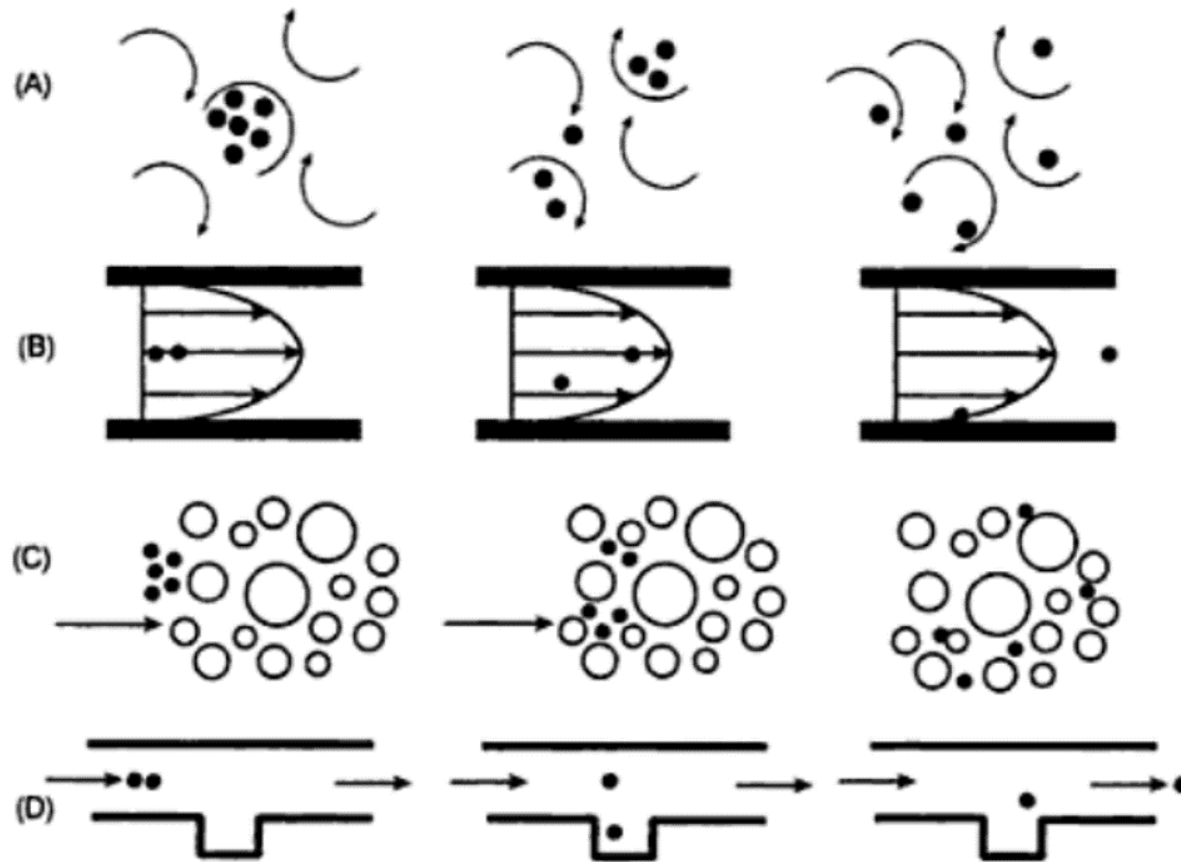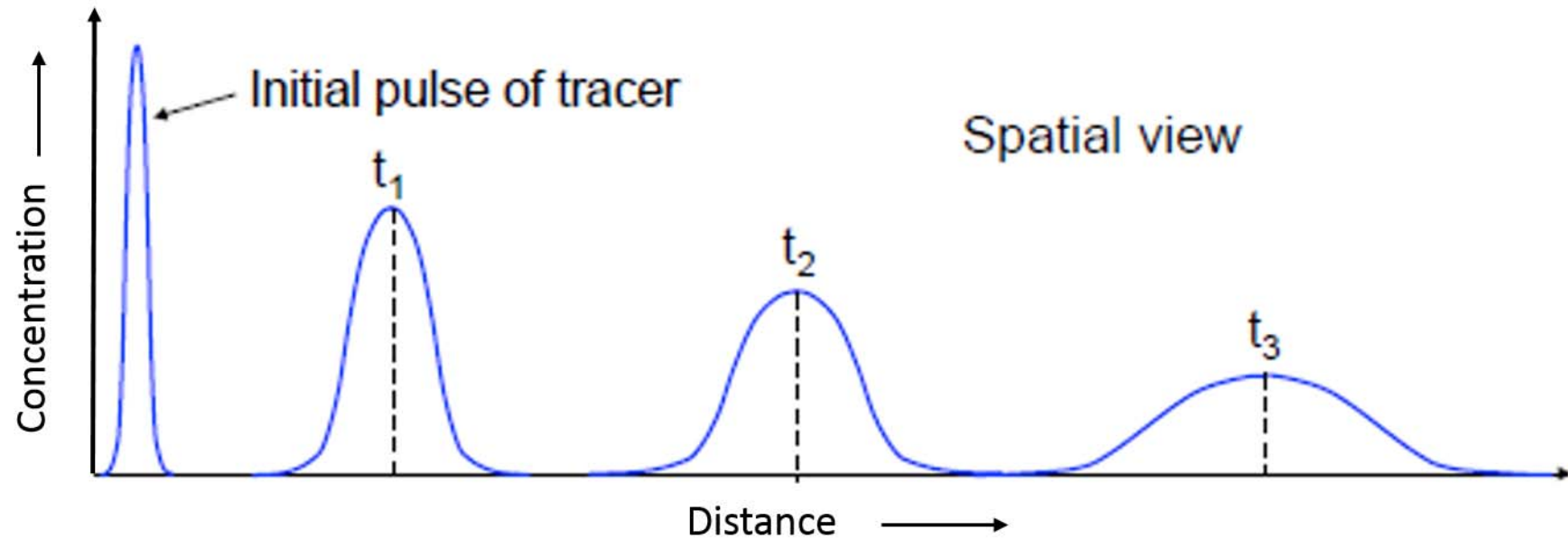