# Dispersion

# Dispersion examples

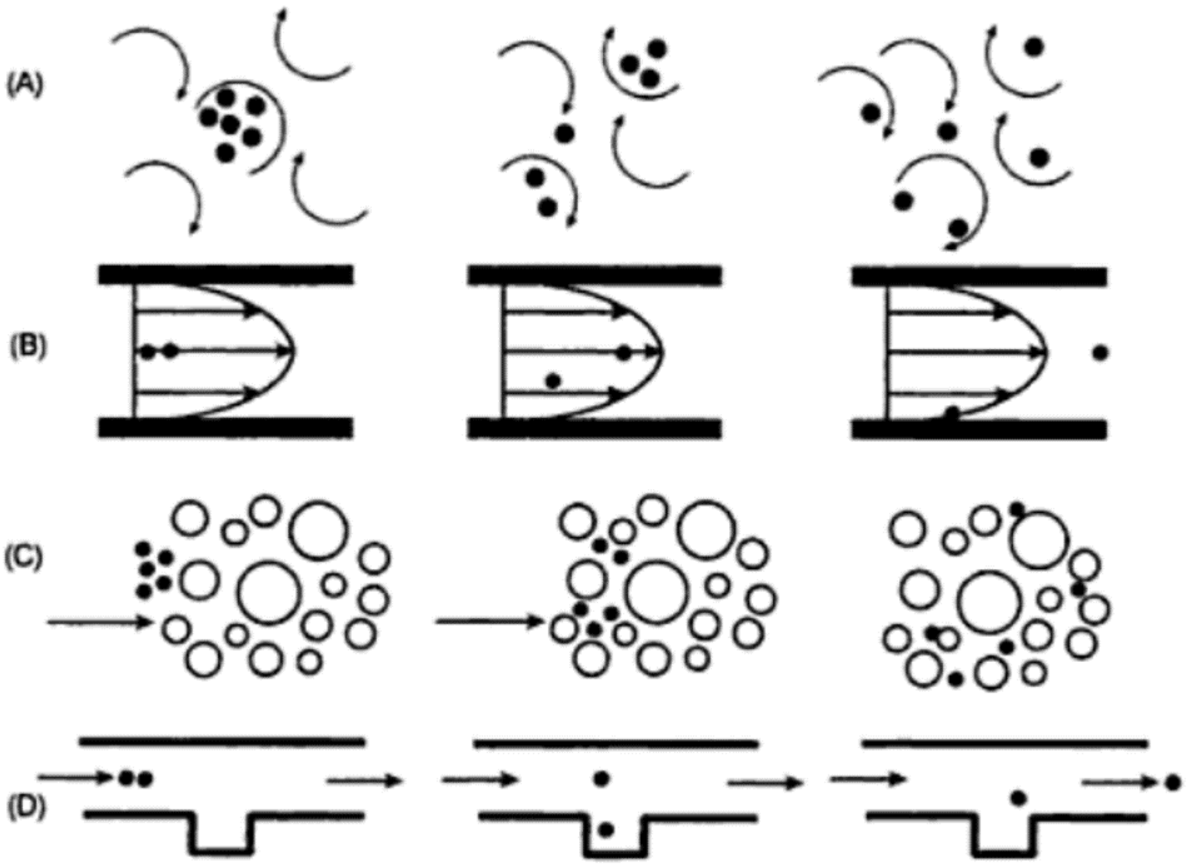
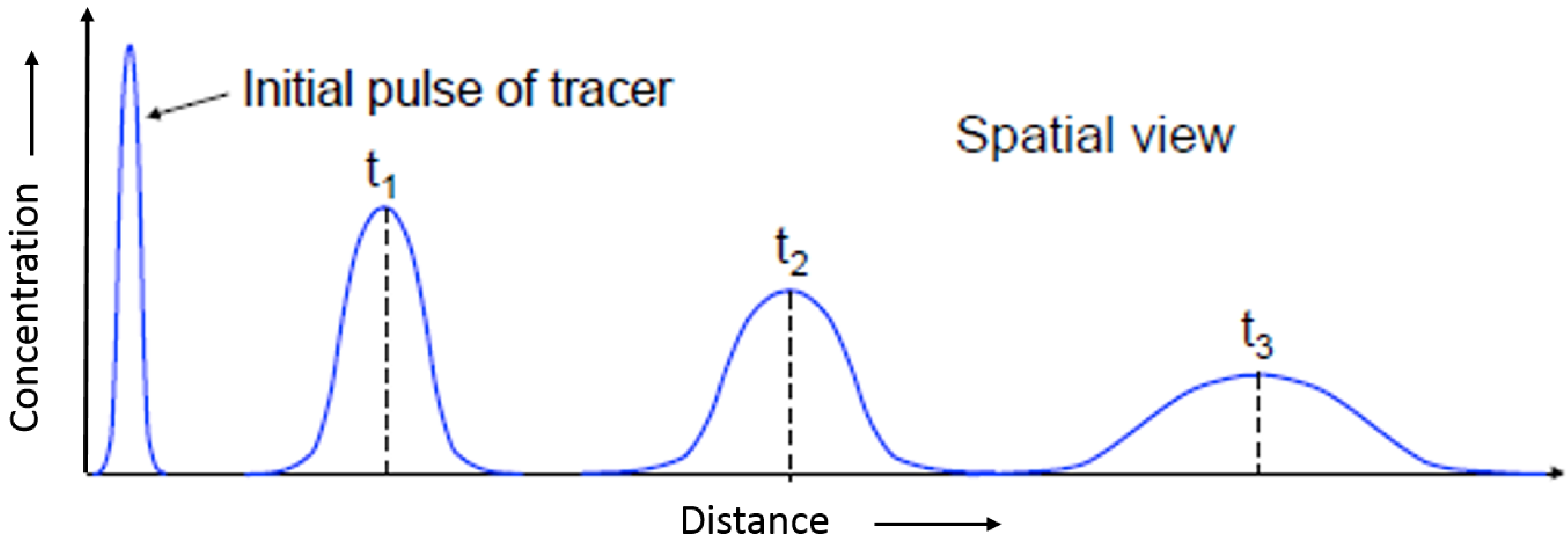


