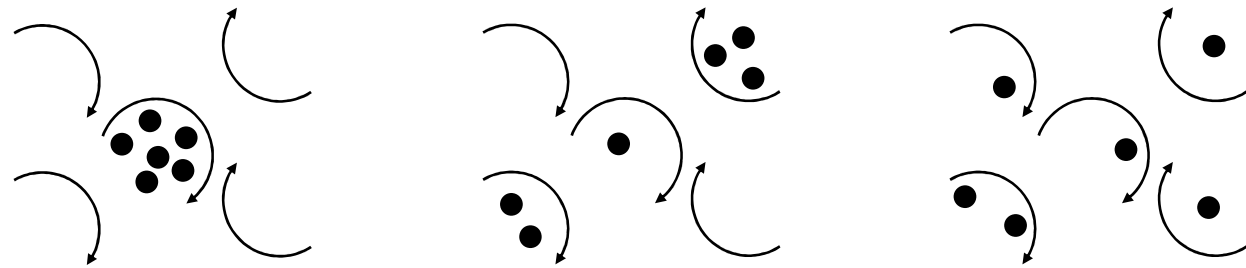


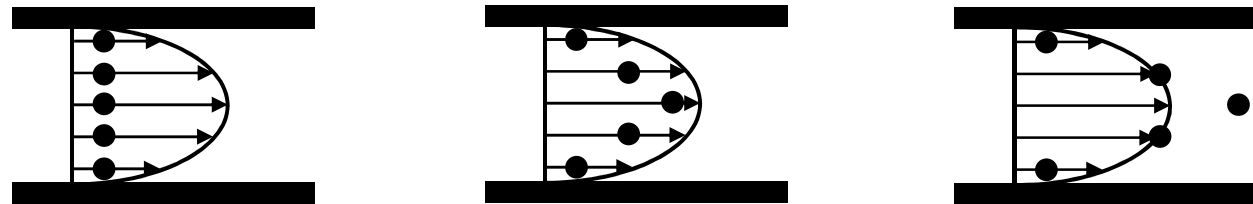
Dispersion

Sources of dispersion

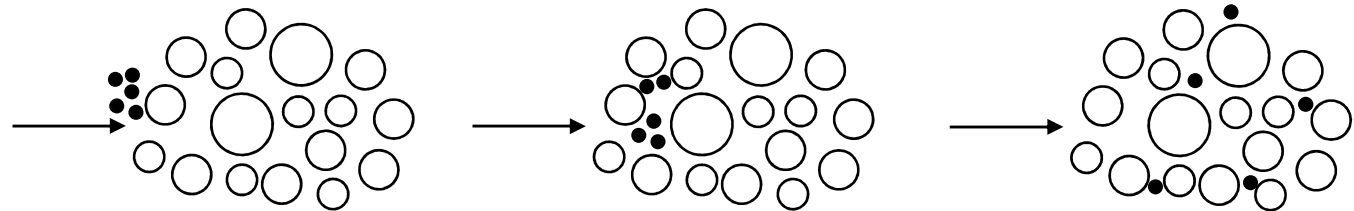
Fluid eddies



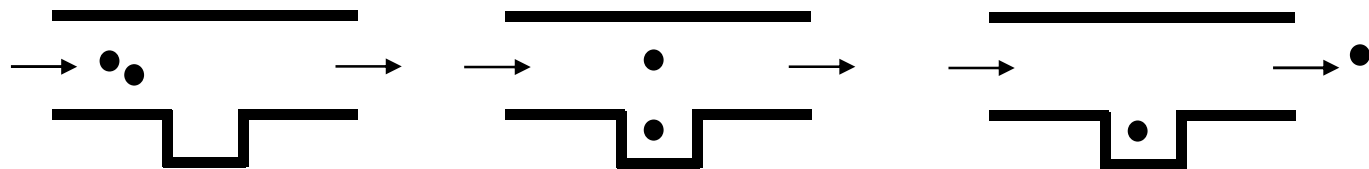
Velocity gradients in flow in a pipe



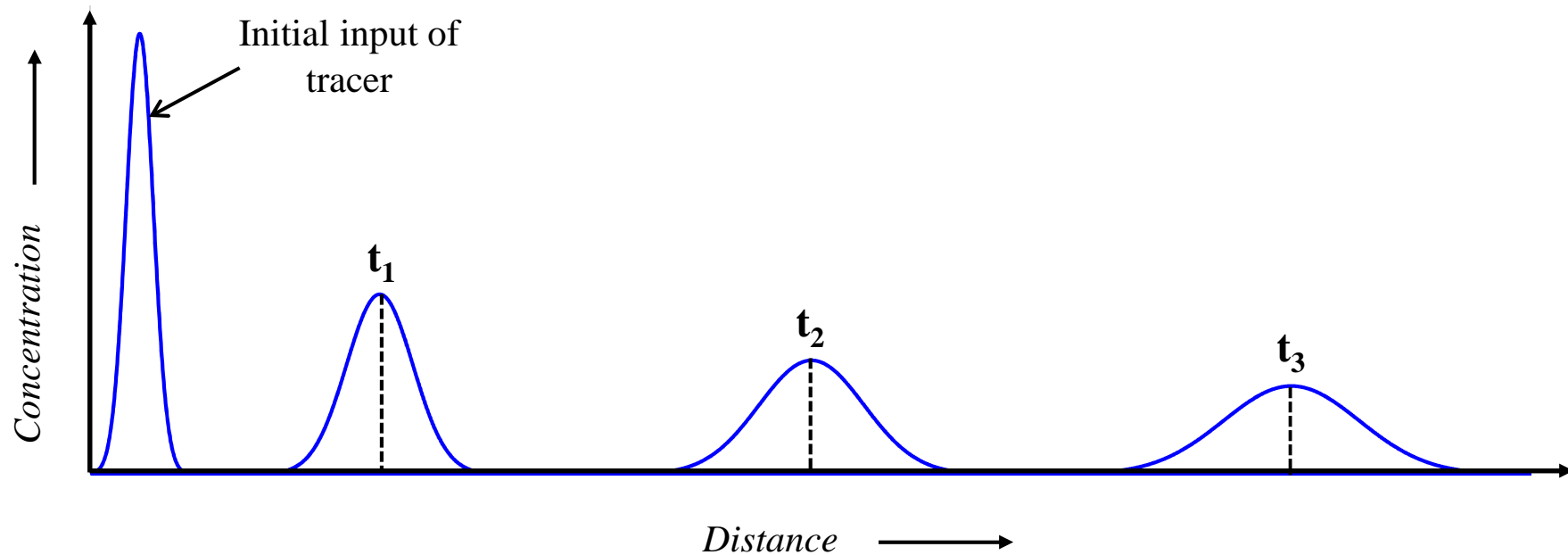
Non-continuous flow & different paths in porous media



