ESE5001: Physical Principles
Lecture 2

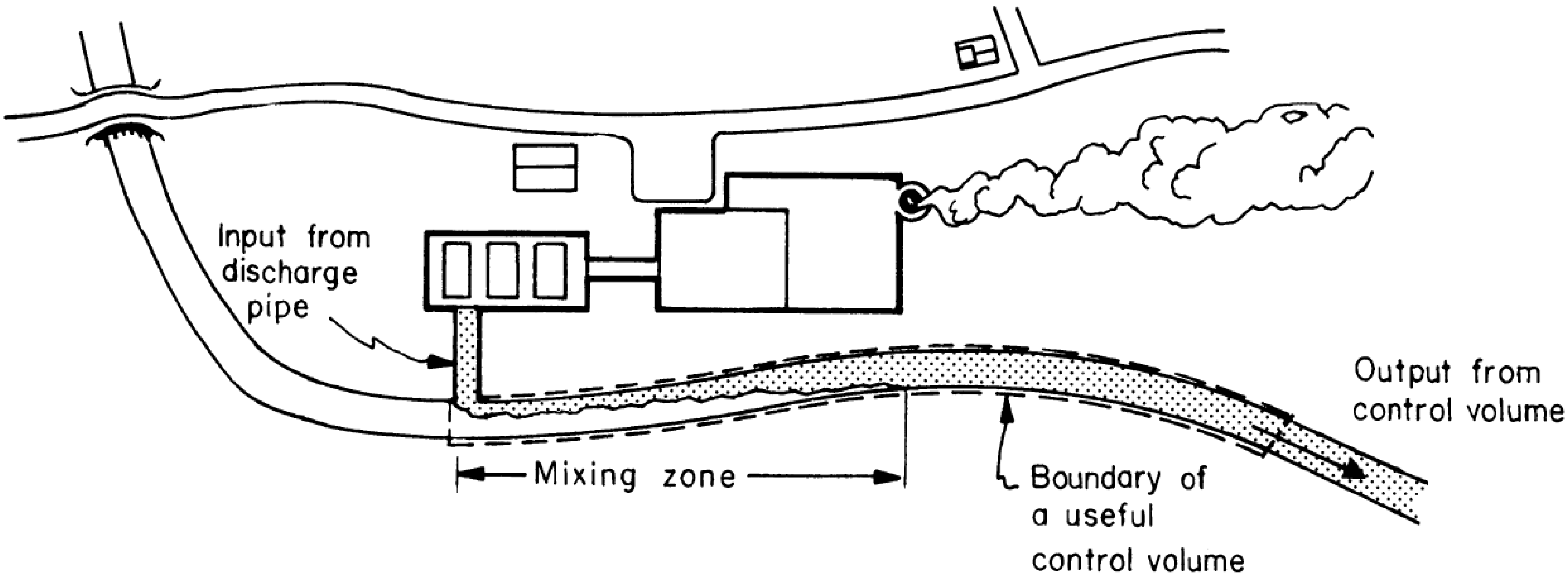
Physical transport of contaminants

Learning outcome

The student would be able to