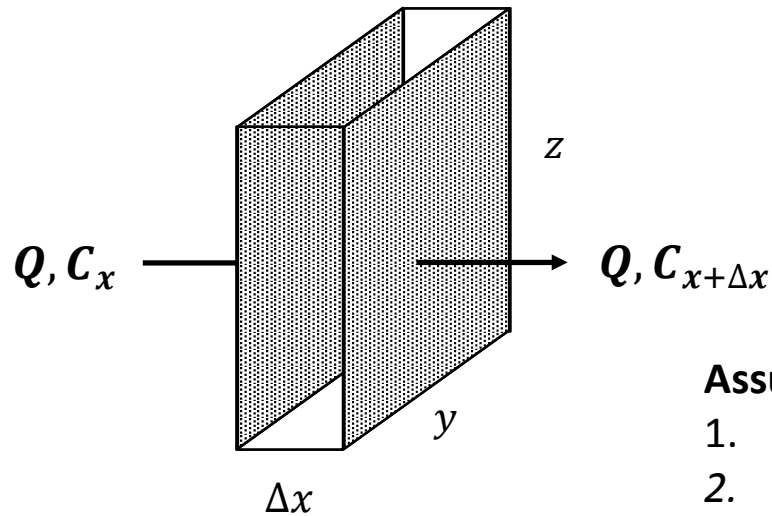# Dispersion