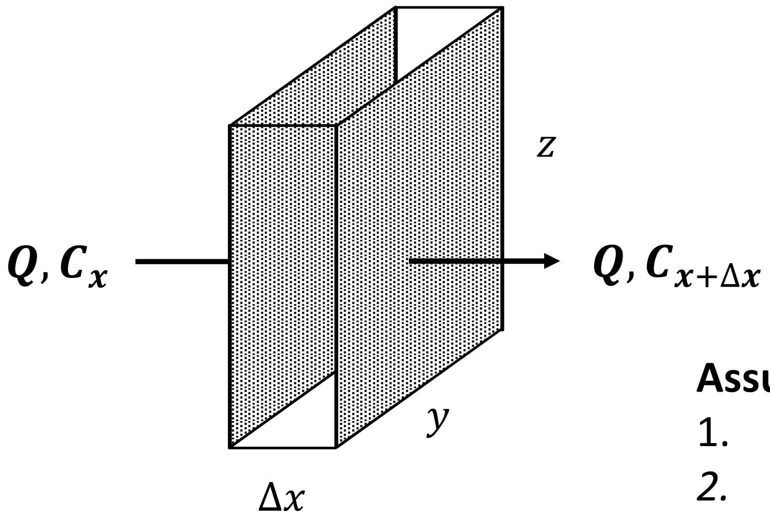

**Figure 10.1** Examples of conditions that generate chemical dispersion (A) fluid eddies; (B) velocity gradients in flow in a pipe; (C) noncontinuous flow field (in porous media); (D) boundary effects.