Boundary effects

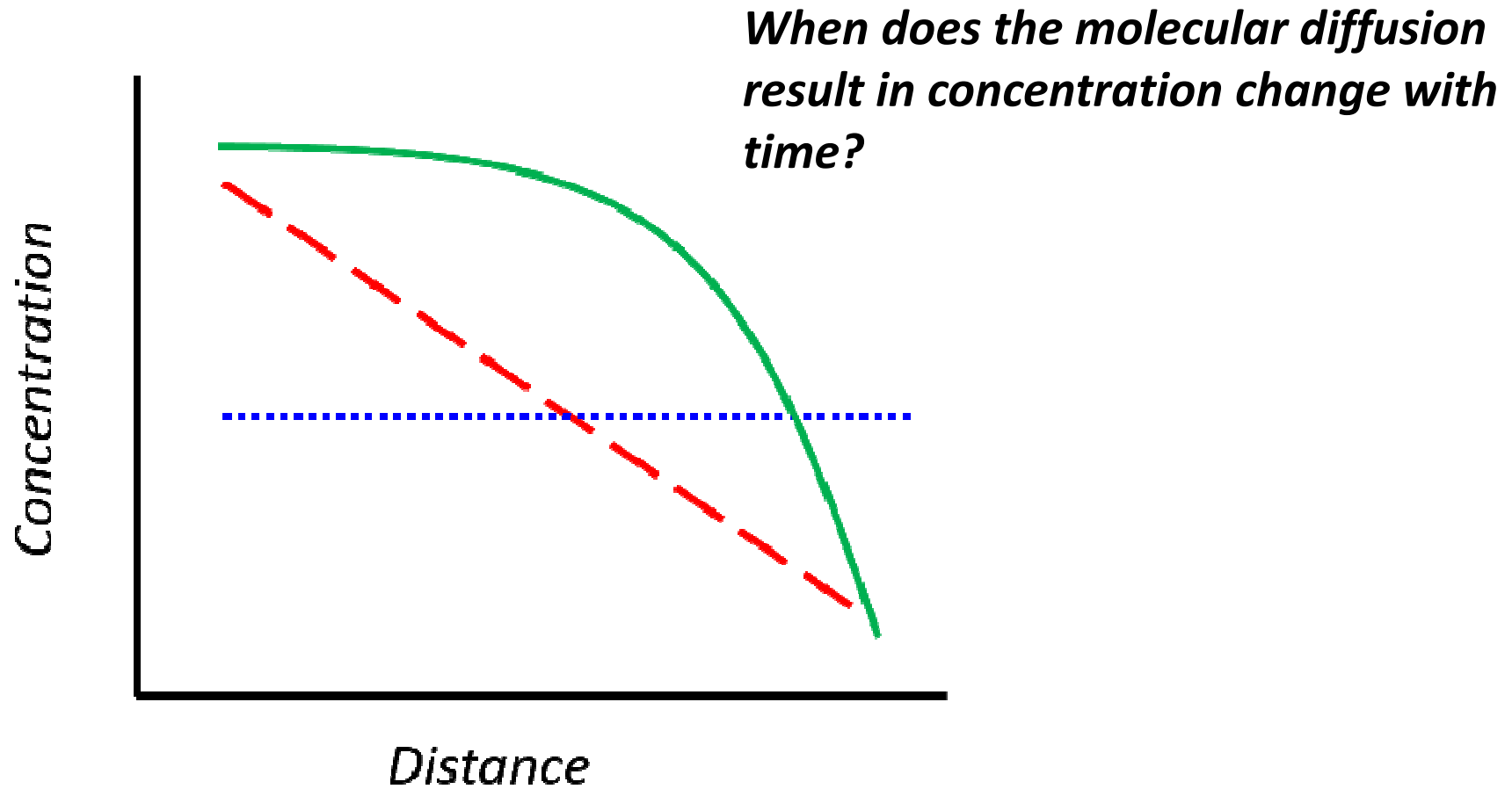


Dispersion from pulse input of a tracer



No change in area (conservative tracer – mass conserved), but gets more spatially dispersed over time