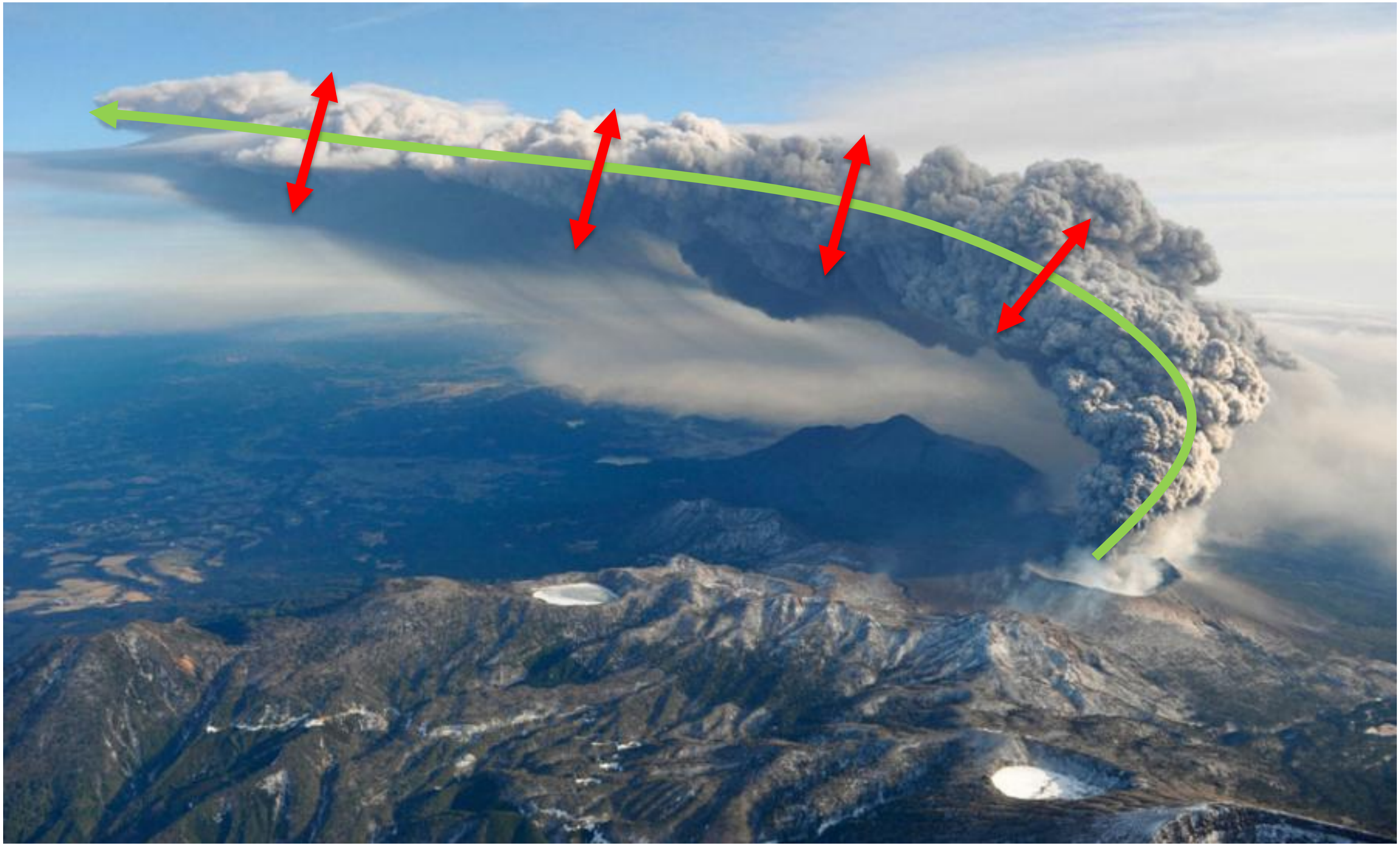
- describe various *physical transport processes* (that move mass from point to point) of contaminants in the environment