# Dispersion from pulse input of a tracer




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

# Mass balance, control volume




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

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

**Assumptions**

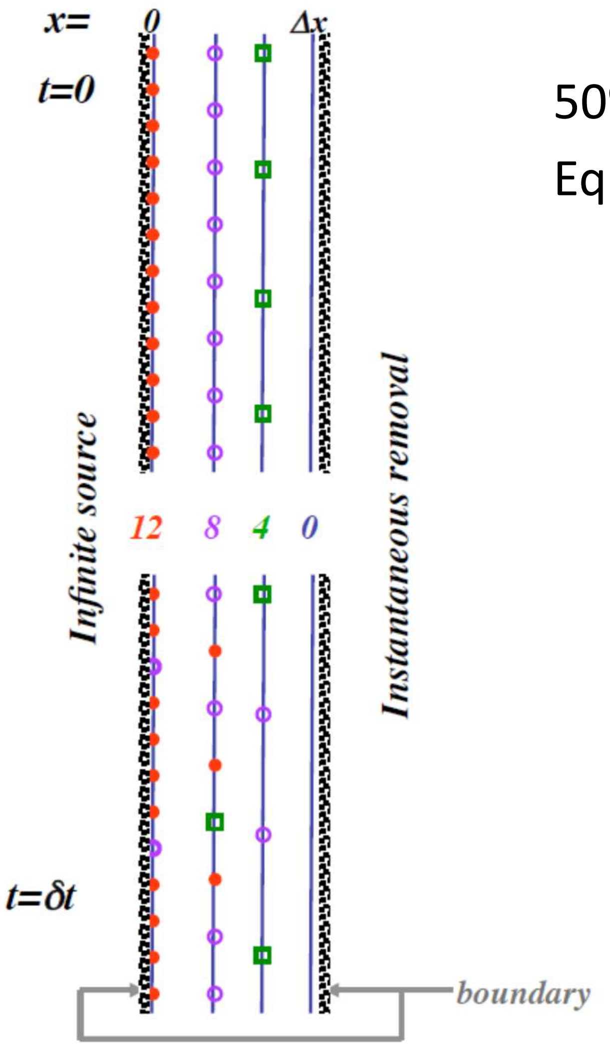
1. Flow only through 2 faces perpendicular to *x*-dir
2. *Q, A* constant
3. Instantaneous mixing within control volume

