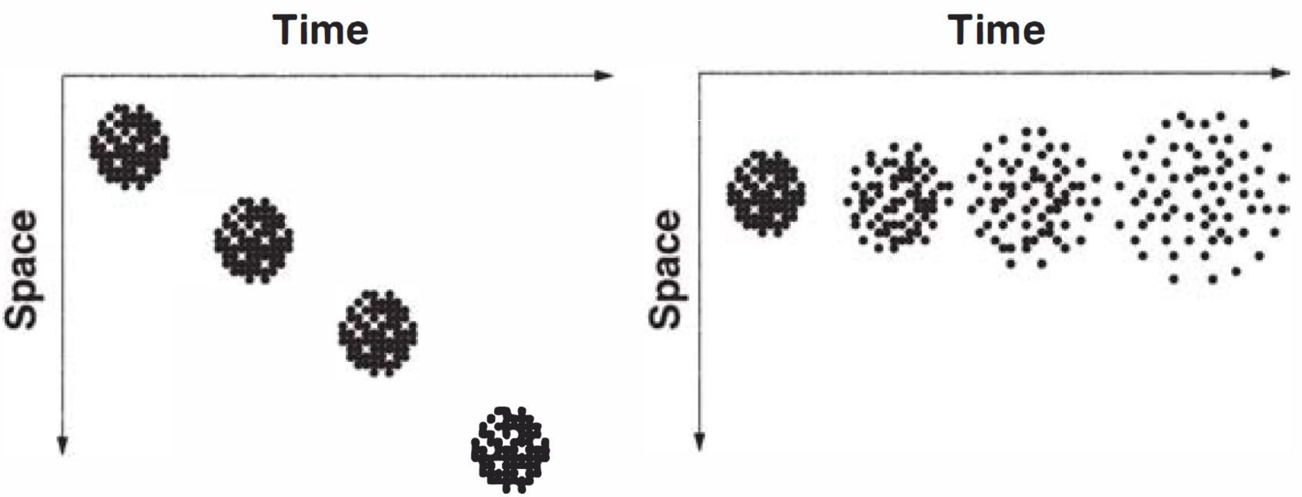
Week 2

Monday, Feb 03, 2020

Incompletely Mixed Systems

Diffusion





(a) Advection
(b) Diffusion

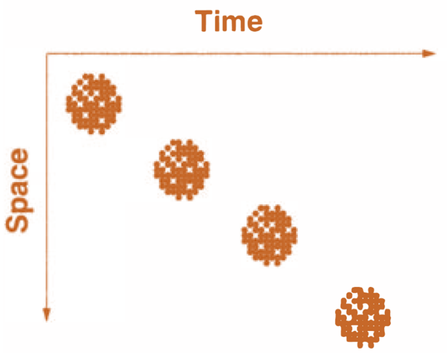
Advection & Diffusion

Experiment

Fick's First Law

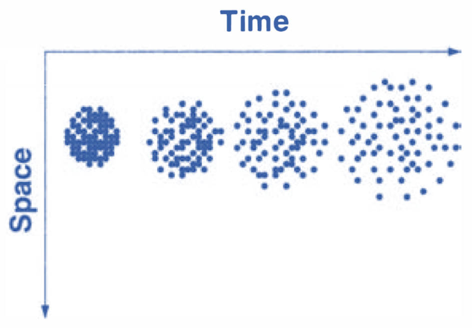
Embayment Model

Advection & Diffusion



(*a*) Advection

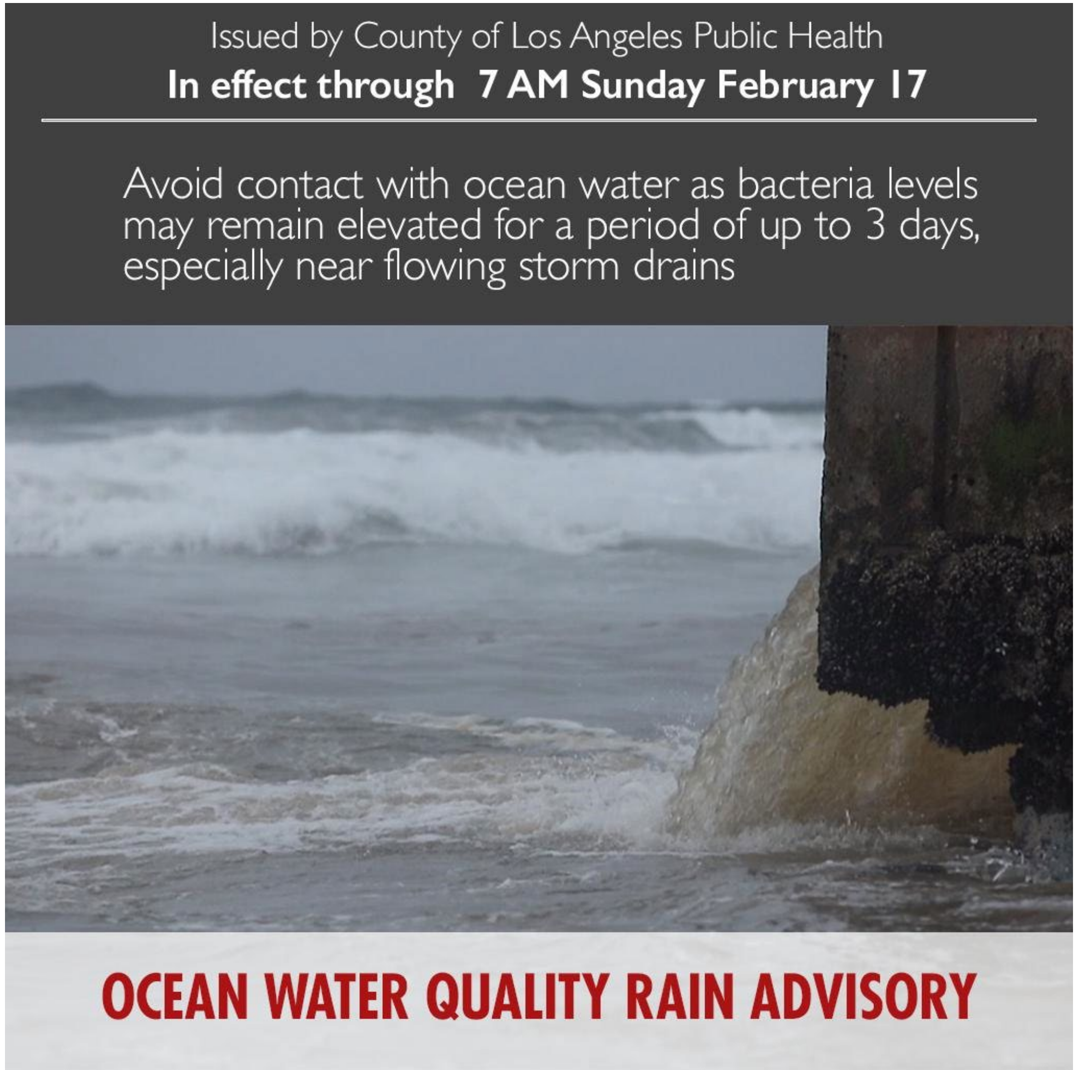
Advection results from flow that is unidirectional and does not change the identity of the substance being transported.