Recap: Material balance analysis

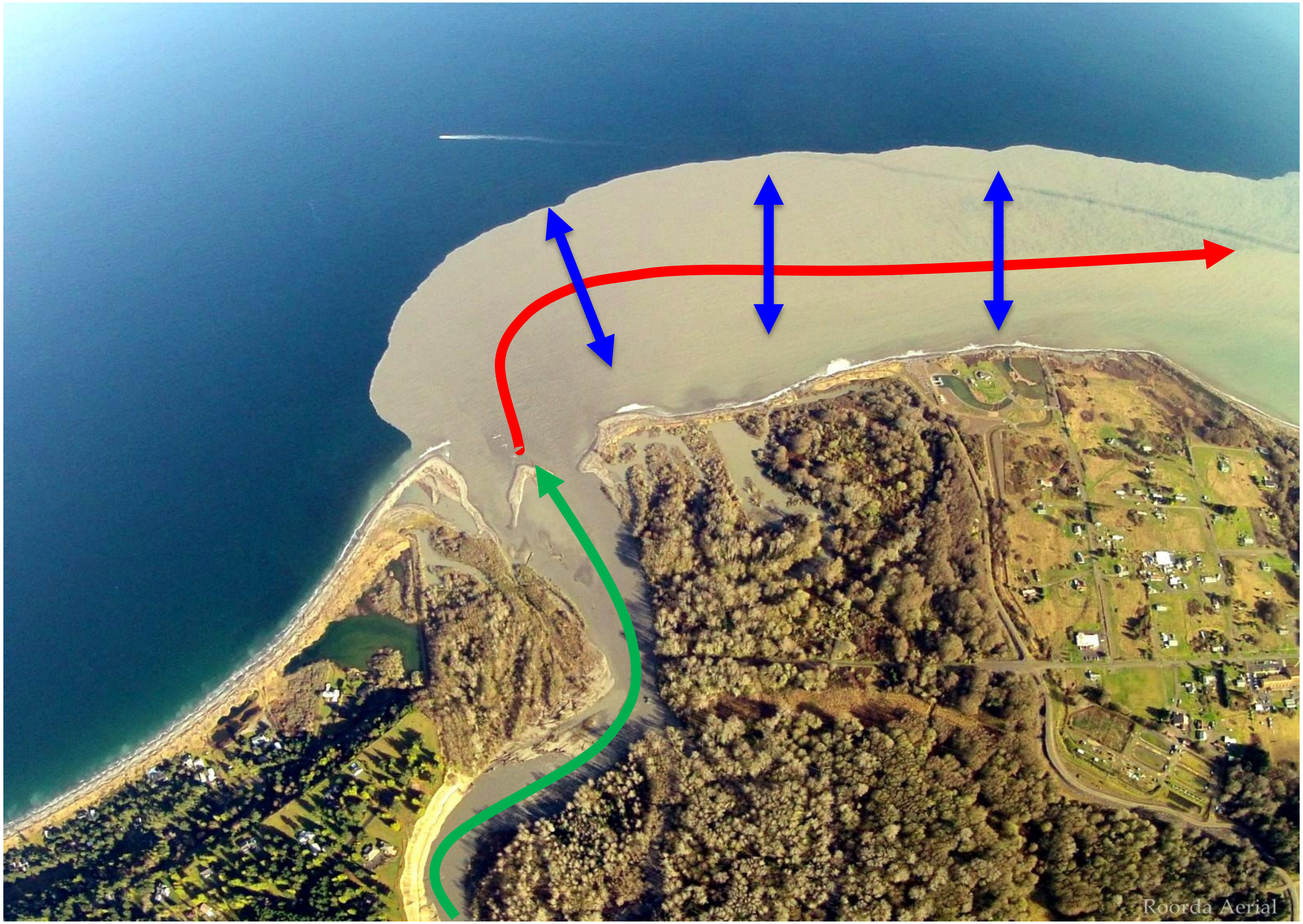


- Accumulation = **Inputs – outputs** + production - consumption
- Control volume
- State of mixing
- Steady and non-steady state
- Performance of batch reactor, CMFR and PFR (Design equations for different reaction orders)