# Dispersion examples



Figure 10.1 Examples of conditions that generate chemical dispersion (A) fluid eddies; (B) velocity gradients in flow in a pipe; (C) noncontinuous flow field (in porous media); (D) boundary effects.

# Dispersion from pulse input of a tracer



Initial pulse of tracer

Spatial view

$t_1$

$t_2$

$t_3$

Concentration

Distance →

- **No change in area (tracer – mass conserved)**
- **Concentration vs. Time at distances $x_1$, $x_2$, $x_3$?**

# Mass balance, control volume

$$C_{x+\Delta x} = C_x + (\Delta C/\Delta x) \cdot \Delta x$$
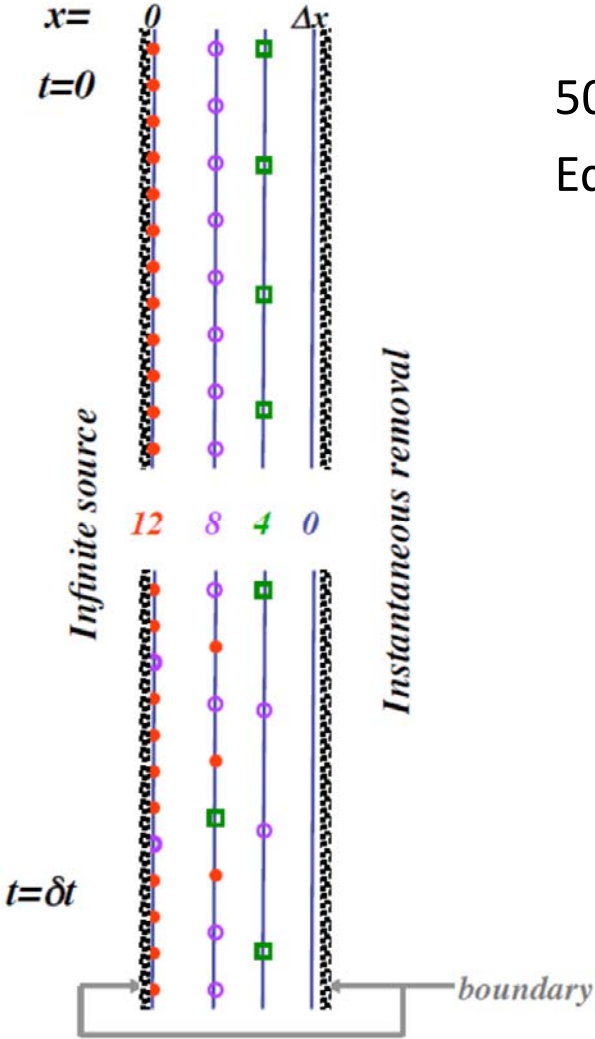
$$\text{control volume,} \quad V = A \cdot \Delta x$$

**Assumptions**

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

$z$

$Q, C_x$

$Q, C_{x+\Delta x}$

$y$

$\Delta x$

**Rate of:**

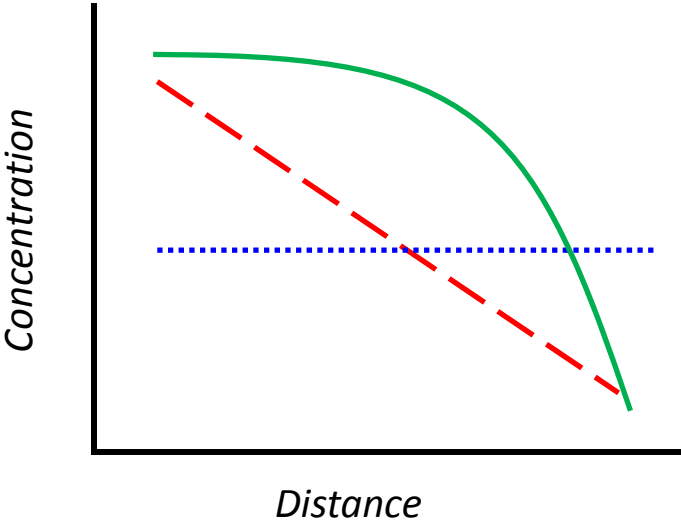***Accumulation = Input − Output + Net dispersion***

