Dispersion

Dispersion examples

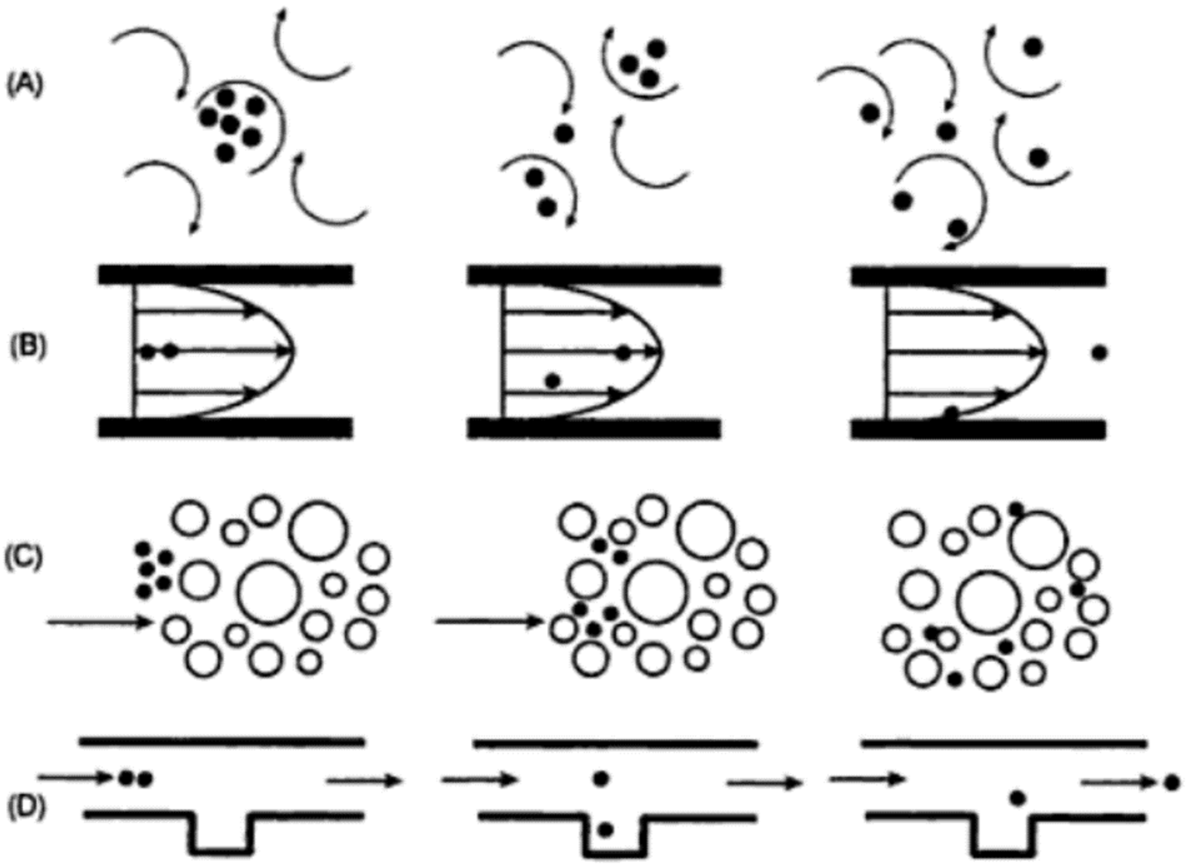
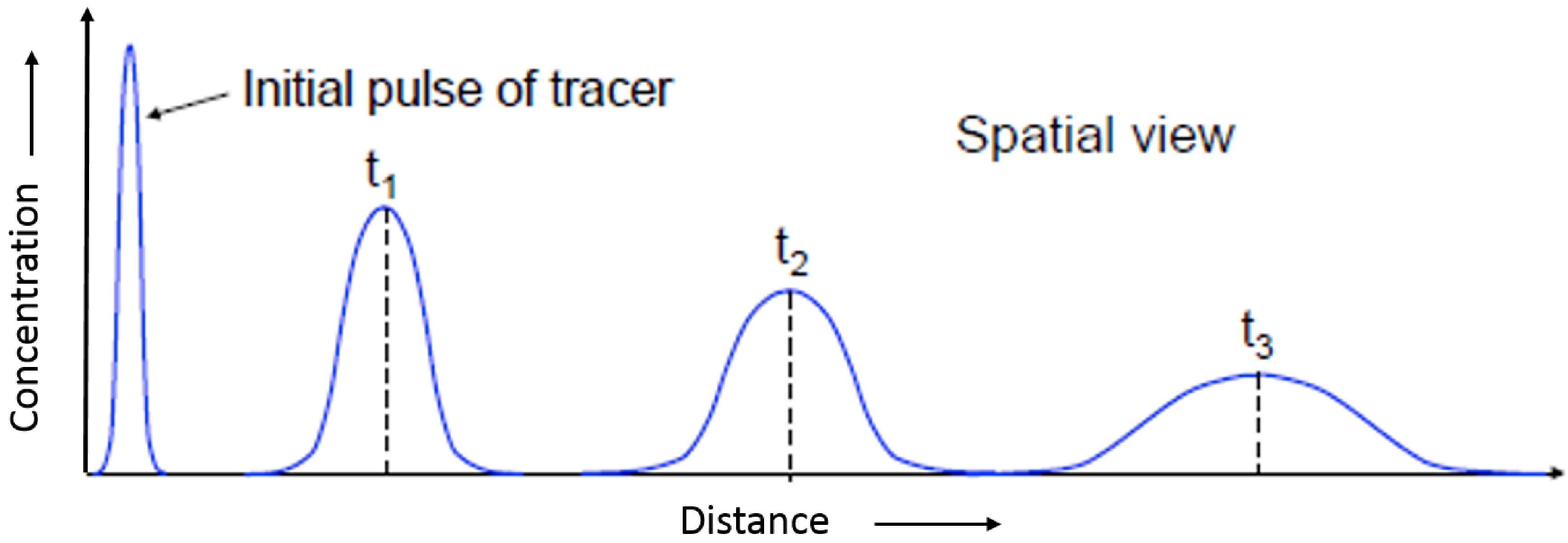