**Rate of:**

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

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

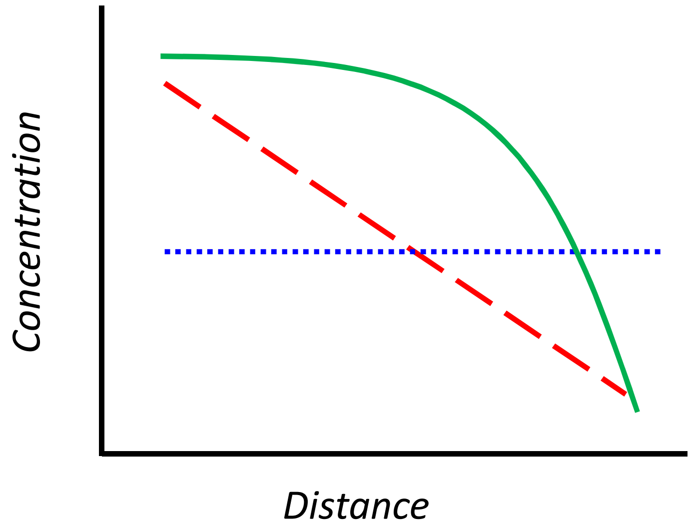
# Recall molecular diffusion




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?***

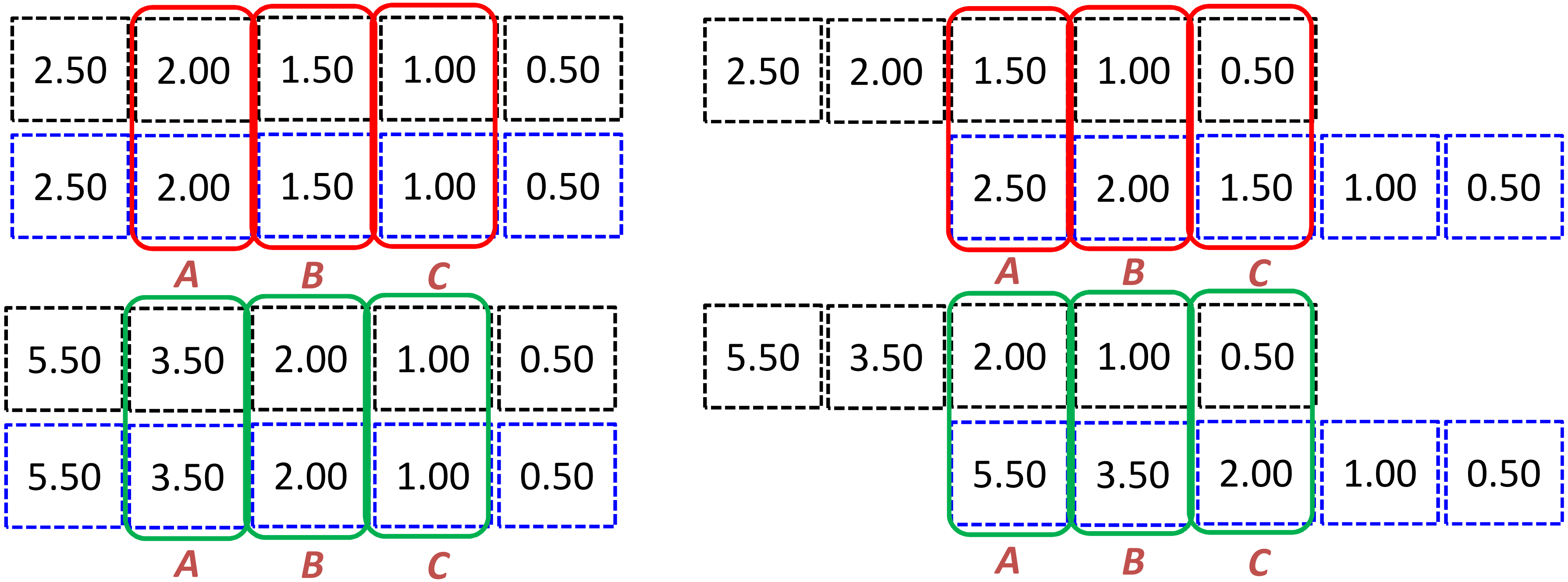


# Dispersion by velocity gradient

- **Turbulence -- creates velocity gradient**

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

$t = 0$ $\qquad\qquad\qquad\qquad$ $t = 1$



# Modeling dispersion

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

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

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

*$D_x'$ = mechanical dispersion coefficient in x-dir [$L^2$/T]*

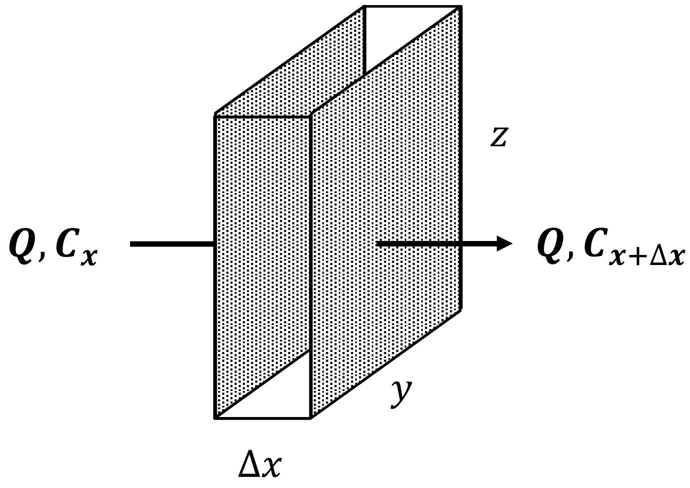
- The overall dispersion coefficient can be defined as the sum of molecular diffusion & mechanical dispersion coeff.