Recall molecular diffusion

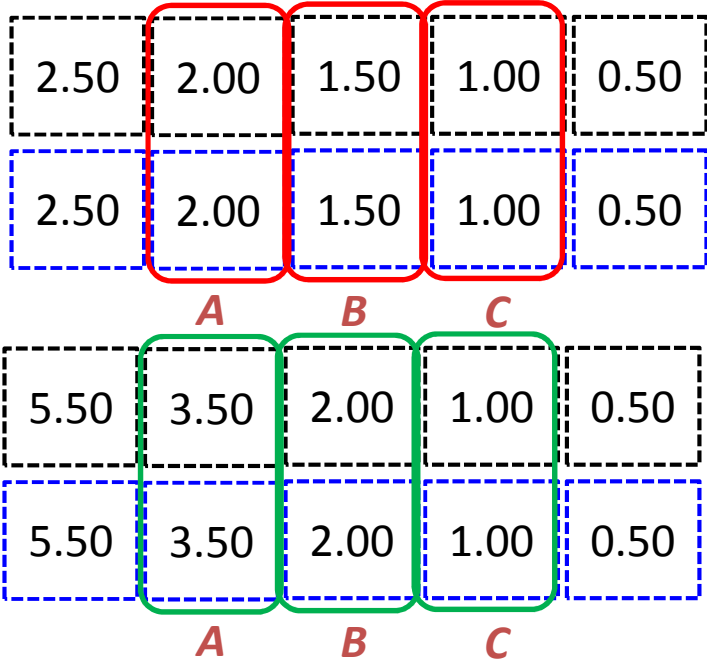


Dispersion by velocity gradient

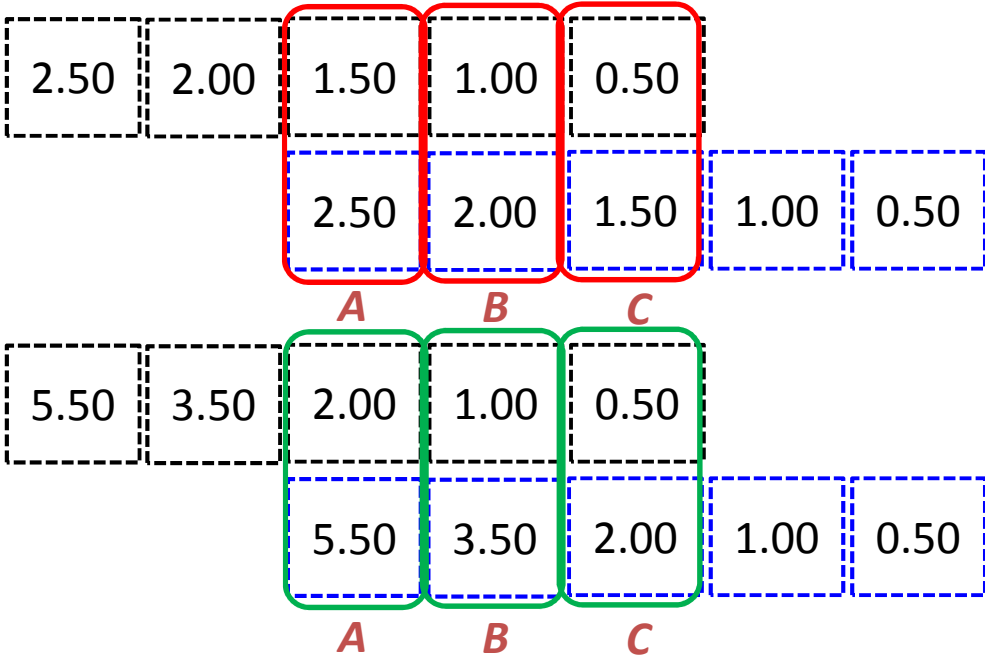
- **Turbulence -- creates velocity gradient**