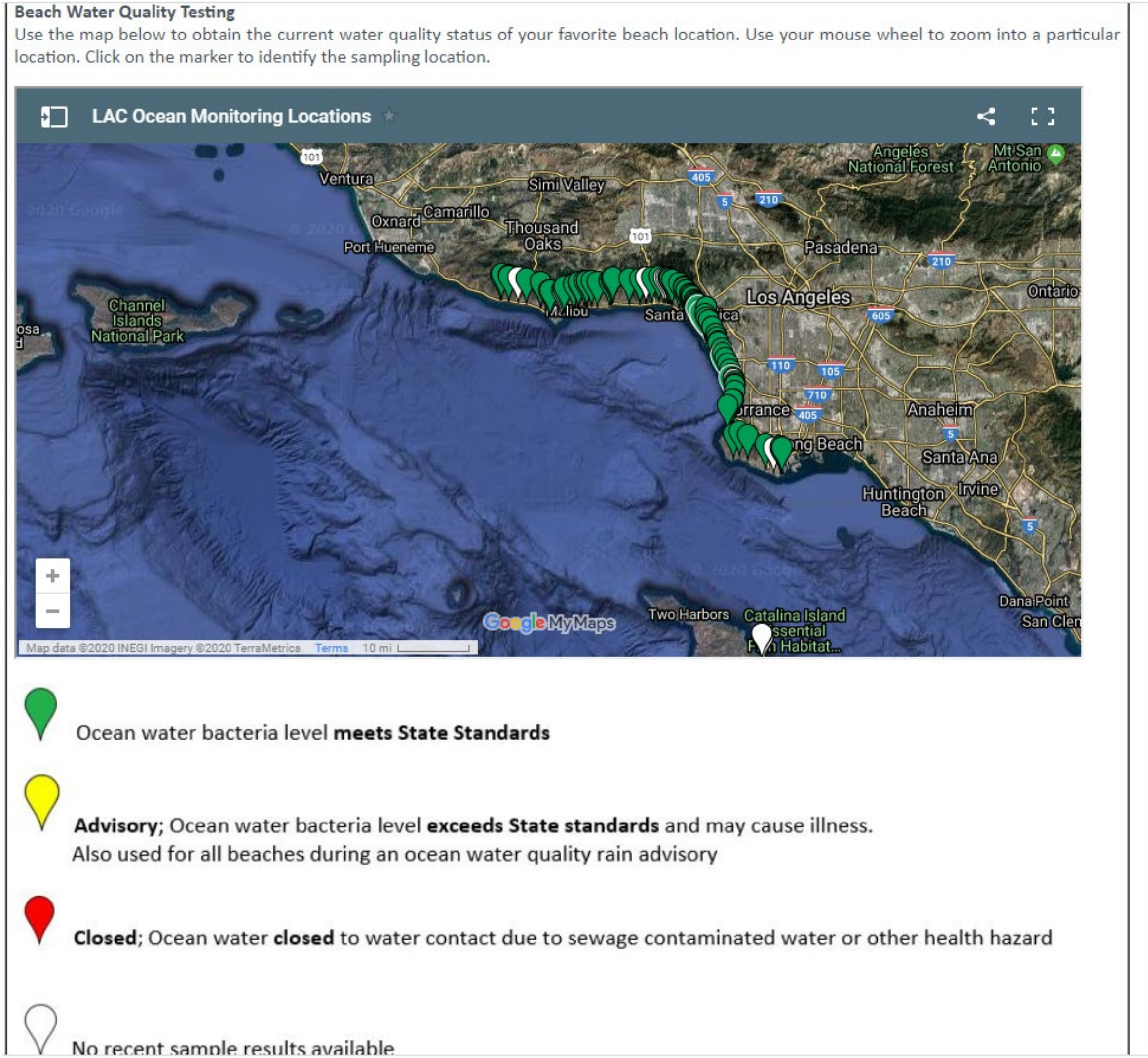


(*b*) Diffusion

Diffusion refers to the movement of the mass due to random water motion or mixing. On a microscopic scale, ***molecular diffusion*** result from the random Brownian motion of water molecules. When this random motion occurs on a larger scale due to eddies it is called ***turbulent diffusion***.

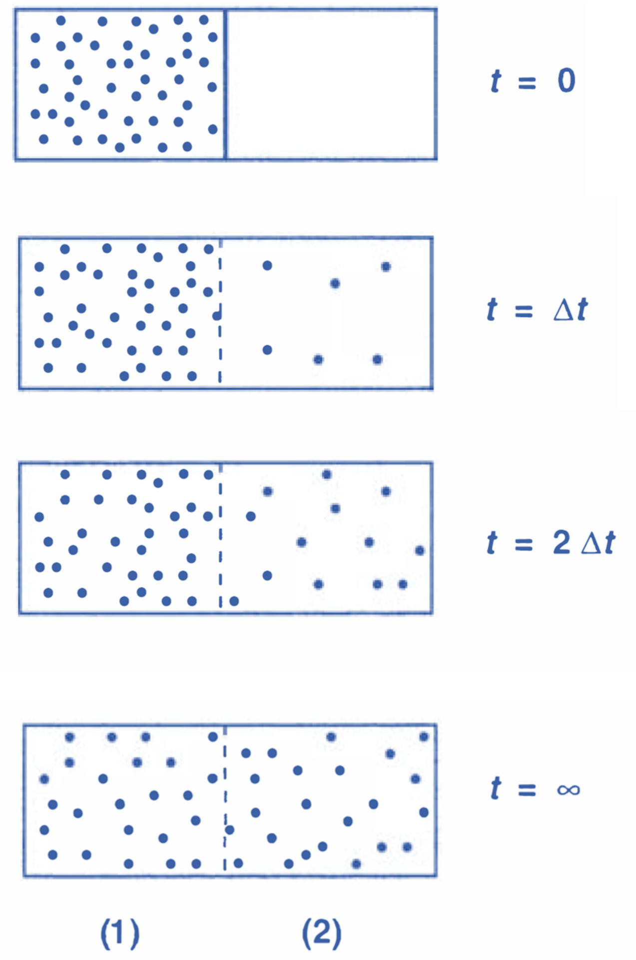
Advection & Diffusion





http://publichealth.lacounty.gov/phcommon/public/eh/water_quality/beach_grades.cfm

Experiment



A tank is divided in half by a removable partition. At the beginning of the experiment ($t = 0$) the partition is gently removed.

After a period of time ($t = \Delta t$), several of the particles will have wandered to the right side.

Later ($t = 2\Delta t$) more would migrate to the right.

Finally the concentrations would be equal.

FIGURE 8.2
The diffusion of mass between two volumes.