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

# Recall molecular diffusion



50% of molecules shift position in time δt

Equal probability of shifting right or left

**When does the molecular diffusion result in concentration change with time?**
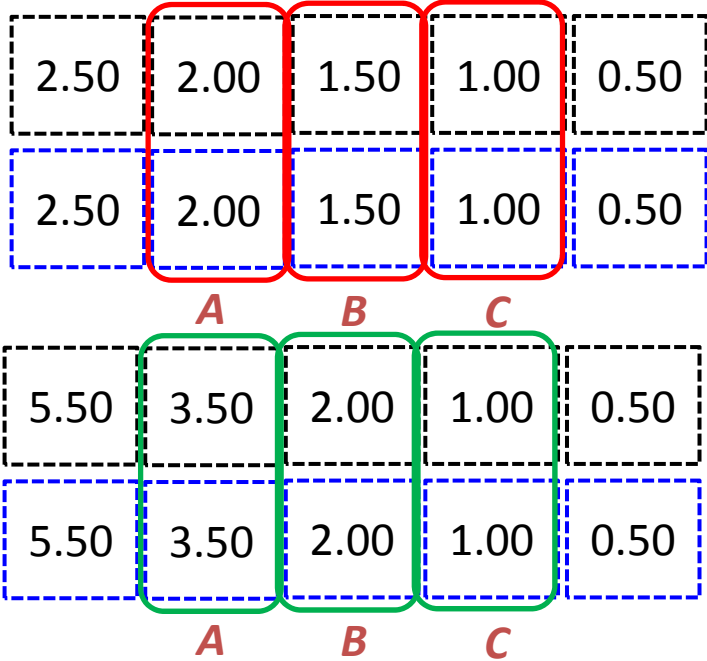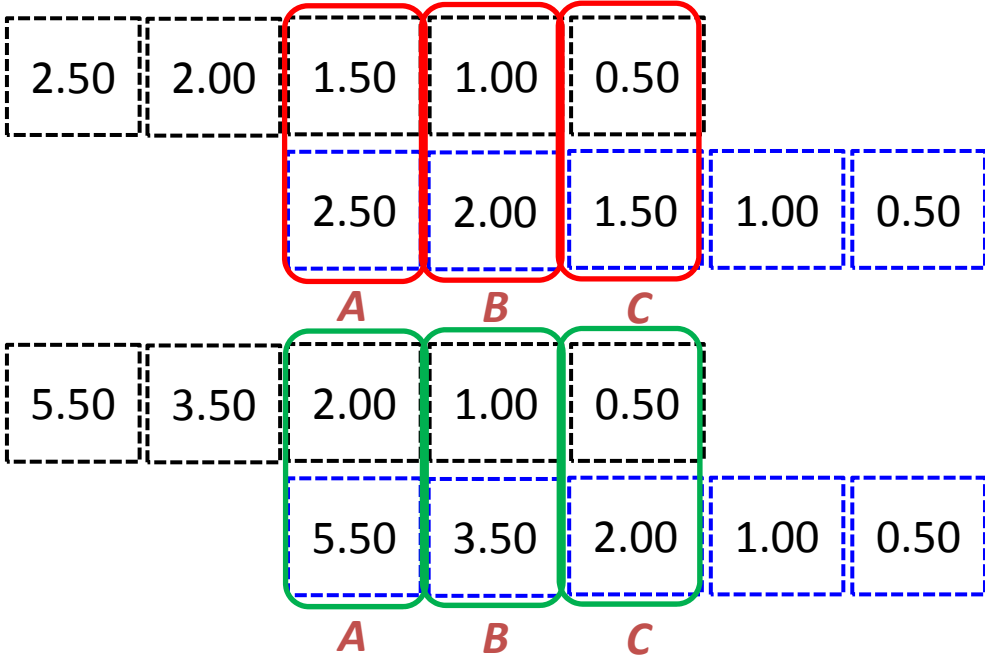
# Dispersion by velocity gradient