Top layer moves 1 grid right & bottom layer moves 1 grid left per unit time by differential velocity

$t = 0$



$t = 1$



Modeling dispersion

- Dispersion by turbulence, etc. can be expressed by the same model as molecular diffusion

- Apply Fick's 1st law:

$$J_x = -D_x' \frac{dC}{dx} \quad D_x' = \text{mechanical dispersion coefficient in } x\text{-dir [L}^2\text{/T]}$$

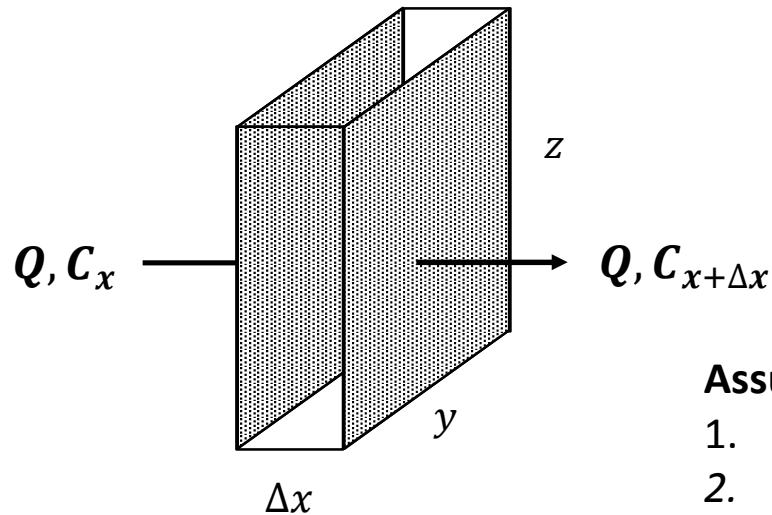
- The overall dispersion coefficient can be defined as the sum of molecular diffusion & mechanical dispersion coeff.

$$J_x = -E_x \frac{dC}{dx}, \quad E_x = D_m + D_x'$$

E_x = overall dispersion coefficient in x-dir [L²/T]

D_m = molecular diffusion coefficient [L²/T]

Mass balance, control volume



$$C_{x+\Delta x} = C_x + (\Delta C / \Delta x) \cdot \Delta x$$

control volume, $V = A \cdot \Delta x$

Assumptions

1. Flow only through 2 faces perpendicular to x-dir
2. Q, A constant
3. Instantaneous mixing within control volume

Rate of:

Accumulation = Input – Output + Net dispersion

$$\frac{V\Delta C}{\Delta t} = QC_x - QC_{x+\Delta x} + \frac{\Delta M_{disp}}{\Delta t}$$

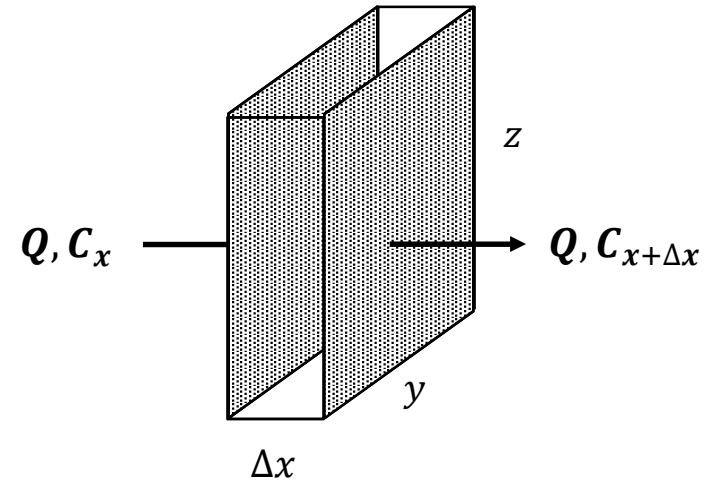
The dispersion term

$$\frac{\Delta M_{disp}}{\Delta t} = ??$$

$$\frac{M_{disp,x_i}}{\Delta t} = -E_x \cdot \left(\frac{\partial C}{\partial x} \right)_{x=x_i} \times A$$