Experiment

Diffusion (such movement of mass due to random water motion) can be quantified mathematically by designating the left side (1) and the right side (2). A mass balance for the left side of the tank is written as:

$$V_1 \frac{dc_1}{dt} = D'(c_2 - c_1)$$

where V_1 = volume of the left side

c_1 and c_2 = concentrations of the particles in the left and right side, respectively

D’ = diffusive flow ($m^3\ yr^{-1}$)

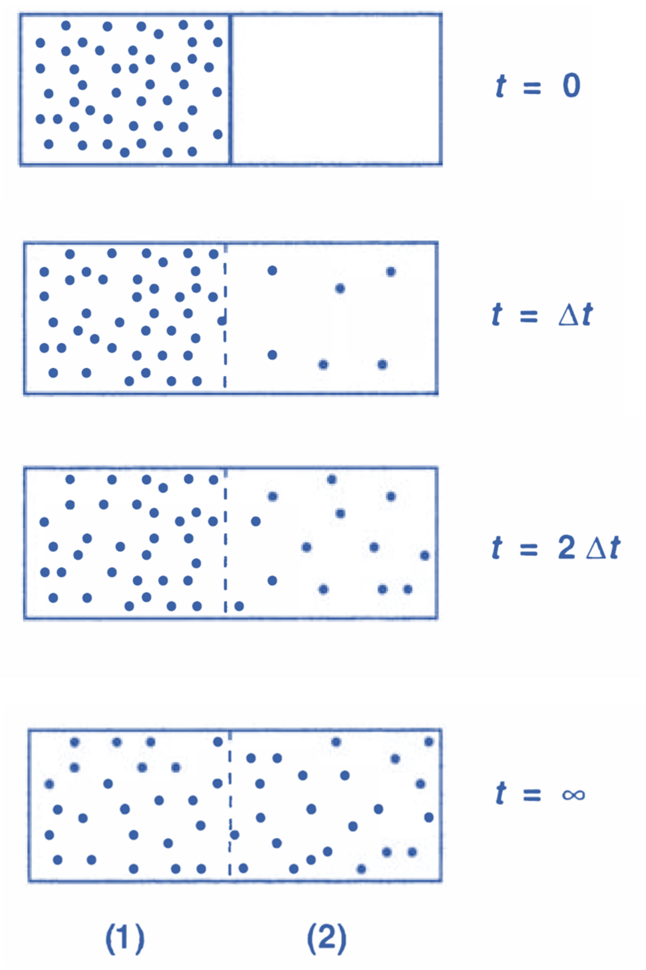


FIGURE 8.2
The diffusion of mass between two volumes.

Experiment

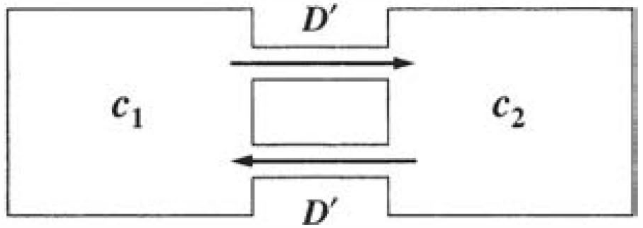


FIGURE 8.3
A two-way flow model of the diffusion of mass.

Thus diffusion is modeled as a two-way flow connecting the volumes. Three factors contribute to the diffusive transport between the two sides:

D’ reflects the intensity of the mixing (small ~weak; large ~vigorous physical mixing).

Interface area is proportional to mixing (mass transport). If interface area were doubled, we would expect twice as many particles to be transported.

The difference in concentration (gradient) influences the diffusive transport.

EXAMPLE 8.1. DIFFUSION OF MASS BETWEEN TWO VOLUMES. Model the time required for the experiment shown in Fig. 8.2 to go to 95% of completion.

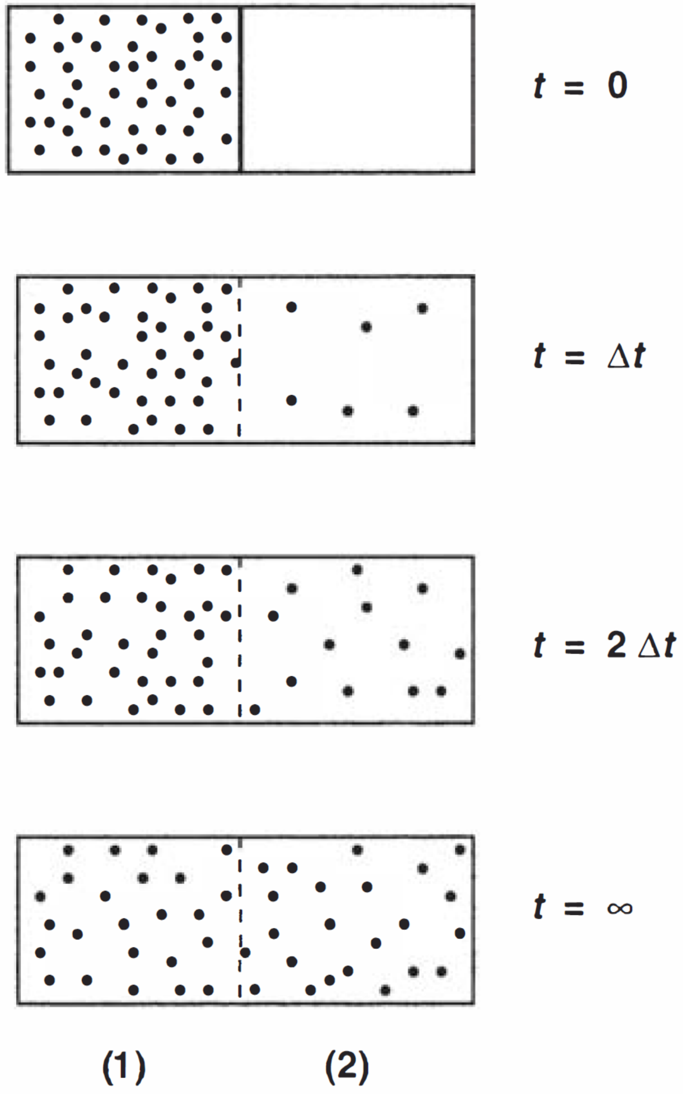
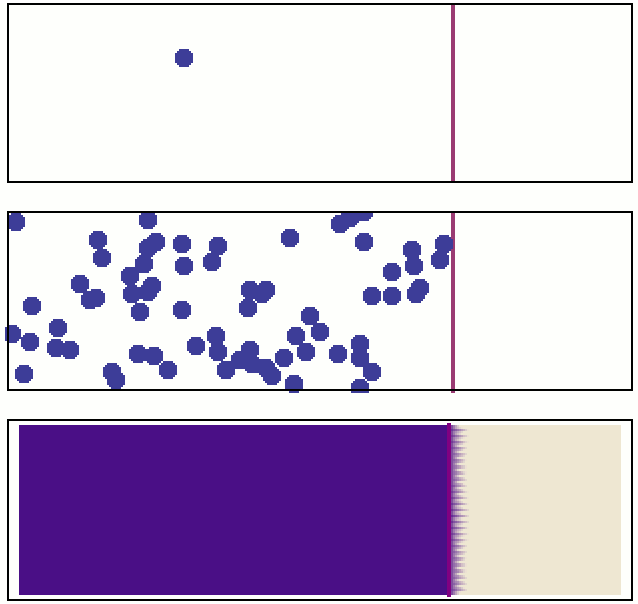
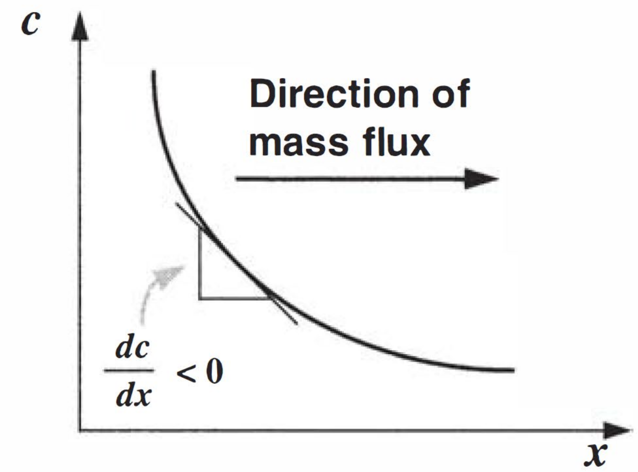
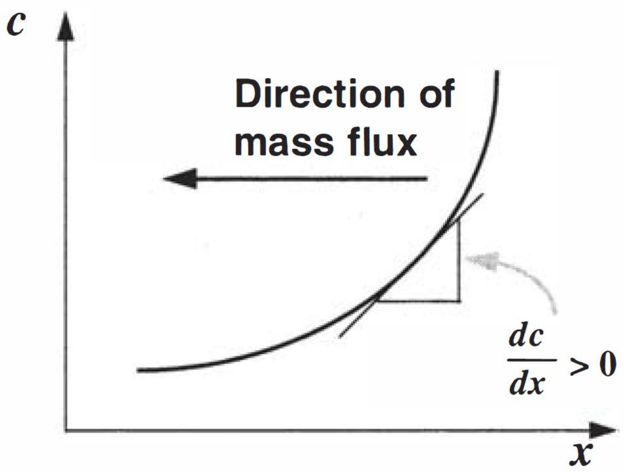