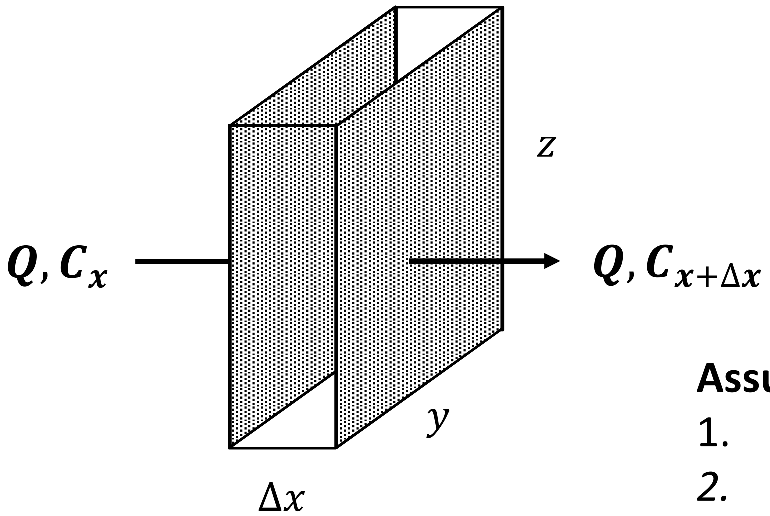
Figure 10.1 Examples of conditions that generate chemical dispersion (A) fluid eddies; (B) velocity gradients in flow in a pipe; (C) noncontinuous flow field (in porous media); (D) boundary effects.