$$\frac{M_{disp,x_i+\Delta x}}{\Delta t} = E_x \cdot \left(\frac{\partial C}{\partial x} \right)_{x=x_i+\Delta x} \times A$$

$$\frac{\Delta M_{disp}}{\Delta t} = E_x \cdot A \cdot \left[\left(\frac{\partial C}{\partial x} \right)_{x=x_i+\Delta x} - \left(\frac{\partial C}{\partial x} \right)_{x=x_i} \right]$$



$$\begin{aligned}\frac{V\Delta C}{\Delta t} &= QC_{x_i} - QC_{x_i+\Delta x} + \frac{\Delta M_{disp}}{\Delta t} \\ &= QC_{x_i} - QC_{x_i+\Delta x} + E_x \cdot A \cdot \left[\left(\frac{\partial C}{\partial x} \right)_{x=x_i+\Delta x} - \left(\frac{\partial C}{\partial x} \right)_{x=x_i} \right]\end{aligned}$$

$$\frac{\Delta C}{\Delta t} = \frac{Q}{V} (C_{x_i} - C_{x_i+\Delta x}) + E_x \cdot \frac{A}{V} \cdot \left[\left(\frac{\partial C}{\partial x} \right)_{x=x_i+\Delta x} - \left(\frac{\partial C}{\partial x} \right)_{x=x_i} \right]$$

use $V = A \cdot \Delta x$ & $u_x = Q/A$:

$u_x = \text{velocity of fluid in } x\text{-dir [L}^2\text{/T]}$

$$\frac{\Delta C}{\Delta t} = u_x \cdot \frac{C_{x_i} - C_{x_i+\Delta x}}{\Delta x} + E_x \cdot \left[\left(\frac{\partial C}{\partial x} \right)_{x=x_i+\Delta x} - \left(\frac{\partial C}{\partial x} \right)_{x=x_i} \right] / \Delta x$$

let $\Delta t \rightarrow 0$ & $\Delta x \rightarrow 0$:

$$\frac{\partial C}{\partial t} = -u_x \frac{\partial C}{\partial x} + E_x \frac{\partial^2 C}{\partial x^2}$$

1-D advection-dispersion equation

$$\frac{\partial C}{\partial t} = \underbrace{-u_x \frac{\partial C}{\partial x}}_{\text{advection term}} + \underbrace{E_x \frac{\partial^2 C}{\partial x^2}}_{\text{dispersion term}}$$

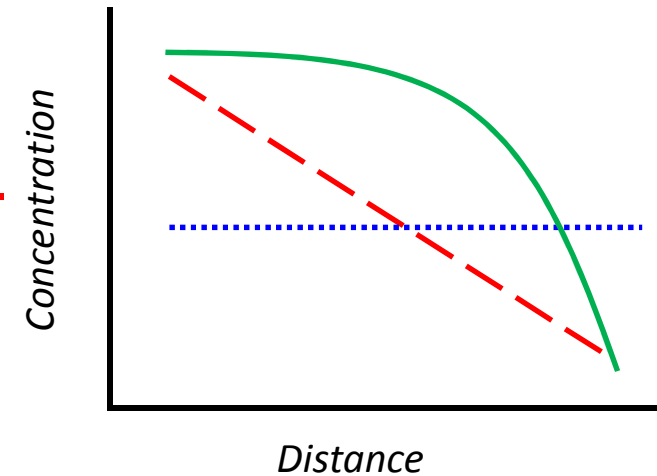
- **Advection:** movement of solutes in the direction of flow, not accounting for mixing
- **Dispersion:** tendency to mix

Dispersion occurs:

- When $\partial^2 C / dx^2 \neq 0$
- By multiple mechanisms
 - Molecular diffusion
 - Variable velocity, turbulence (mechanical dispersion)
 - In surface water, molecular diffusion often very small compared to mechanical dispersion
- With or without a net advective velocity

1-D advection dispersion equation

$$\frac{\partial C}{\partial t} = -u_x \frac{\partial C}{\partial x} + E_x \frac{\partial^2 C}{\partial x^2}$$



Dispersion from a pulse input of tracer

Governing eq.:
$$\frac{\partial C}{\partial t} = -u_x \frac{\partial C}{\partial x} + E_x \frac{\partial^2 C}{\partial x^2}$$

BC's & IC's: $C = 0$ at $x > 0$ & $t = 0$

$M_0 = \text{finite mass pulse at } x = 0 \text{ \& } t = 0, \quad C(0,0) = \infty$