FIGURE 8.2
The diffusion of mass between two volumes.

Fick's First Law







By Anton Klamroth, gestorben 11. Feb. 1929

Fick's First Law

In 1855 the physiologist Adolf Fick proposed the following model of diffusion:

$$J_x = -D \frac{dc}{dx}$$

where J_x = mass flux in the x direction ($M\ L^{-2}T^{-1}$) and D = a diffusion coefficient ($L^2\ T^{-1}$). This model is called Fick's first law. Fick's law states that mass flows from regions of high to low concentration.

The diffusion coefficient D is a parameter used to quantify the rate of the diffusive process.

Fick's First Law

Fick's law can be used to model the situation depicted previously with the two-sided tank. The mass balance for the left side of the reactor is:

$$V_1 \frac{dc_1}{d1} = -J\,A_c$$

where A_c= cross-sectional area of the interface between the two sides (m^2) and J= flux between the volumes.

$$V_1 \frac{dc_1}{d1} = -(-D\,\frac{dc}{dx})\,A_c$$

$$\frac{dc}{dx} \cong \frac{c_2 - c_1}{\ell}$$

$$V_1 \frac{dc_1}{d1} = \frac{DA_c}{\ell}(c_2 - c_1)$$

Fick’s First Law

$$V_1 \frac{dc_1}{d1} = \frac{DA_c}{\ell}(c_2 - c_1)$$

where now we see that we have defined the diffusion flow in fundamental parameters:

$$V_1 \frac{dc_1}{dt} = D'(c_2 - c_1)$$

$$D' = \frac{DA_c}{\ell}$$

D reflects the vigor of the mixing process. The area A_c accounts for the fact that the mass transport should be directly proportional to the size of the interface across which the mixing occurs. The mixing length (ℓ) defines the distance across which the mixing takes place.

Fick’s First Law

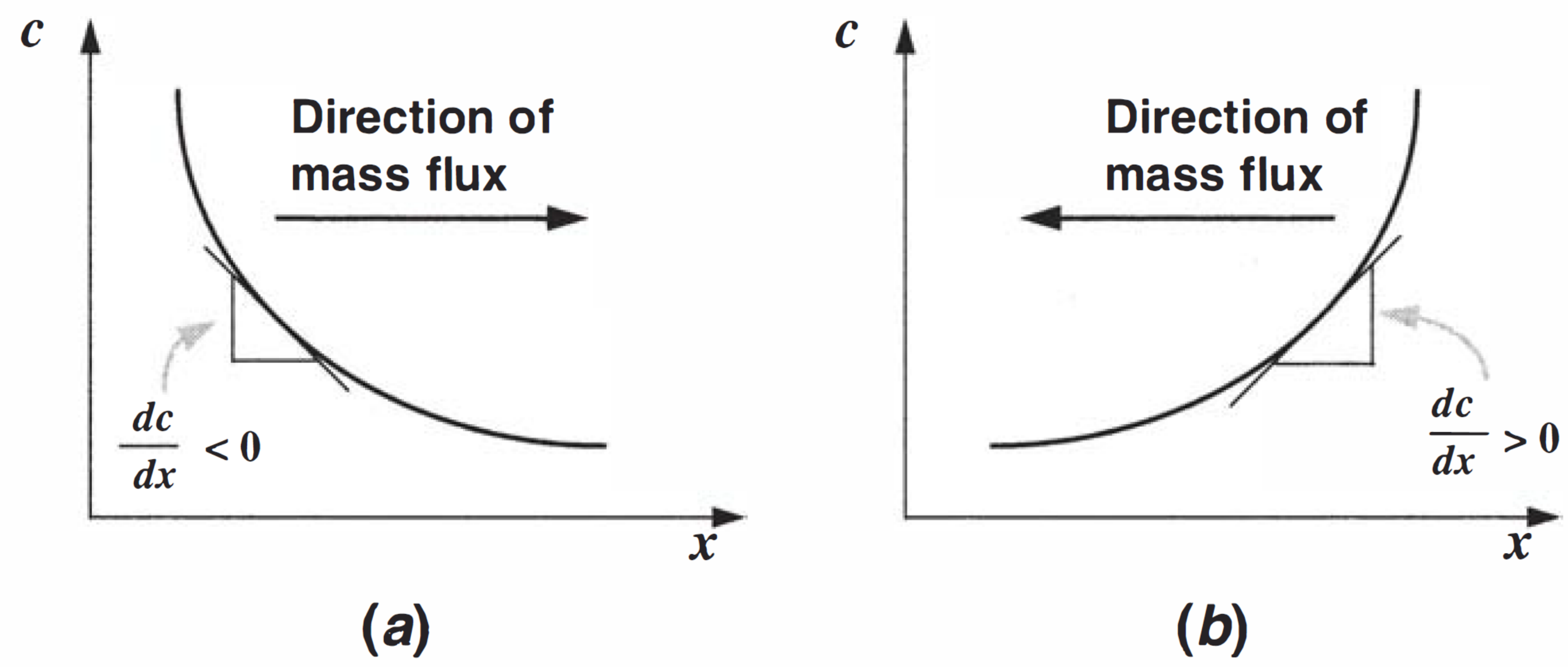


FIGURE 8.4
Graphical depiction of the effect of the concentration gradient on the mass flux. Because mass moves “downhill” from high to low concentrations, the flow in (*a*) is from left to right in the positive *x* direction. However, due to the orientation of cartesian coordinates, the slope is negative for this case. Thus a negative gradient leads to a positive flux. This is the origin of the negative sign in Fick’s first law. The reverse case is depicted in (*b*), where the positive gradient leads to a negative mass flow from right to left.