- **Turbulence -- creates velocity gradient**

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

# Modeling dispersion

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

- **Apply Fick's 1st law:**

$$J_x = D_x{}' \frac{dC}{dx}$$

$D_x{}'$ = mechanical dispersion coefficient in x-dir [L²/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]

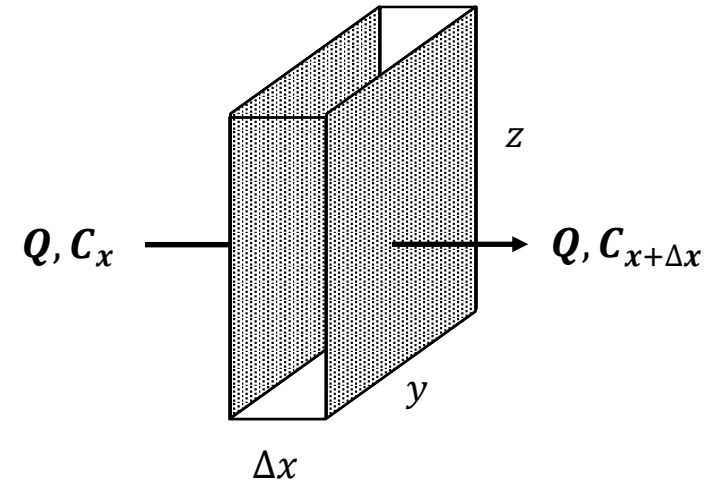$D_m$ = molecular diffusion coefficient [L²/T]

# 1-D advection dispersion equation

$$\frac{V \Delta C}{\Delta t} = Q C_x - Q C_{x+\Delta x} + \frac{\Delta M_{disp}}{\Delta t}$$



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

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

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

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

*u = velocity of fluid (in x-dir) [L$^2$/T]*

# Dispersion occurs:



Concentration

Distance

- **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*

$$\frac{\partial C}{\partial t} = -u \frac{\partial C}{\partial x} + E_x \frac{\partial^2 C}{\partial x^2}$$
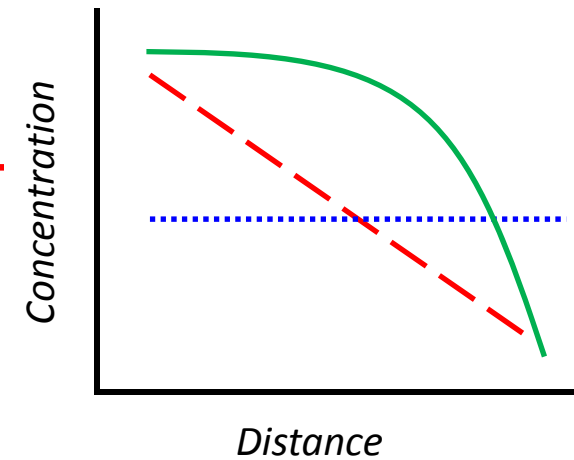
# Dispersion from a pulse input of tracer