$C = 0$ at $x \rightarrow \infty$ for all t

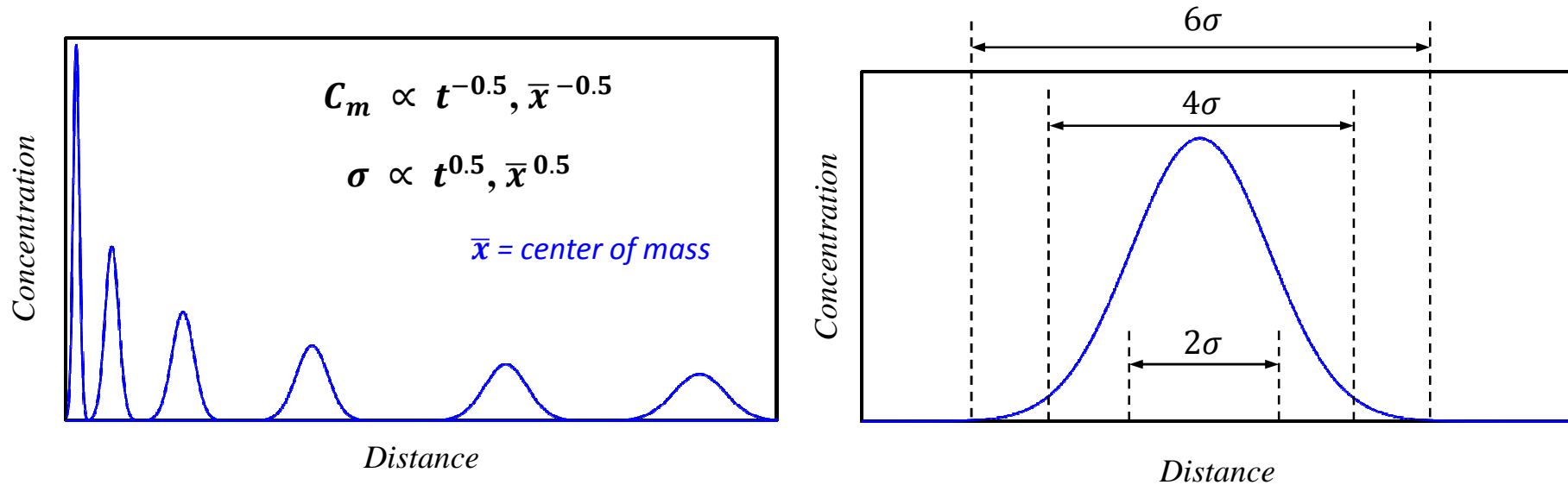
define new, dimensionless variable η and solve:

$$\eta = \frac{x - u_x t}{\sqrt{4E_x t}} \quad C(x, t) = C_{max} e^{-\eta^2} = \frac{M_0}{A \sqrt{4\pi E_x t}} e^{-\left[\frac{(x - u_x t)^2}{4E_x t}\right]}$$

A = cross-sectional area

- Solution is symmetric in space, centered at $u_x t$
- Solution is in the form of a normal distribution with **mean** = $u_x t$ & **$\sigma = (2E_x t)^{0.5}$**

Dispersion from a pulse input of tracer



- Mass is conserved → areas under all curves are the same
- 95% of the mass is located within $x \pm 1.96\sigma$; 99% between $x \pm 2.58\sigma$
- $C_x = 0.01C_m @ x \pm 3.03\sigma$
 → if we define plume as the range of $C_x \geq 0.01C_m$, $\Delta x_{plume} = 6\sigma$

What if the concentration is observed at a certain distance, L_x , over time?

Observation @ $x=L_x$ over time

Let's introduce a dimensionless number, **Pe**, defined as:

$$Pe = \frac{t_{disp}}{t_{advect}} = \frac{L_x^2/E_x}{L_x/u_x} = \frac{L_x u_x}{E_x} = \frac{L_x}{\alpha_x}$$

Pe = Peclet #

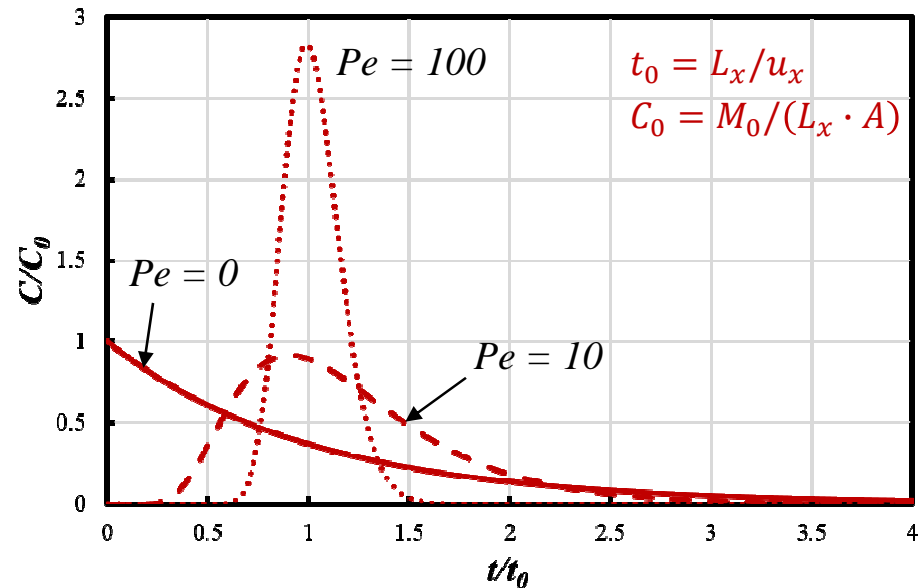
t_{disp} = characteristic time for dispersion [T]