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, $V = A \cdot \Delta x$

Assumptions

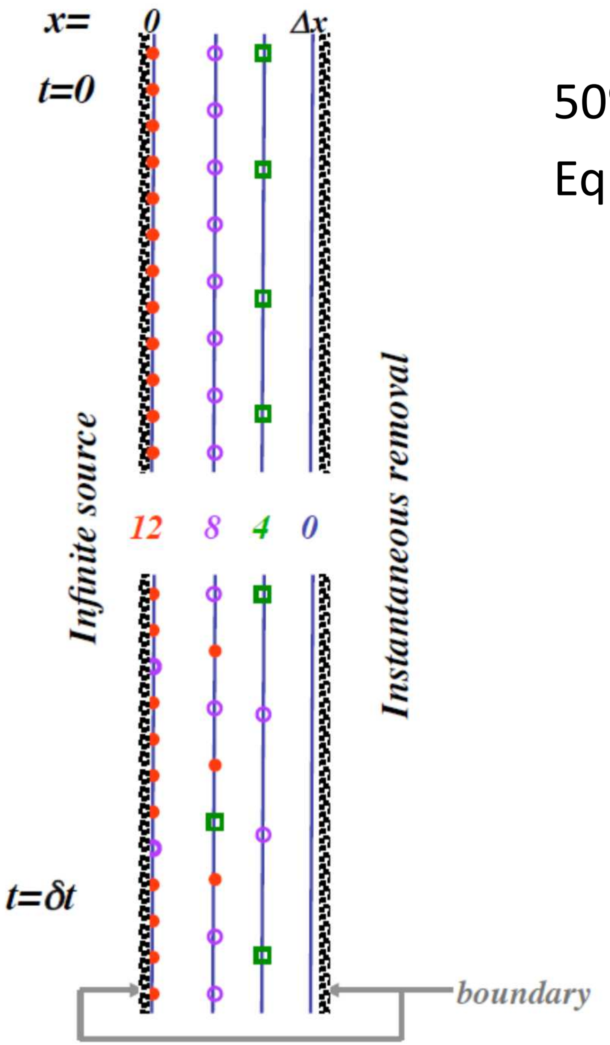
1. Flow only through 2 faces perpendicular to *x*-dir
2. *Q, A* constant
3. Instantaneous mixing within control volume

Rate of:

Accumulation = Input − Output + Net dispersion

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

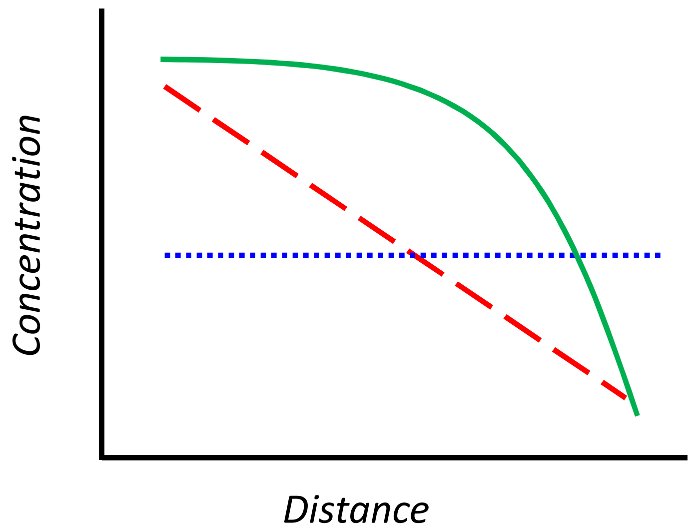
Recall molecular diffusion



50% of molecules shift position in time δt

Equal probability of shifting right or left

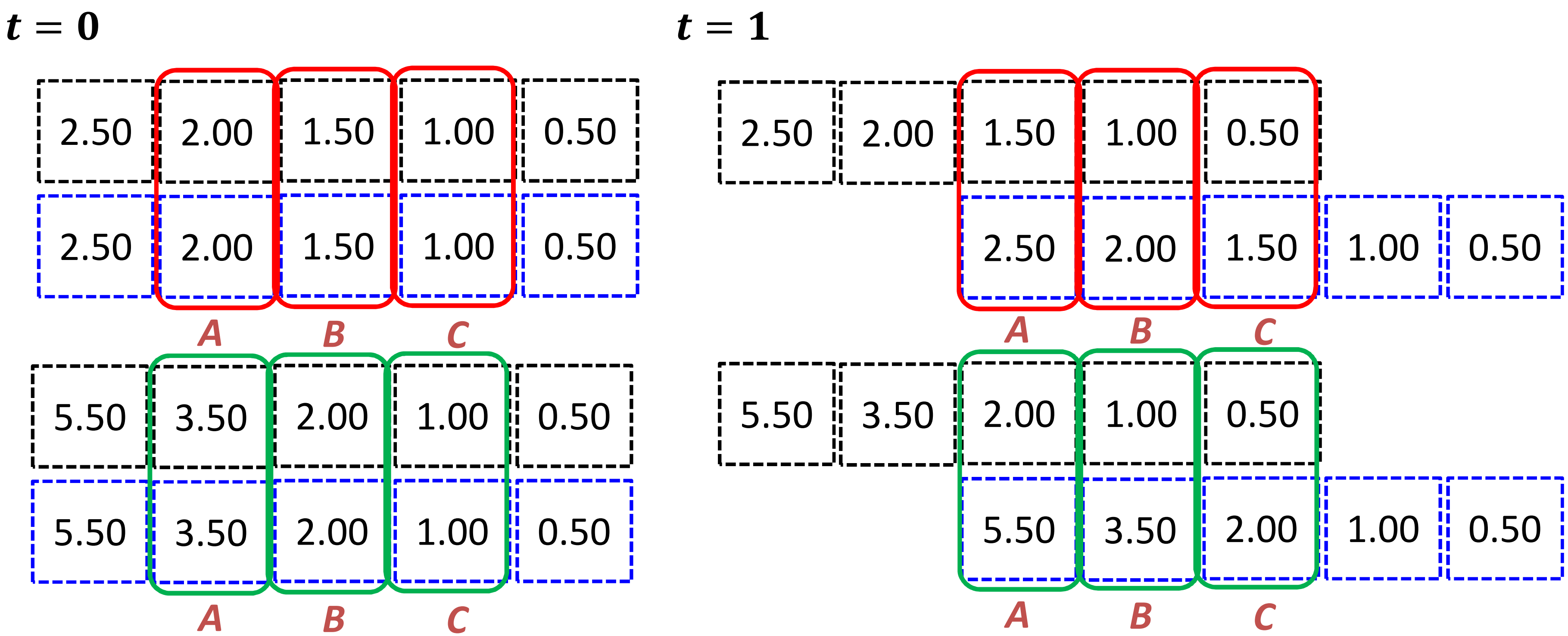
When does the molecular diffusion result in concentration change with time?



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



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]

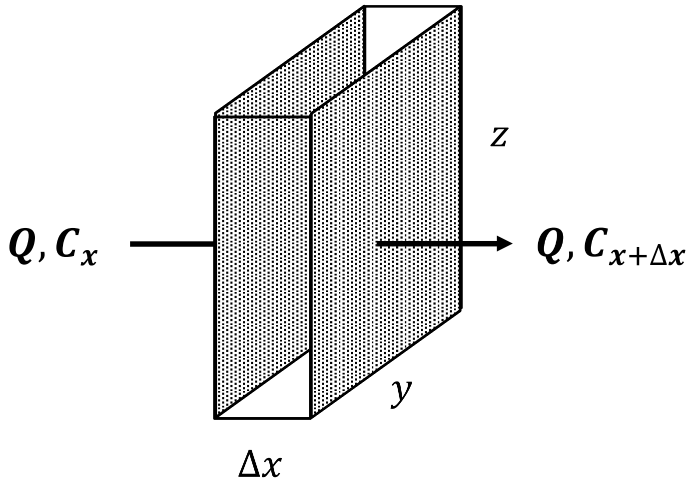
- The overall dispersion coefficient can be defined as the sum of molecular diffusion & mechanical dispersion coeff.