Fick's First Law

Often other parameterizations and nomenclature are used. E.g. the distinction between molecular diffusion and turbulence mixing is often made. Usually D is taken for molecular, E for turbulent diffusion.

For diffusion **mass-transfer coefficient** (v_d; L T^{-1}) grouping, the length is often combined with the diffusion coefficient.

$$v_d = \frac{D}{\ell} \quad or \quad v_d = \frac{E}{\ell}$$

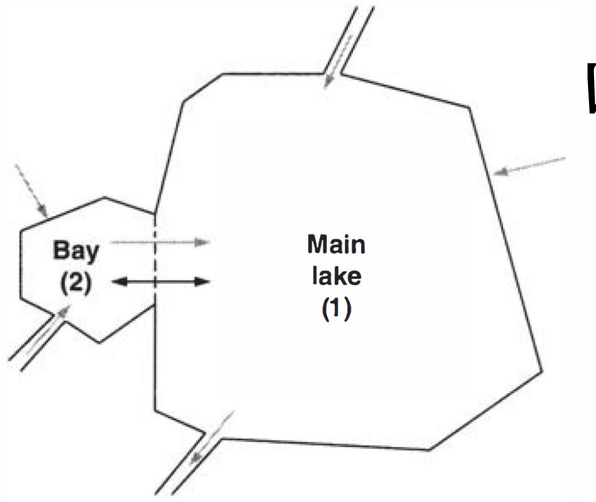
Also, the **bulk diffusion coefficient** D' or E' is frequently used for mathematical convenience.

$$D' = \frac{DA_c}{\ell} \qquad E' = \frac{DA_c}{\ell}$$

Embayment Model

A well-mixed bay (2) connected to a large lake (1) is a simple illustration of an incompletely mixed system. This is comparable to the completely mixed lake model described in previous lectures.

$$V_1 \frac{dc_1}{dt} = W_1 - Q_1 c_1 - k_1 V_1 c_1 + Q_2 c_2 + E'(c_2 - c_1)$$



$$V_2 \frac{dc_2}{dt} = W_2 - Q_2 c_2 - k_2 V_2 c_2 + E'(c_1 - c_2)$$

Estimation of Diffusion

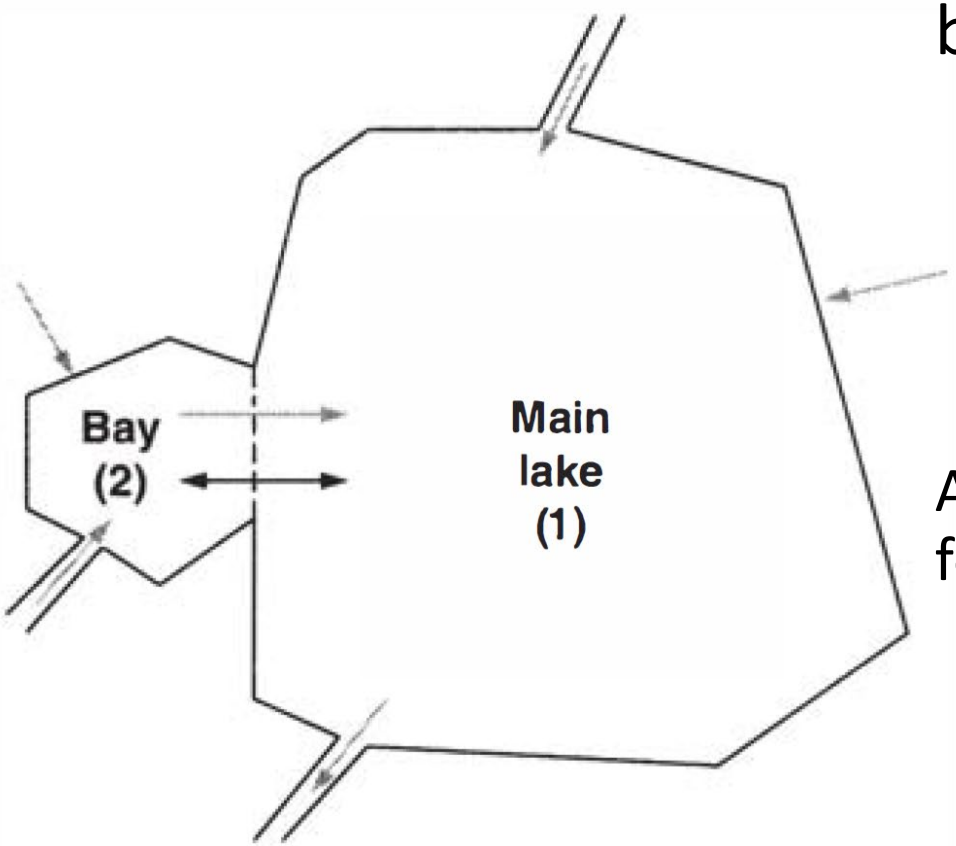


FIGURE 8.5
A lake/embayment system.

Where the substance is conservative ($k = 0$) the bay/lake model can be written as a mass balance :

$$V_2 \frac{ds_2}{dt} = W_2 - Q_2 s_1 - k_2 V_2 s_2 + E'(s_1 - s_2)$$

$$V_2 \frac{ds_2}{dt} = W_2 - Q_2 s_2 + E'(s_1 - s_2)$$

At steady state, the bulk diffusion coefficient can be solved for:

$$E' = \frac{Q_2 s_2 - W_2}{(s_1 - s_2)} = \frac{W_2 - Q_2 s_2}{(s_2 - s_1)}$$

EXAMPLE 8.2. USING NATURAL TRACERS TO ESTIMATE DIFFUSION. For Saginaw Bay the bulk diffusion coefficient can be estimated by using the gradient of the conservative substance chloride. Estimate the diffusion coefficient and the mass-transfer coefficient for the process.

EXAMPLE 8.3. STEADY-STATE TOTAL P BUDGET FOR LAKE HURON AND SAGINAW BAY. Information for the Lake Huron/Saginaw Bay system is summarized in Table 8.1. The sedimentation loss of total phosphorus can be parameterized by an apparent settling velocity v of approximately 16 m yr^{-1} (Chapra 1977). Use the models described in Lec. 6 to determine (*a*) the inflow concentration and (*b*) the steady-state concentration.