t_{advect} = characteristic time for advection [T]

L_x = length in x-dir [L]

α_x = dispersivity in x-dir [L]

(note $E_x = \alpha_x \cdot u_x$)



For given α_x ; Pe increases with increasing length of system (river, reactor, etc.)

Plug flow vs. Completely mixed

- **Plug flow**

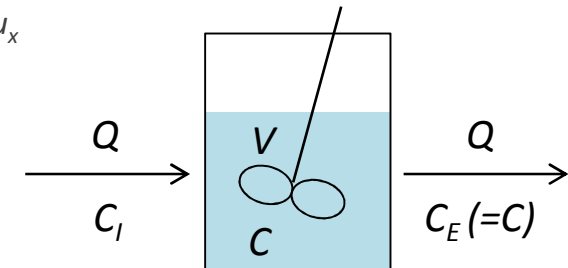
- Assume no mixing in the direction of flow; complete mixing in the direction perpendicular to the flow
- Long reactors (e.g., disinfection), rivers, aqueducts, pipes, etc.



A very thin patch of water, completely mixed within its volume, moving at a velocity of u_x without any substance movement into/out of the patch

- **Completely-mixed, flow-through**

- Complete mixing of the contents of the system
- Common reactor setting for biological reactions, lakes, reservoirs, etc.



$Pe \rightarrow \infty$ Plug flow; $Pe \rightarrow 0$ Completely mixed

+ Reaction (1st order)

Governing eq.:
$$\frac{\partial C}{\partial t} = -u \frac{\partial C}{\partial x} + E_x \frac{\partial^2 C}{\partial x^2} - kC$$

BC's & IC's: $C = 0$ at $x > 0$ & $t = 0$

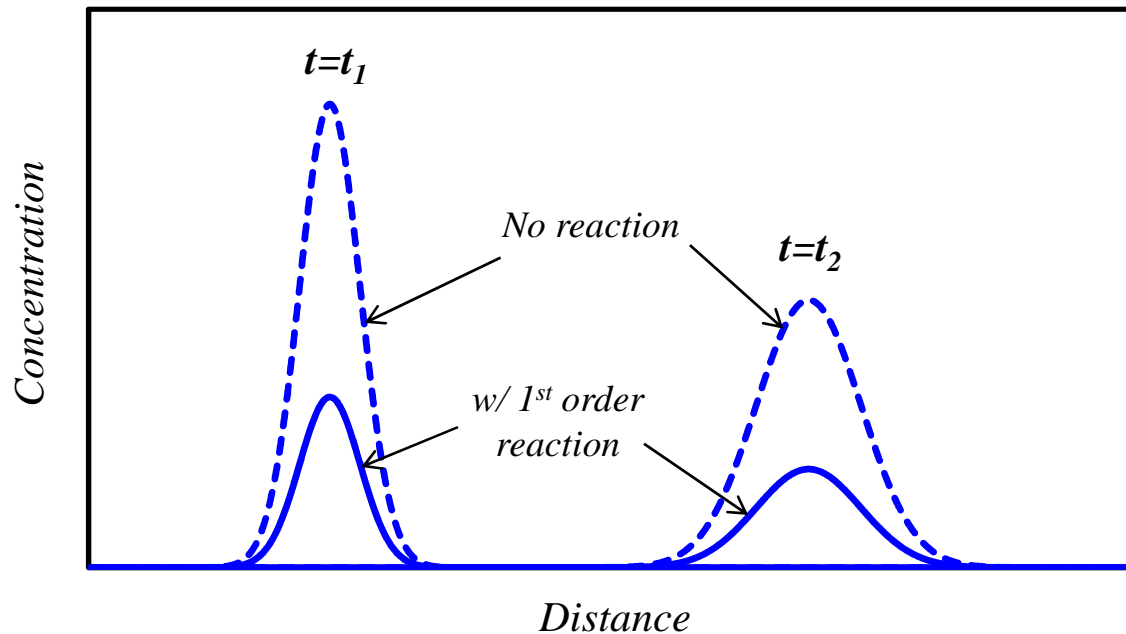
$$M_0 = \text{finite mass pulse at } x = 0 \text{ \& } t = 0, \quad C(0,0) = \infty$$