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

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

$M_0 =$ finite mass pulse at $x = 0$ & $t = 0$,   $C(0,0) = \infty$
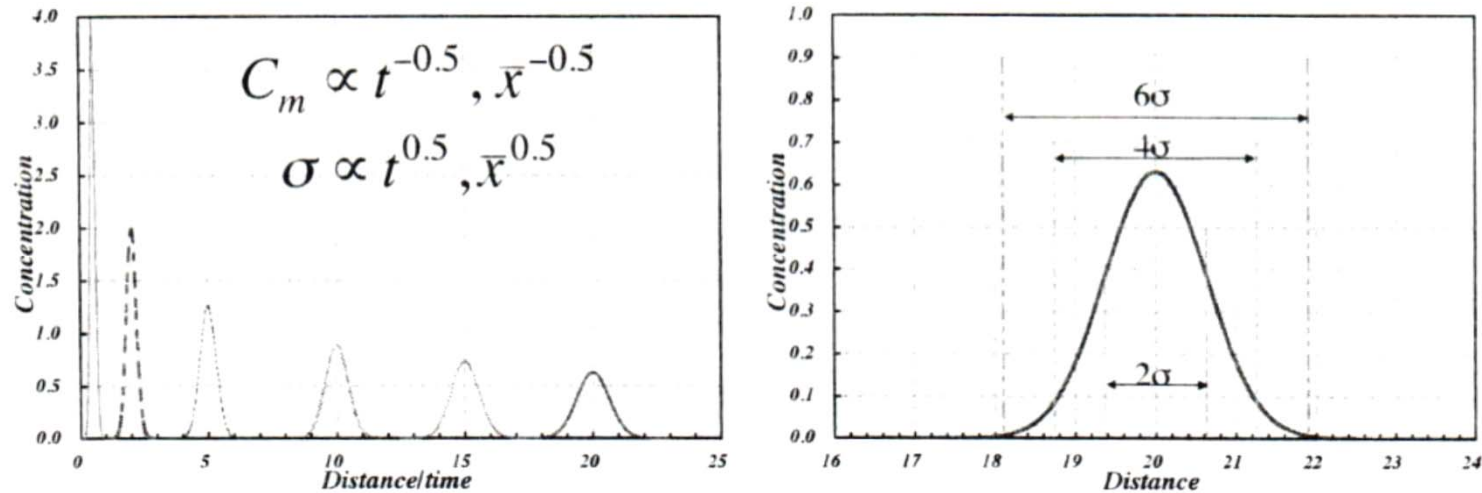
$C = 0$   at   $x \to 0$   for all t

*define new, dimensionless variable $\eta$ and solve:*

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

*A = cross-sectional area*

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

# Dispersion from a pulse input of tracer



$$C_m \propto t^{-0.5}, \bar{x}^{-0.5}$$

$$\sigma \propto t^{0.5}, \bar{x}^{0.5}$$

*Mass is conserved, i.e., areas under all curves are the same*

*95% of the mass is located between x±2σ; 99% between x±2.6σ*

$C_x = 0.01 C_m$ @ x±3σ

*We define:* $\Delta x_{plume} = 6\sigma$

**What if the concentration is observed at a certain distance, L, over time?**
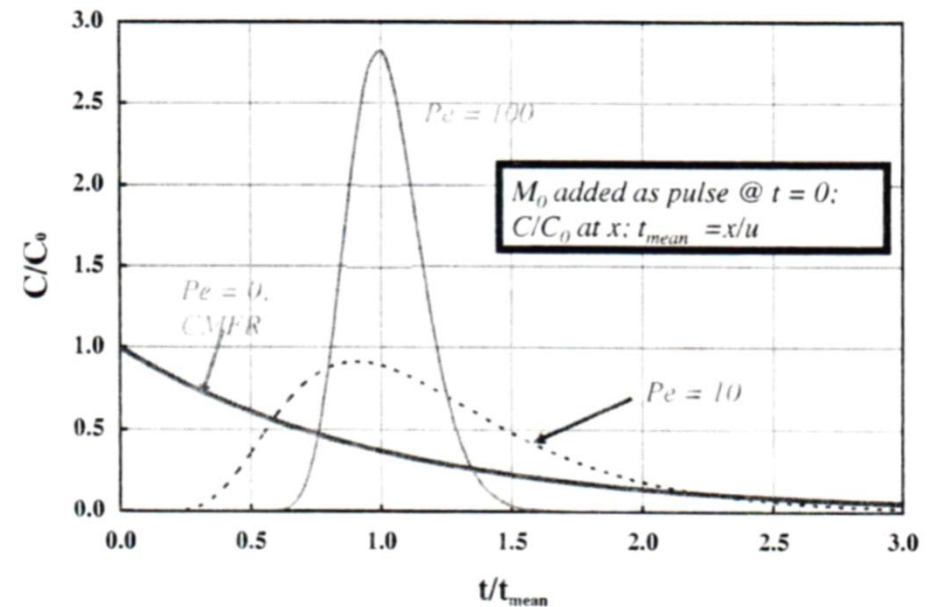
# Peclet #