Steady-State Solution

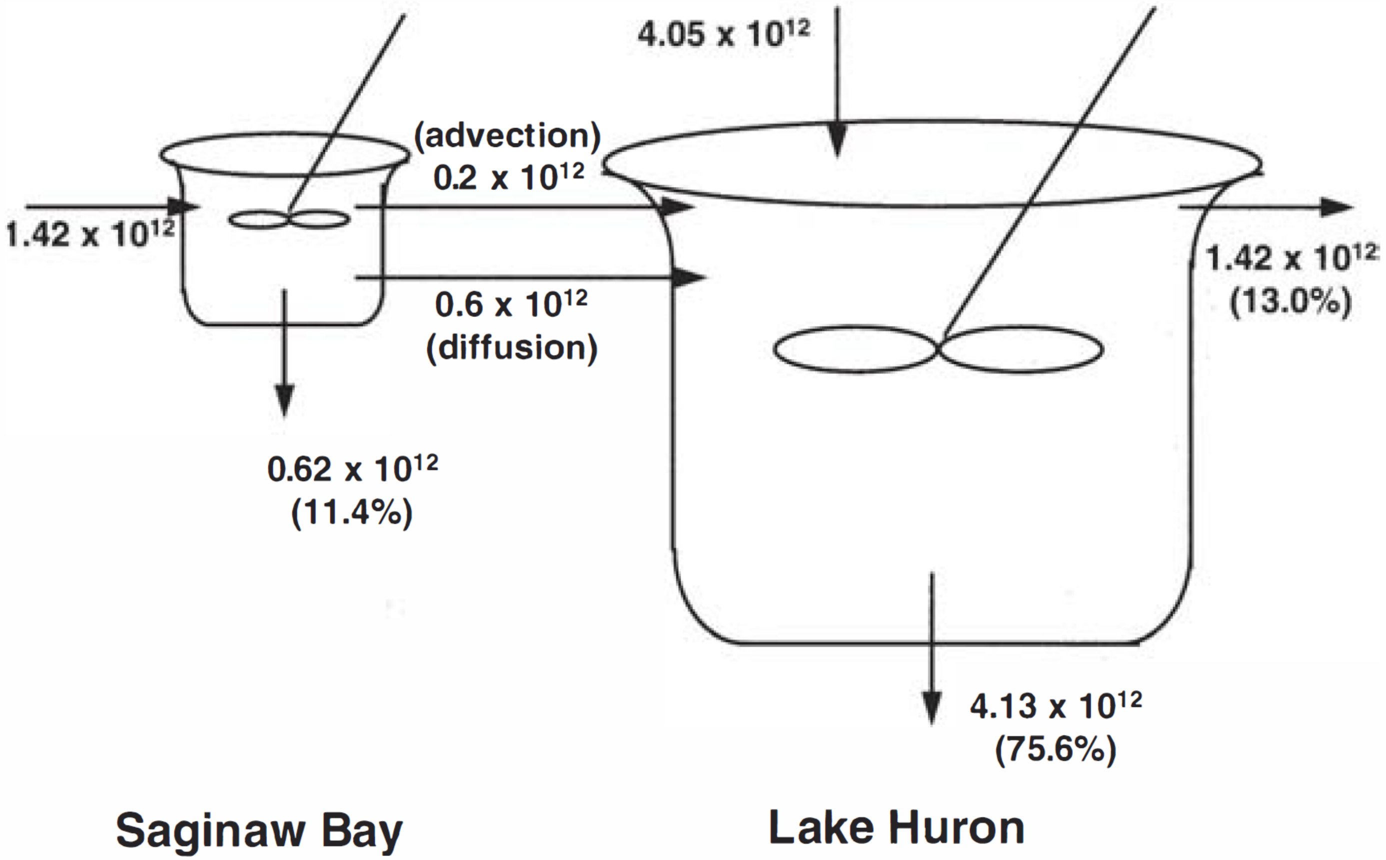


FIGURE 8.6
A total phosphorus budget for Lake Huron and Saginaw Bay computed in Example 8.3. Note that the percentages are based on the total loading to the system.

EXAMPLE 8.4. TIME-VARIABLE SOLUTION FOR LAKE HURON AND SAGINAW BAY. Determine the temporal response of the Saginaw Bay/Lake Huron system following termination of loads. Assume that the system is initially at the steady-state concentrations determined in Example 8.3.

Time-Variable Solution

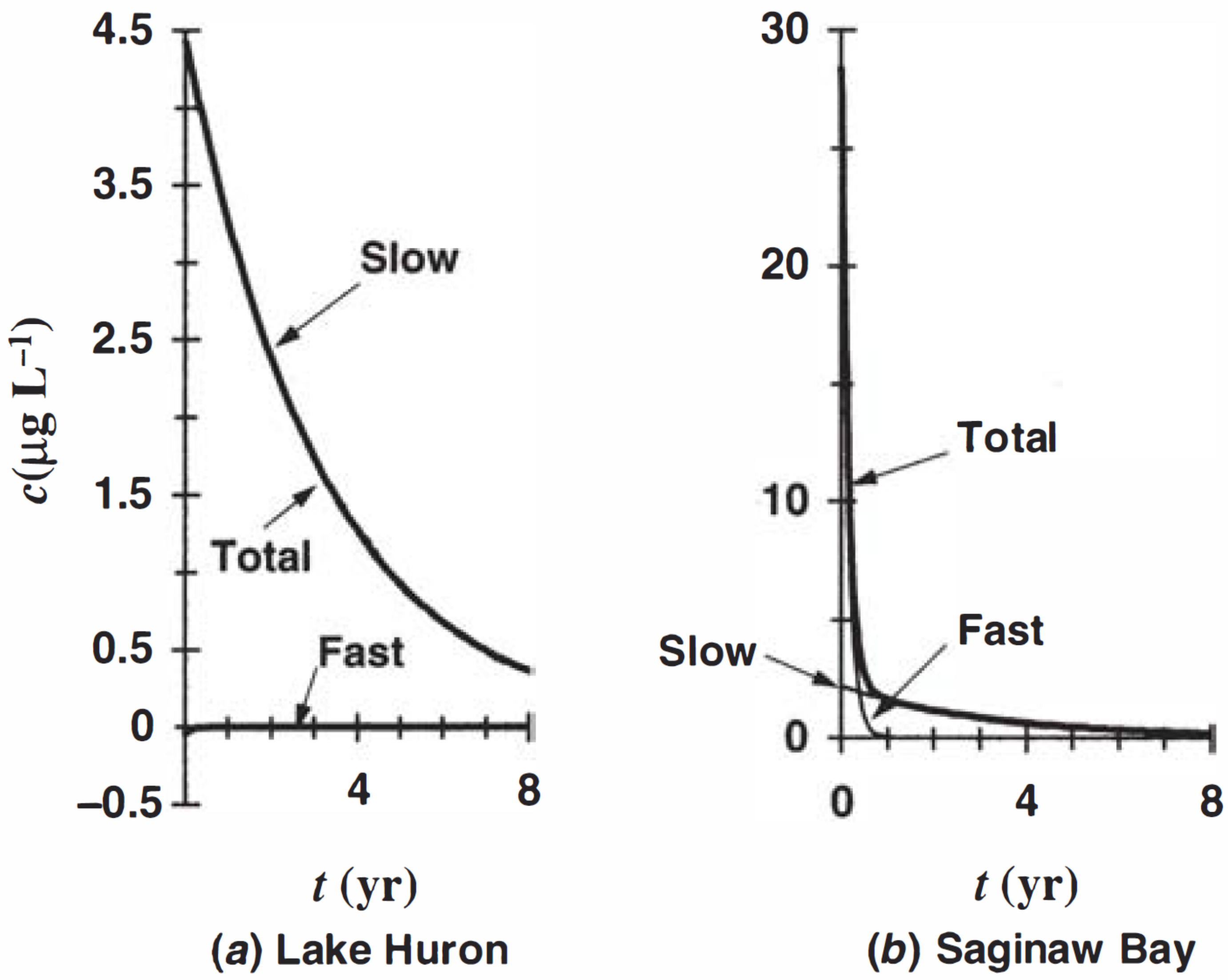


FIGURE 8.7
General solutions for (*a*) Lake Huron and (*b*) Saginaw Bay following the termination of loadings of total phosphorus.