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

*$E_x$ = overall dispersion coefficient in x-dir [$L^2$/T]*
*$D_m$ = molecular diffusion coefficient [$L^2$/T]*

# 1-D advection dispersion equation

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




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

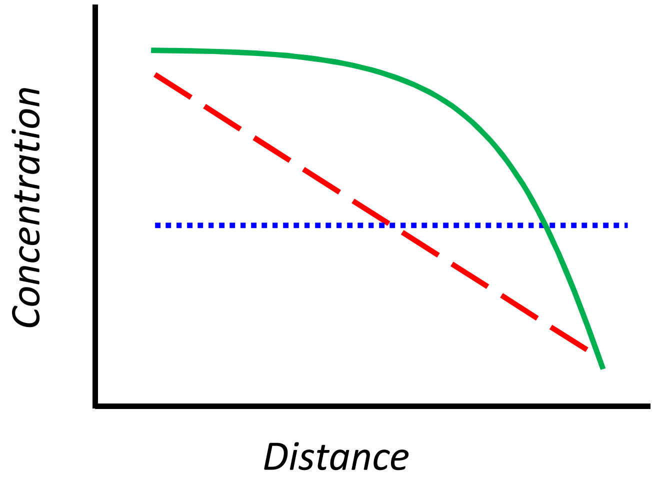
$$\frac{M_{disp,x_i+\Delta x}}{\Delta t} = E_x \cdot \left(\frac{\partial C}{\partial x}\right)_{x=x_i+\Delta x} \times A$$

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

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

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

# Dispersion occurs:




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

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

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

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

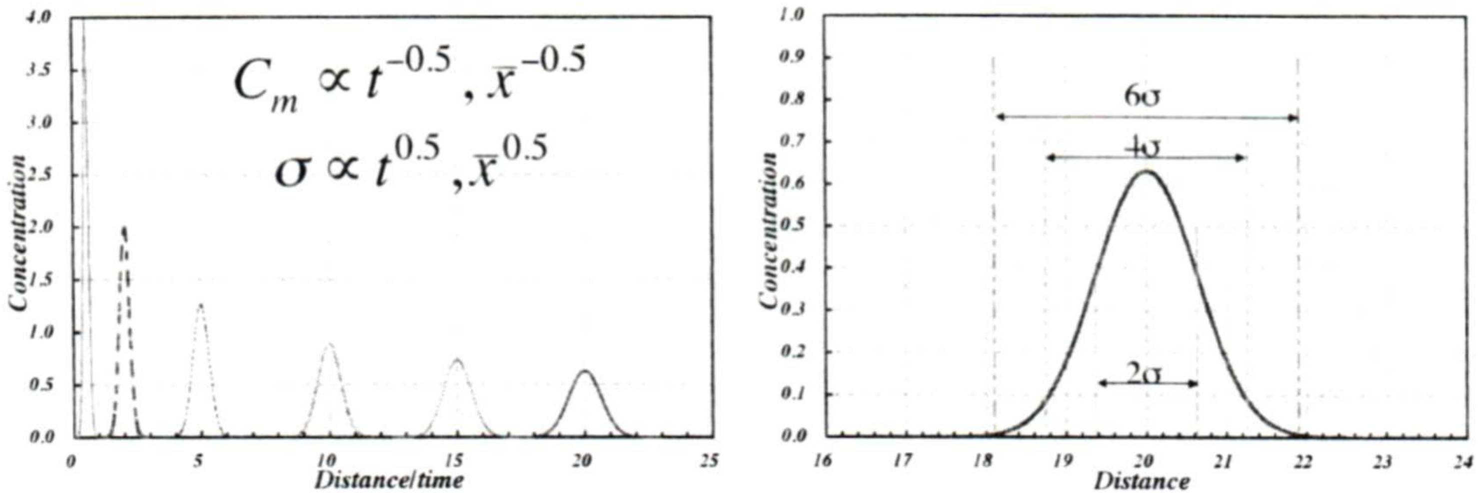
*<u>define new, dimensionless variable η and solve</u>:*

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

*A = cross-sectional area*

*Solution is symmetric in space, centered at **ut***
*Solution is in the form of a normal distribution with*
***mean = ut** & **σ=(2E<sub>x</sub>t)<sup>0.5</sup>***