$$t_{advect} = \frac{L_x}{u_x} \qquad t_{disp} = \frac{L_x{}^2}{E_x}$$

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

For given $\alpha_x$; Pe increases with increasing length of system (river, reactor, etc.)
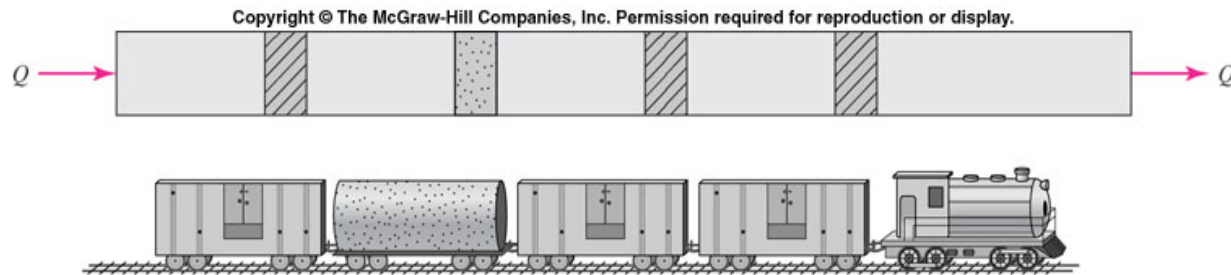
| $Pe \rightarrow \infty$ | Plug flow |
| $Pe \rightarrow 0$ | Completely mixed |



$M_0$ added as pulse @ $t = 0$: $C/C_0$ at $x$: $t_{mean} = x/u$

$Pe = 100$

$Pe = 0,$ CMFR

$Pe = 10$

C/C₀

t/t_mean

# Plug flow vs. Completely mixed reactors

- **Plug-flow reactor (PFR)**
  - 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.



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- **Completely-mixed flow reactors (CMFR) or continuously-stirred tank reactors (CSTR)**
  - Complete mixing of the contents of the reactors
  - Common reactor setting for biological reactions, lakes, reservoirs, etc.
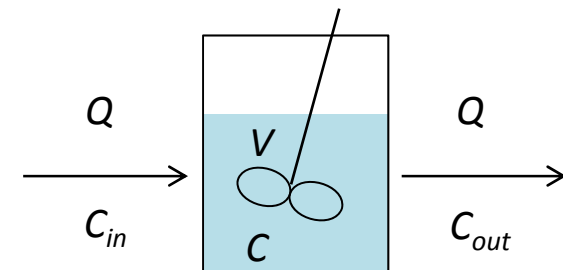
# Advection, dispersion & reaction