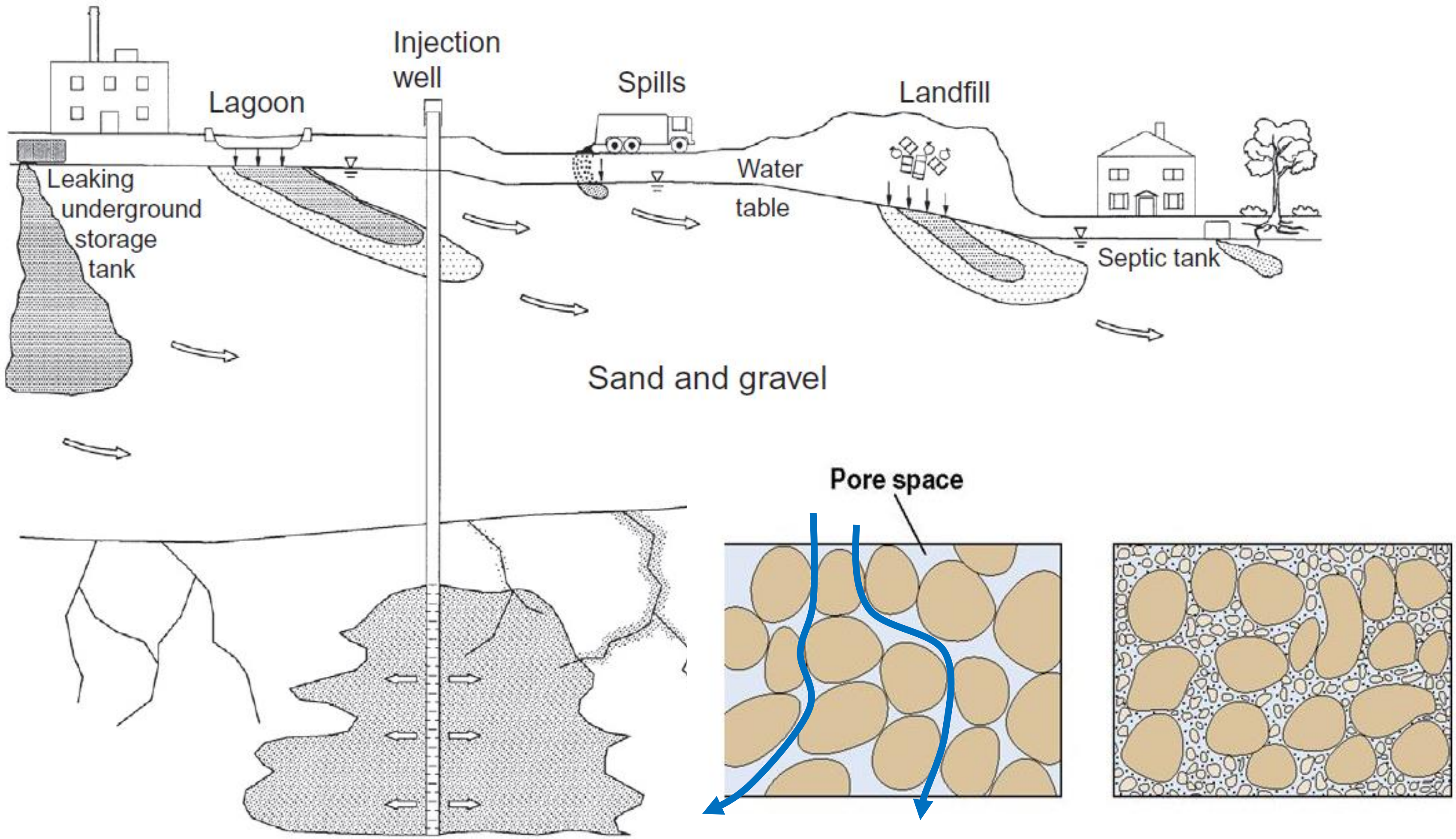
Transport of fine particles in air



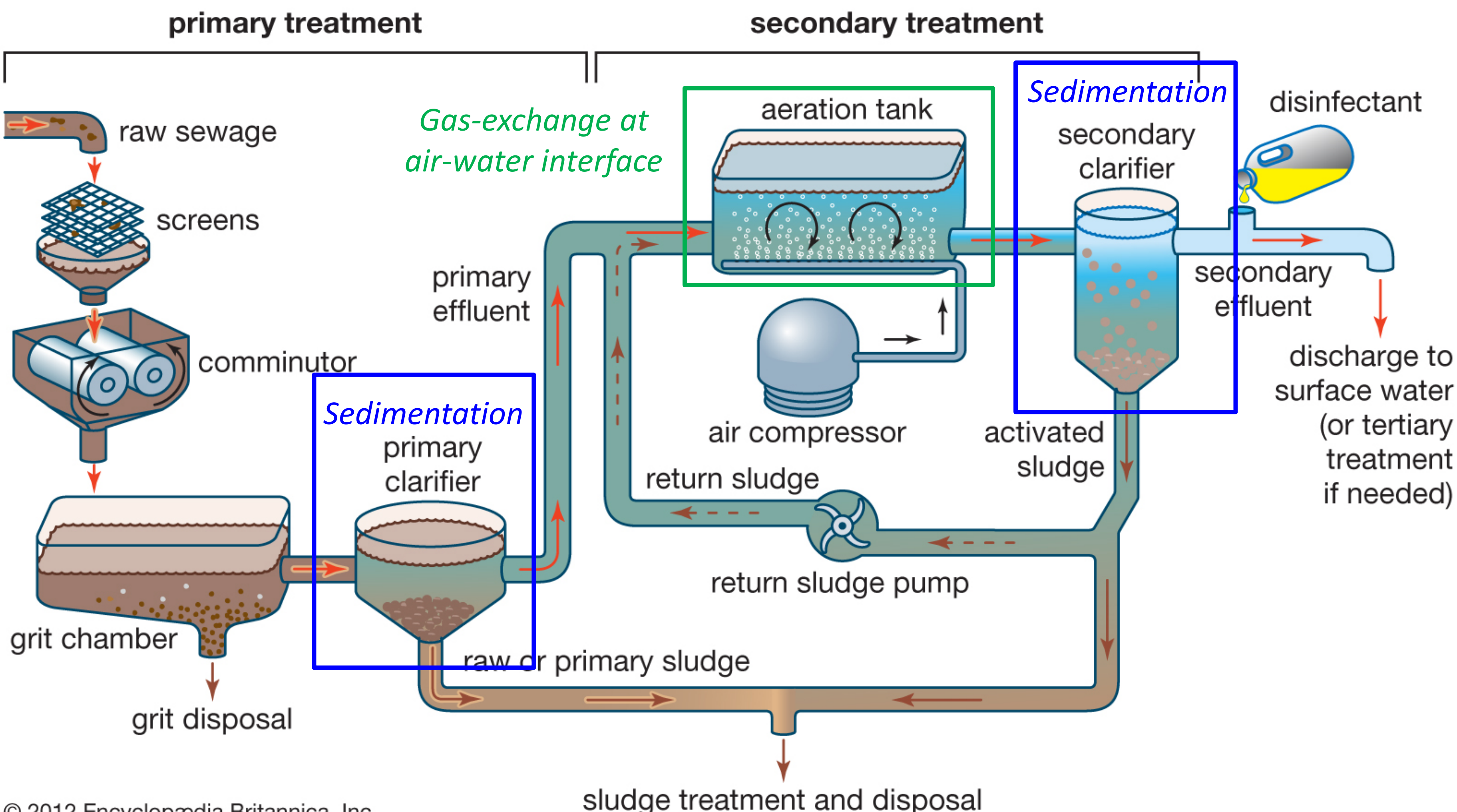