# Dispersion from a pulse input of tracer




*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*

$C_x = 0.01C_m$ *@ x±3σ*

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

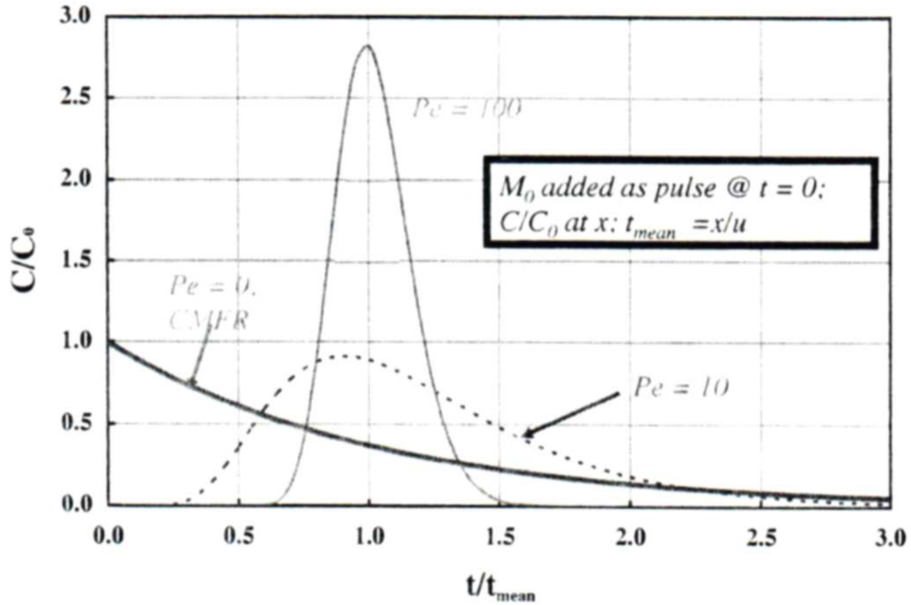
***What if the concentration is observed at a certain distance, L, over time?***

# 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.)

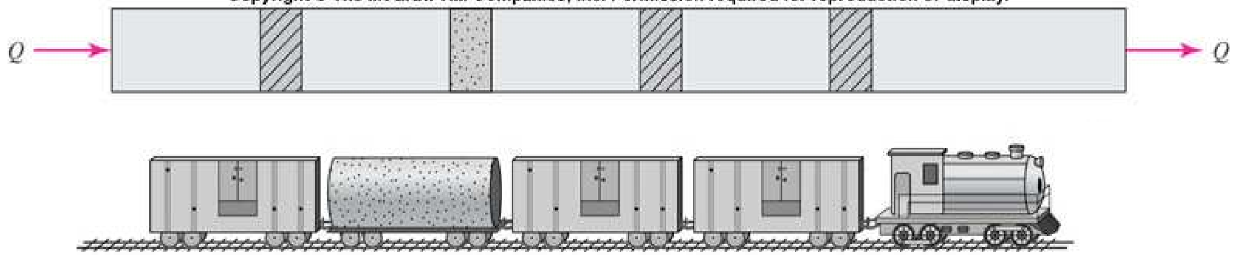



| | | |
|---|---|---|
| $Pe \rightarrow \infty$ | | *Plug flow* |
| $Pe \rightarrow 0$ | | *Completely mixed* |

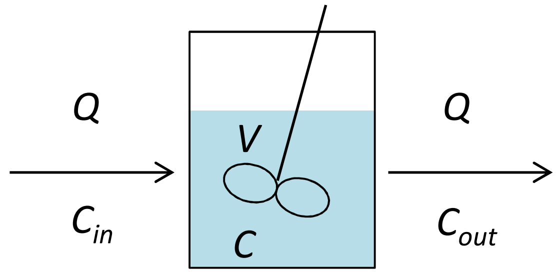
# Plug flow vs. Completely mixed

- **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.