Time-Variable Solutions

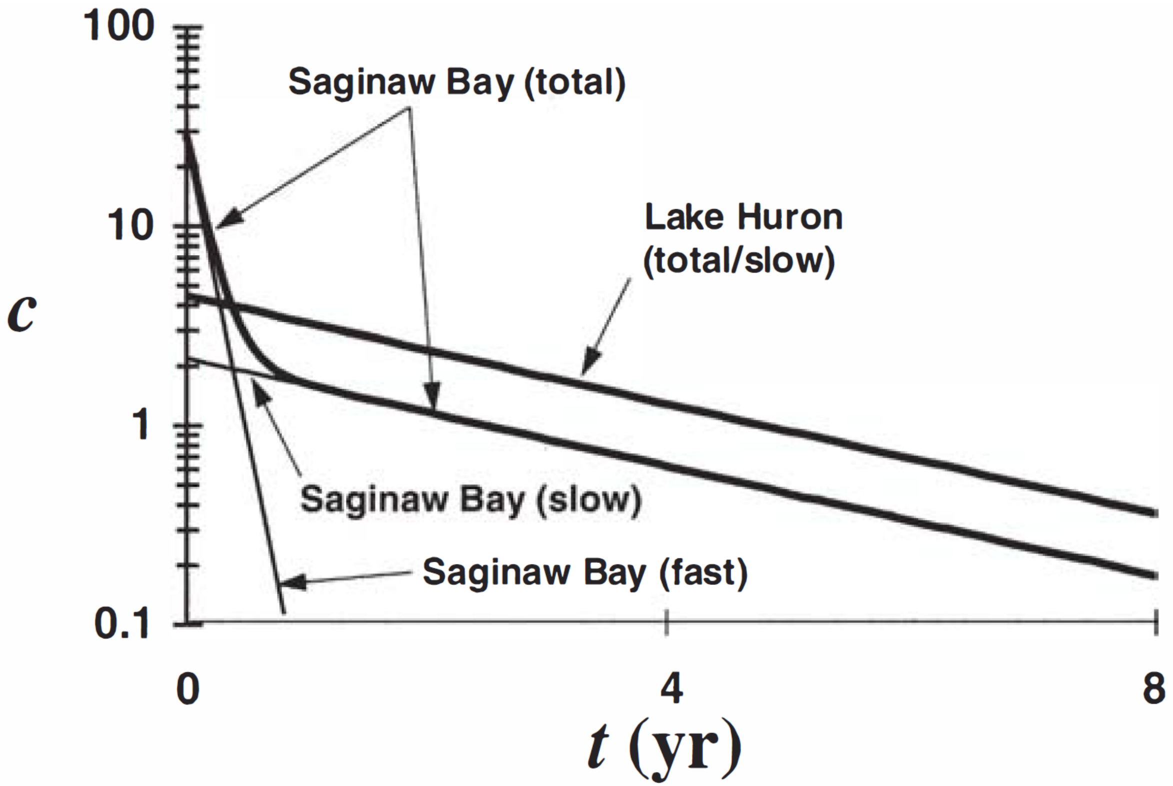


FIGURE 8.8
General solutions for Lake Huron and Saginaw Bay following the termination of loadings of total phosphorus. In this case the responses are displayed on a semi-logarithmic plot to make the eigenvalues obvious.

Additional Transport Mechanisms: Turbulent Diffusion

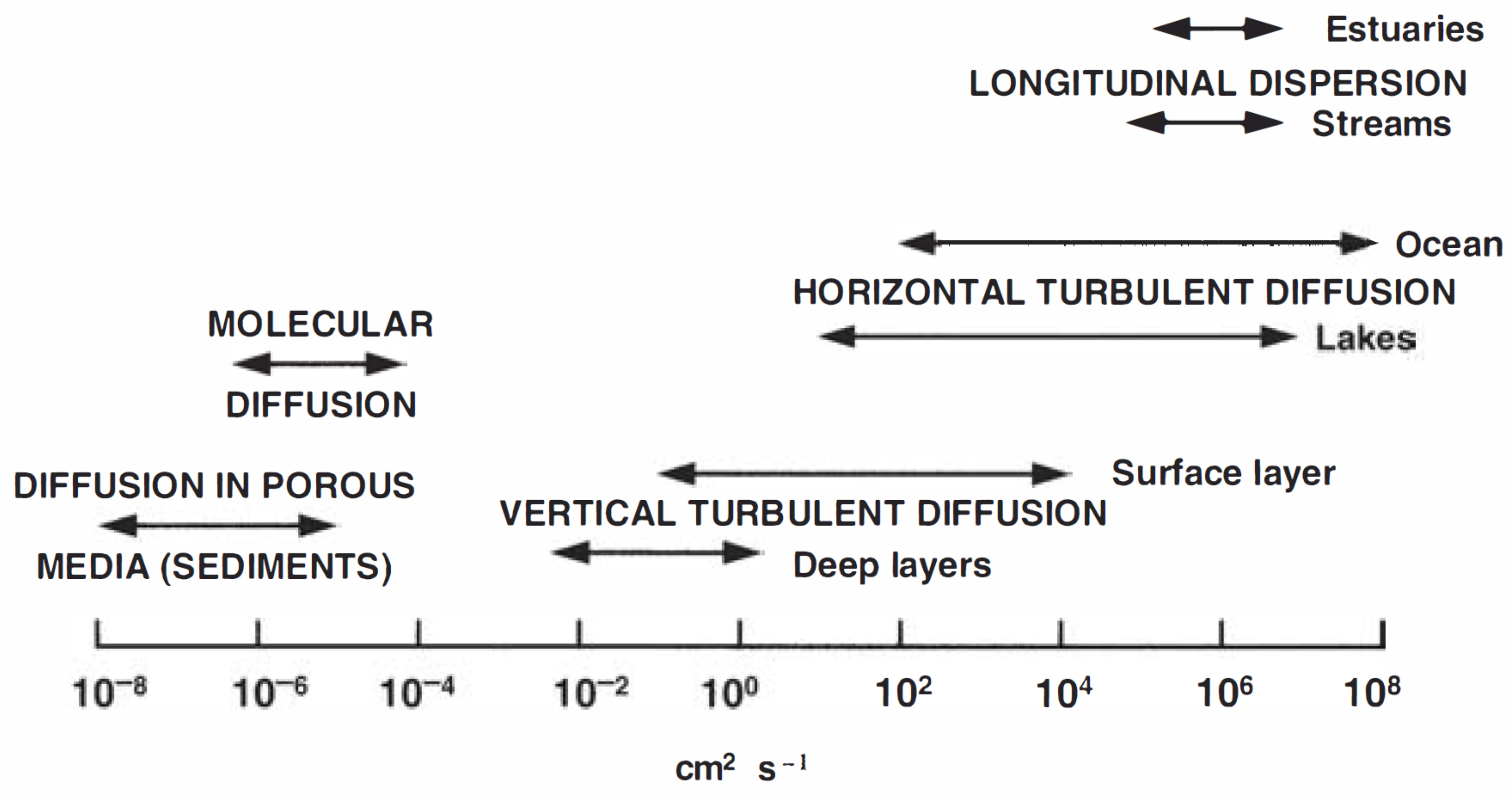


FIGURE 8.10
Typical ranges of the diffusion coefficient in natural waters and sediments.