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

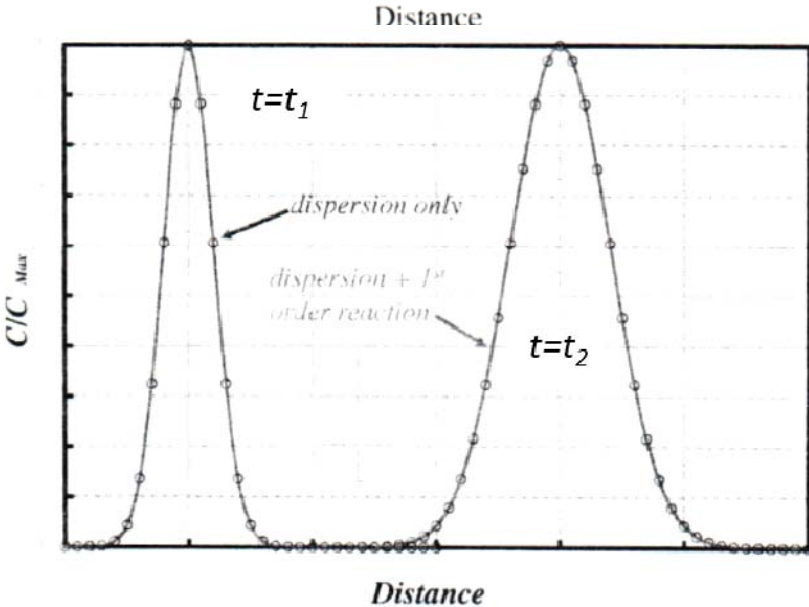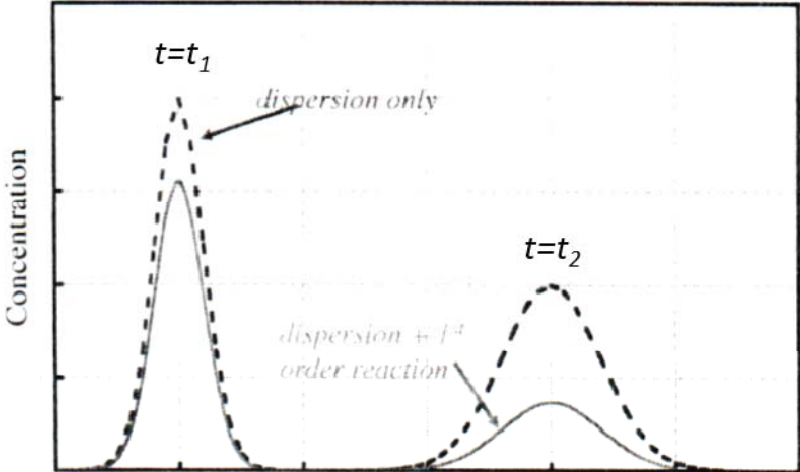**BC's & IC's:**   $C = 0$   $at$   $x > 0$   &   $t = 0$

$M_0 = $ *finite mass pulse at* $x = 0$   &   $t = 0,$   $C(0,0) = \infty$

$C = 0$   $at$   $x \to 0$   *for all t*

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

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

# Dispersion + 1st order reaction



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

Dispersion

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

Dispersion

Reaction

# Steady state response for reactor at x=L

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:

$C = 0 \quad at \quad x \geq 0 \quad \& \quad t = 0$

$C = C_I \quad at \quad x = 0 \quad \& \quad t > 0$

**Steady state solution:**

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

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

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

*Calculations show plug flow approximation is accurate to within 1% if $Pe \geq 100$ and $(k\bar{t}/Pe) \leq 0.01$*

*$\bar{t}$ = hydraulic retention time = V/Q*

PFR solution: $C_E/C_I = e^{-k\bar{t}}$
Steady-state CSTR solution: $C_E/C_I = (1 + k\bar{t})^{-1}$

# 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
  - $t_{disp} \sim L^2$

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

  $H = 4\,m$      $E_x = 15\,m^2/s$

  $W = 40\,m$      $E_y = 0.12\,m^2/s$

  $L = 40{,}000\,m$      $E_z = 0.12\,m^2/s$

  $u_x = 0.5\,m/s$

  *Travel time = 80,000 seconds*

  $t_{disp,x} = 1.1 \times 10^8\,s$

  $t_{disp,y} = 13{,}000\,s$

  $t_{disp,z} = 130\,s$

# Dispersion coefficients in aqueous systems

| Environment | $E$, m$^2$/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 bioturbed sediments | $10^{-9} - 10^{-8}$ |
| Solutes in compacted soils, sediments | $10^{-10} - 10^{-12}$ |