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

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

1-D advection dispersion equation

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



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

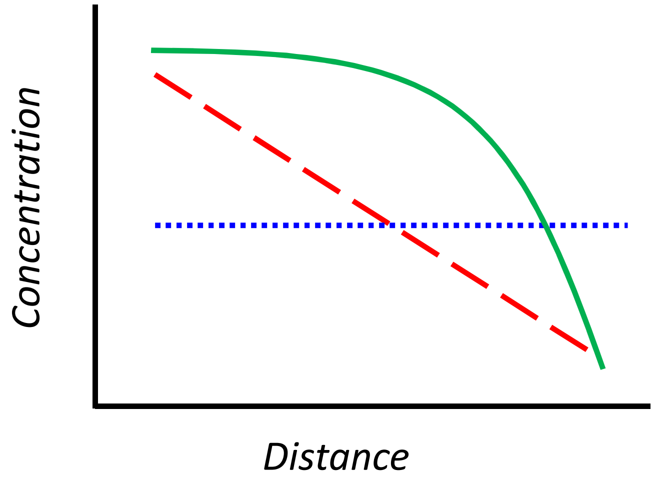
$$\frac{M_{disp,x_i+\Delta x}}{\Delta t} = E_x \cdot \left(\frac{\partial C}{\partial x}\right)_{x=x_i+\Delta x} \times A$$

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

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

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* $x \to 0$ *for all t*

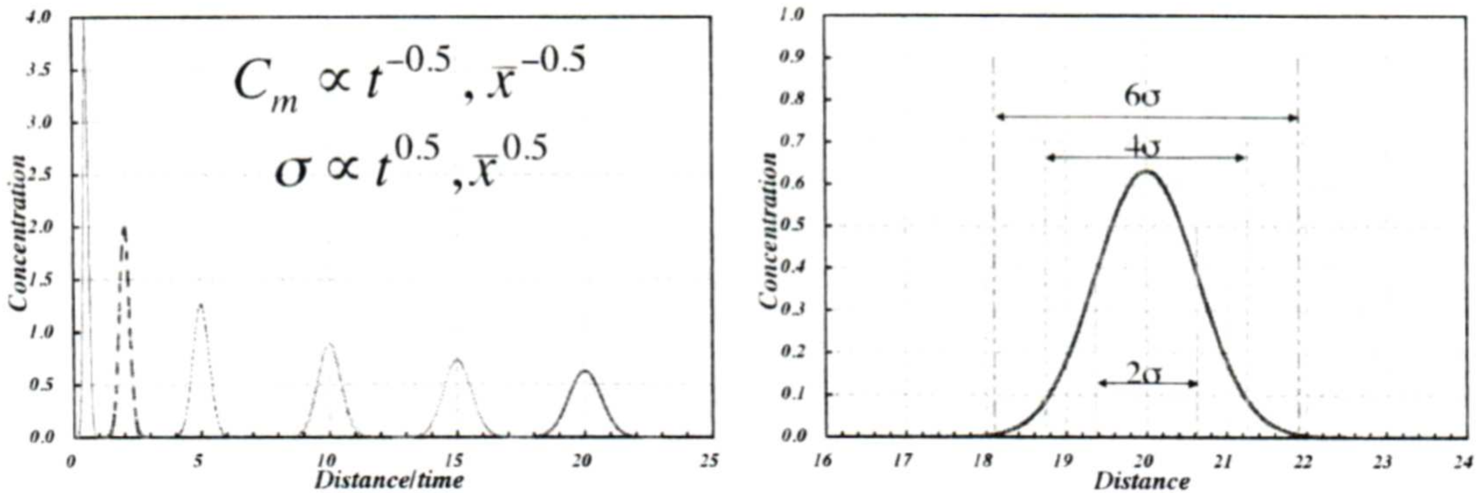
define new, dimensionless variable η and solve:

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

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$_x$t)$^{0.5}$

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

$C_x = 0.01C_m$ @ $x \pm 3\sigma$

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

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

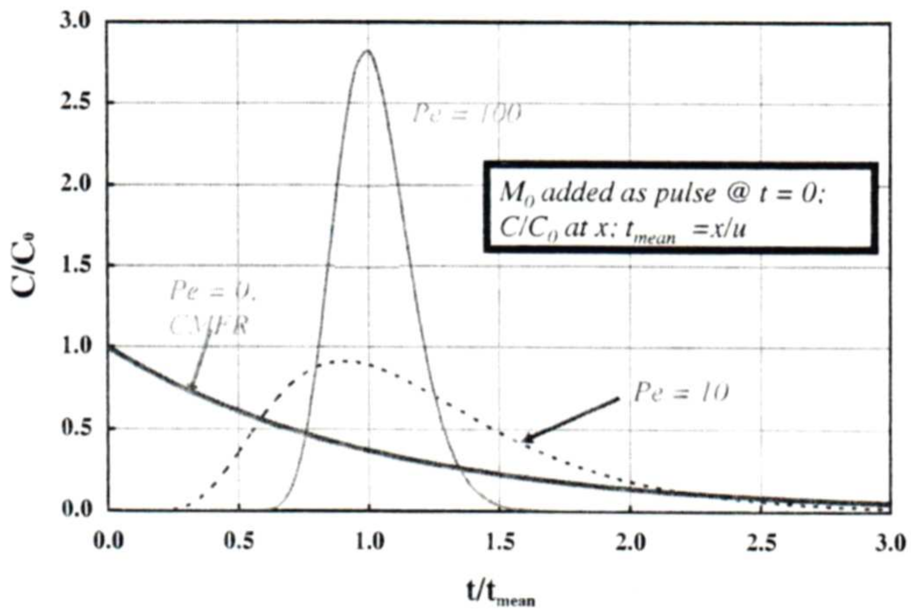
Peclet

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

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

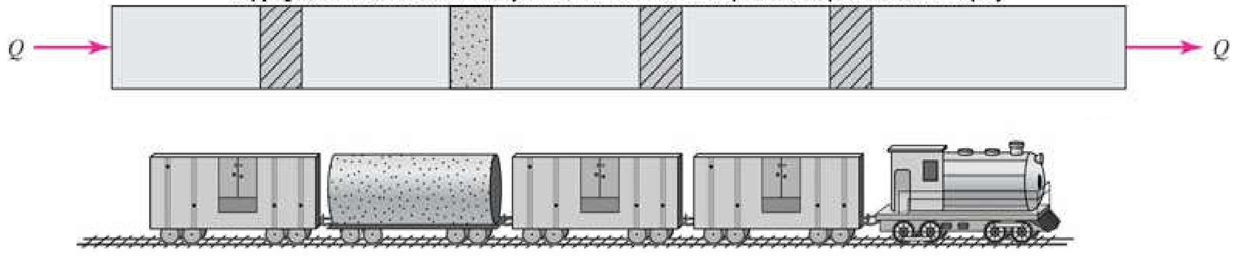
For given α_x; Pe increases with increasing length of system (river, reactor, etc.)