Transport Diffusion

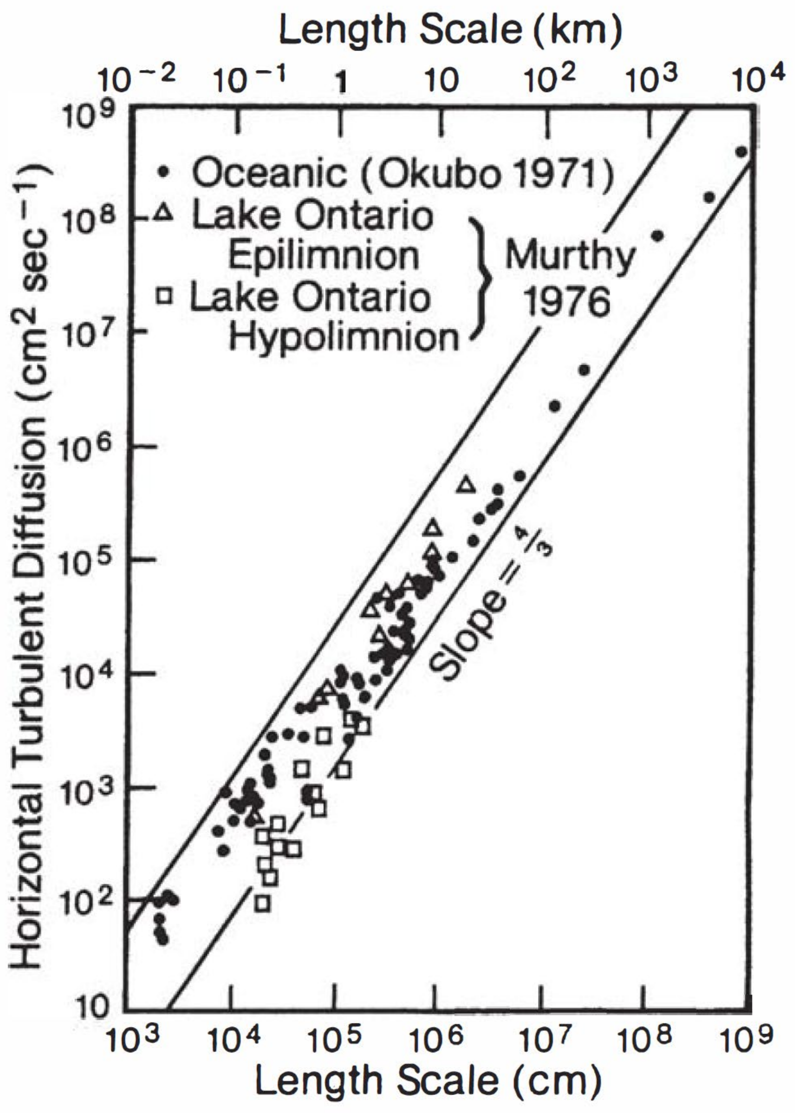


FIGURE 8.11
Relationship of horizontal diffusivity and scale length in the ocean and Lake Ontario. Lines define an envelope around the oceanic data with a slope of 4/3 (Okubo 1971, with additional data from Murthy 1976).

Dispersion

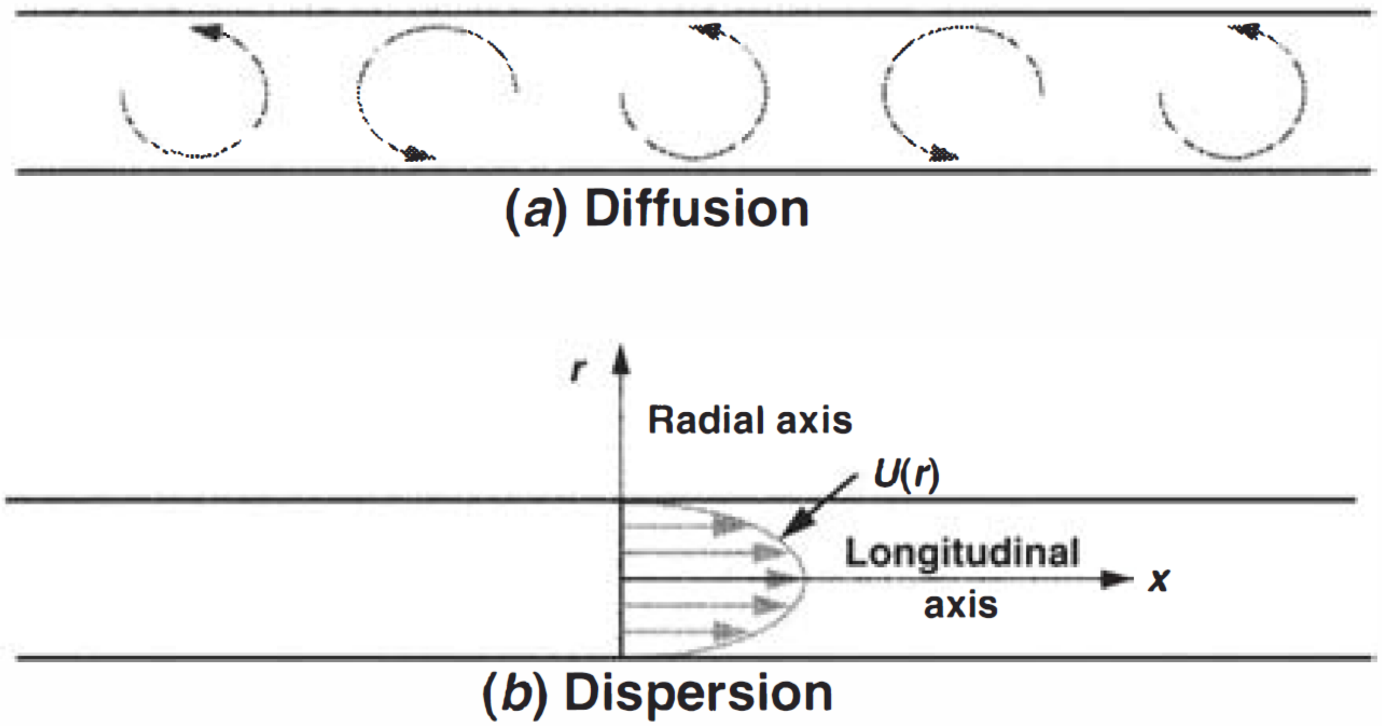


FIGURE 8.12
Contrast between diffusion and dispersion. Both tend to “spread out” pollutants. Diffusion is due to random motion of the water in time, whereas dispersion is due to differential movement of the water in space.

Dispersion is the result of velocity differences in space. In the remainder of the book, dispersion will be used for narrow, flooding bodies of waters (such as streams, estuaries).

Conduction/Convection

Conduction refers to the transfer of heat by molecular activity from one substance to another.

Convection generally refers to the motions in a fluid that result in the transport and mixing of the fluid's properties. Free convection refers to vertical atmospheric motions due to the buoyancy of heated or cooled fluid. In contrast, forced convection is due to external forces. An example is the lateral movement of heat or mass due to the wind. Forced ***convection*** is akin to ***advection***.