Transport of sediment in water



Transport of pollutants in soil

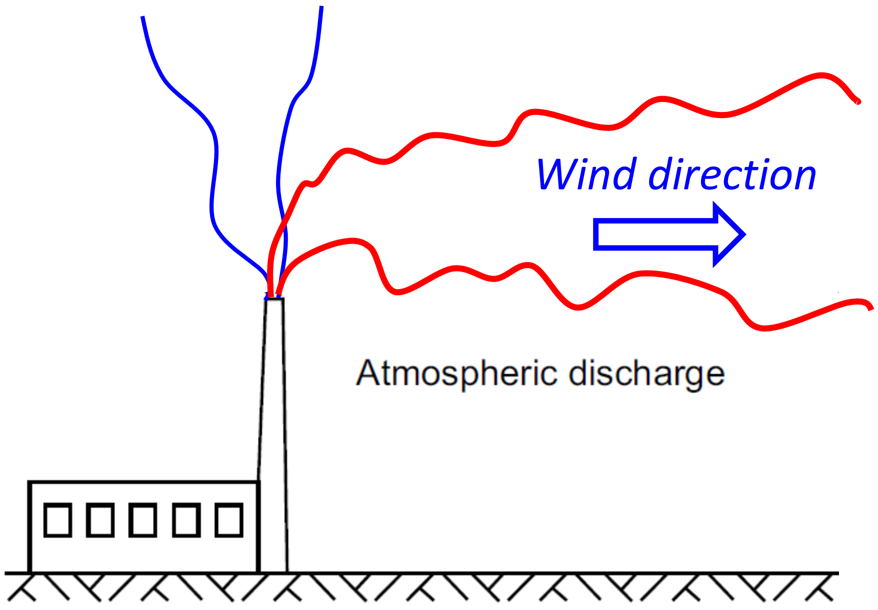