$$C = 0 \text{ at } x \rightarrow 0 \text{ for all } t$$

Because reaction is 1st order, $M_{tot,t} = M_0 e^{-kt}$

$$C(x, t) = \frac{M_0 e^{-kt}}{A \sqrt{4\pi E_x t}} e^{-\left[\frac{(x-ut)^2}{4E_x t}\right]} = \frac{M_0}{A \sqrt{4\pi E_x t}} e^{-\left[\frac{(x-ut)^2 + kt}{4E_x t}\right]}$$

Dispersion + 1st order reaction



$$C(x, t) = C_{max} e^{-\left[\frac{(x-ut)^2}{4E_x t}\right]}$$

Dispersion

$$C_{max} = \frac{M_0}{A\sqrt{4\pi E_x t}} \times e^{-kt}$$

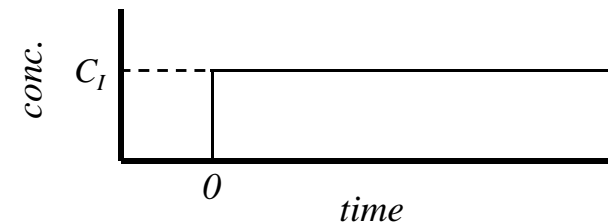
Reaction

- Total mass and peak concentration is reduced to be $\times e^{-kt}$ of the value @ $t=0$
- σ is still $(2E_x t)^{0.5}$

Step input, steady state @ at $x=L_x$

Governing eq.:
$$\frac{\partial C}{\partial t} = -u \frac{\partial C}{\partial x} + E_x \frac{\partial^2 C}{\partial x^2} - kC$$

BC's & IC's: $C = 0$ at $x \geq 0$ & $t = 0$
 $C = C_I$ at $x = 0$ & $t > 0$



Steady state solution:

$$\frac{C_E}{C_I} = \frac{4a \cdot e^{Pe/2}}{[(1+a)^2 \cdot e^{(a \cdot Pe/2)} - (1-a)^2 \cdot e^{-(a \cdot Pe/2)}]}$$

$$a = \left[1 + \frac{4kt_0}{Pe} \right]^{0.5}$$

$$Pe = \frac{u_x L}{E_x}$$

Calculations show plug flow approximation is accurate to within 1% if $Pe \geq 100$ and $(kt_0/Pe) \leq 0.01$

$$t_0 = \text{hydraulic retention time} \\ = L_x/u_x = V/Q$$

Plug flow reactor (PFR) solution: $C_E/C_I = e^{-kt_0}$

Steady-state completely mixed flow reactor (CMFR) solution: $C_E/C_I = (1 + kt_0)^{-1}$

Rivers as plug flow reactors

- **Rivers are typically relatively long, narrow & shallow**
 - Even if transverse dispersion is substantially less than longitudinal dispersion, vertical and transverse mixing is likely to be complete
 - Characteristic time of dispersion, $t_{disp,i} = L_i^2/E_i$

Consider the following river setting (Sacramento River, USA):

<i>Flow velocity</i>	$u_x = 0.5 \text{ m/s}$		<i>Travel time = 80,000 s</i>
<i>Length</i>	$L_x = 40,000 \text{ m}$	$E_x = 15 \text{ m}^2/\text{s}$	$t_{disp,x} = 1.1 \times 10^8 \text{ s}$
<i>Width</i>	$L_y = 40 \text{ m}$	$E_y = 0.12 \text{ m}^2/\text{s}$	$t_{disp,y} = 13,000 \text{ s}$
<i>Height</i>	$L_z = 4 \text{ m}$	$E_z = 0.12 \text{ m}^2/\text{s}$	$t_{disp,z} = 130 \text{ s}$

Dispersion coefficients in aqueous systems

Environment	$E, \text{m}^2/\text{sec}$
Estuaries (longitudinal)	$10^2 - 10^3$
Rivers (longitudinal)	$10^0 - 10^2$
Rivers (lateral)	$10^{-2} - 10^{-1}$
Surface waters (vertical)	$10^{-6} - 10^{-3}$
Pipes, ducts (normal to flow)	$10^{-5} - 10^{-2}$
Solutes in water	$10^{-10} - 10^{-8}$
Solutes in bioturbated sediments	$10^{-9} - 10^{-8}$
Solutes in compacted soils, sediments	$10^{-10} - 10^{-12}$

Course review