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

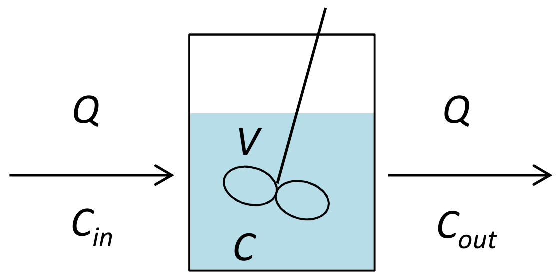


Plug flow vs. Completely mixed reactors

- **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.



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

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

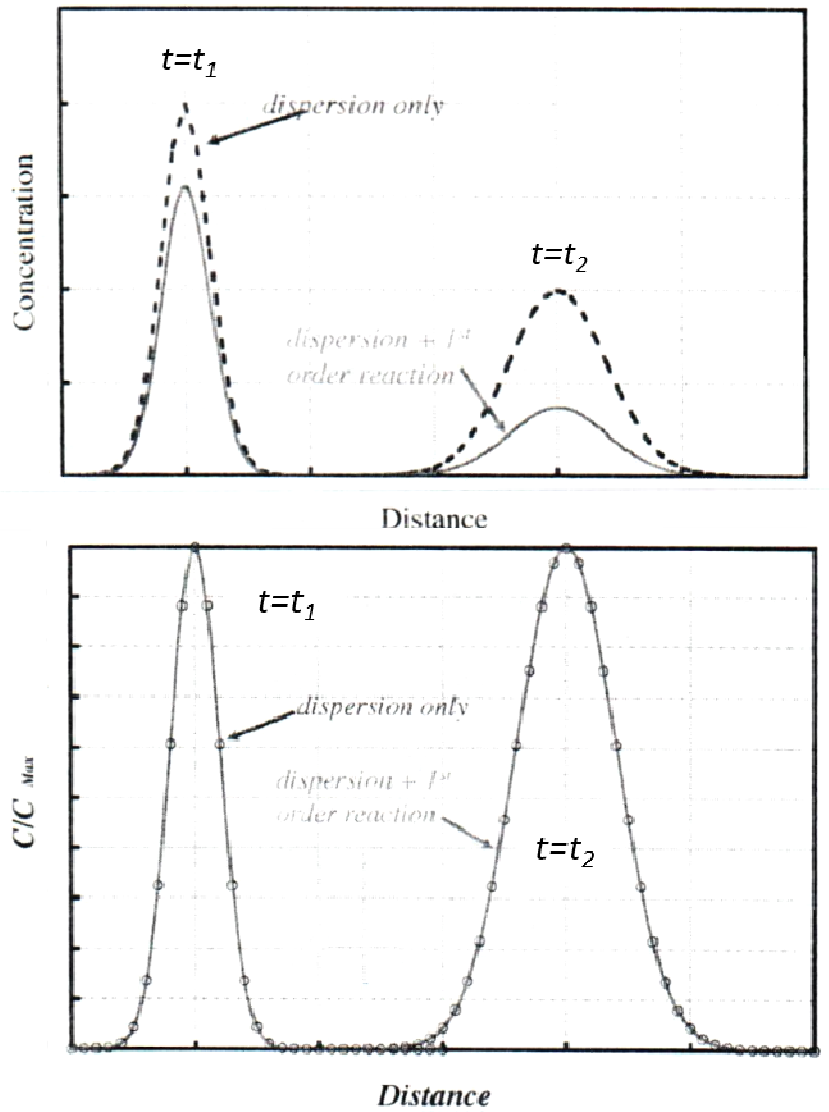
$M_0 =$ *finite mass pulse at* $x = 0$ & $t = 0,$ $C(0,0) = \infty$

$C = 0$ *at* $x \rightarrow 0$ *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:

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

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

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

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} ~ L^2

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

$H = 4\ m$

$W = 40\ m$

$L = 40{,}000\ m$

$u_x = 0.5\ m/s$

$E_x = 15\ m^2/s$

$E_y = 0.12\ m^2/s$

$E_z = 0.12\ m^2/s$

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, 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	$10^{-10} – 10^{-12}$