- **Completely-mixed, flow-through**
  - Complete mixing of the contents of the reactors
  - Common reactor setting for biological reactions, lakes, reservoirs, etc.



# Advection, dispersion & reaction

**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* $x > 0$ & $t = 0$

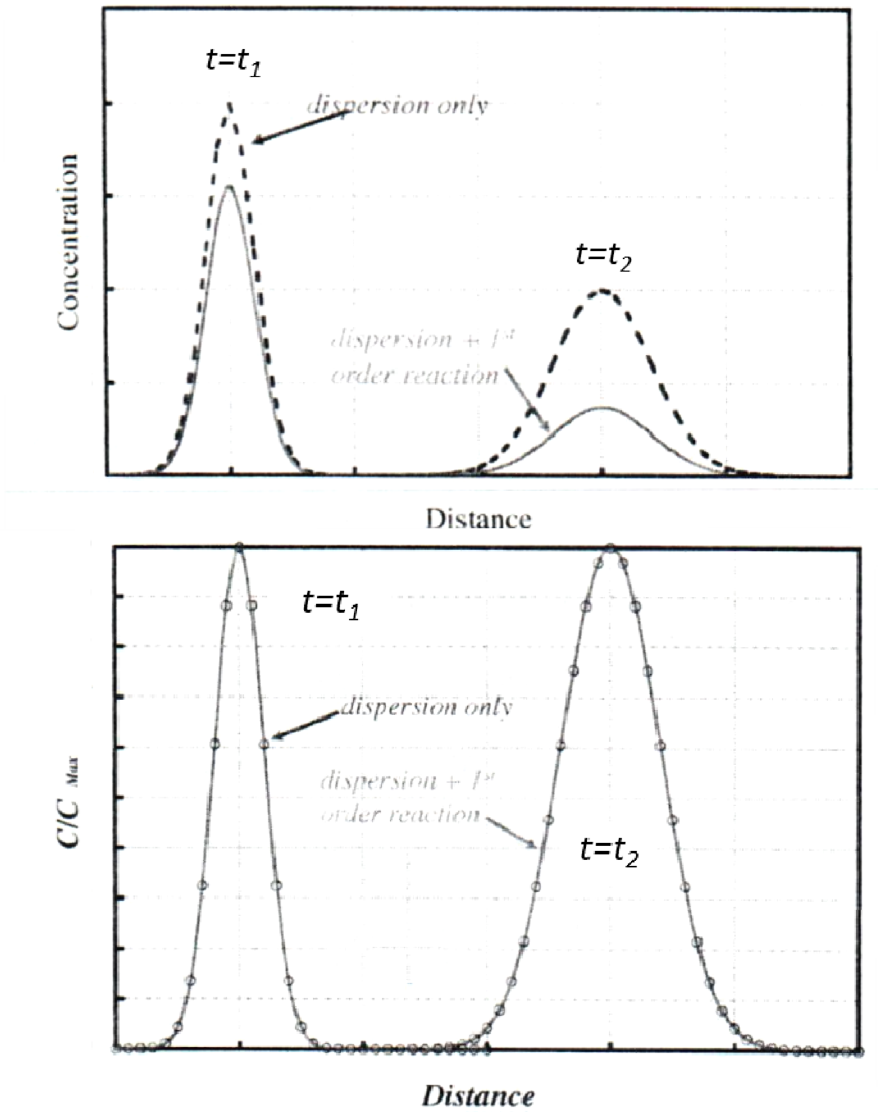
$M_0 =$ *finite mass pulse at* $x = 0$ & $t = 0,$ $C(0,0) = \infty$

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

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

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

# Dispersion + 1st order reaction




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

Dispersion

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

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: $C = 0$ *at* $x \geq 0$ & $t = 0$

$C = C_I$ *at* $x = 0$ & $t > 0$

**Steady state solution:**

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

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

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

*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
  - Characteristic time of dispersion, $t_{disp,i} = L_i^2/E_i$

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

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

# Dispersion coefficients in aqueous systems

| Environment | $E$, m²/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 | $10^{-10} – 10^{-12}$ |