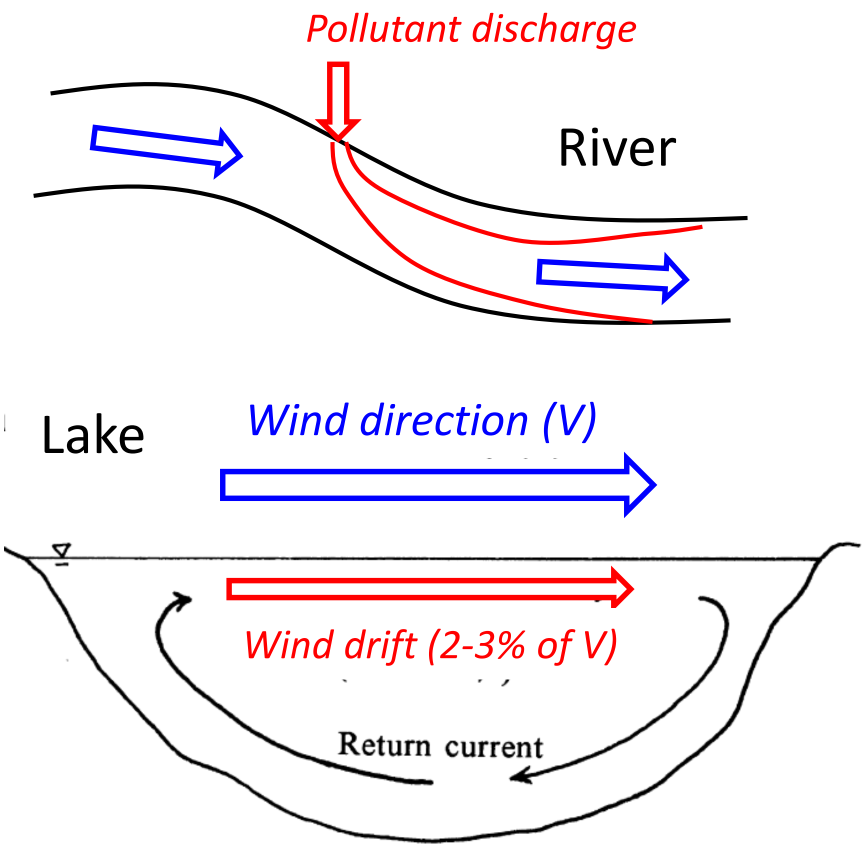
Removal of pollutants by physical process



Advective transport

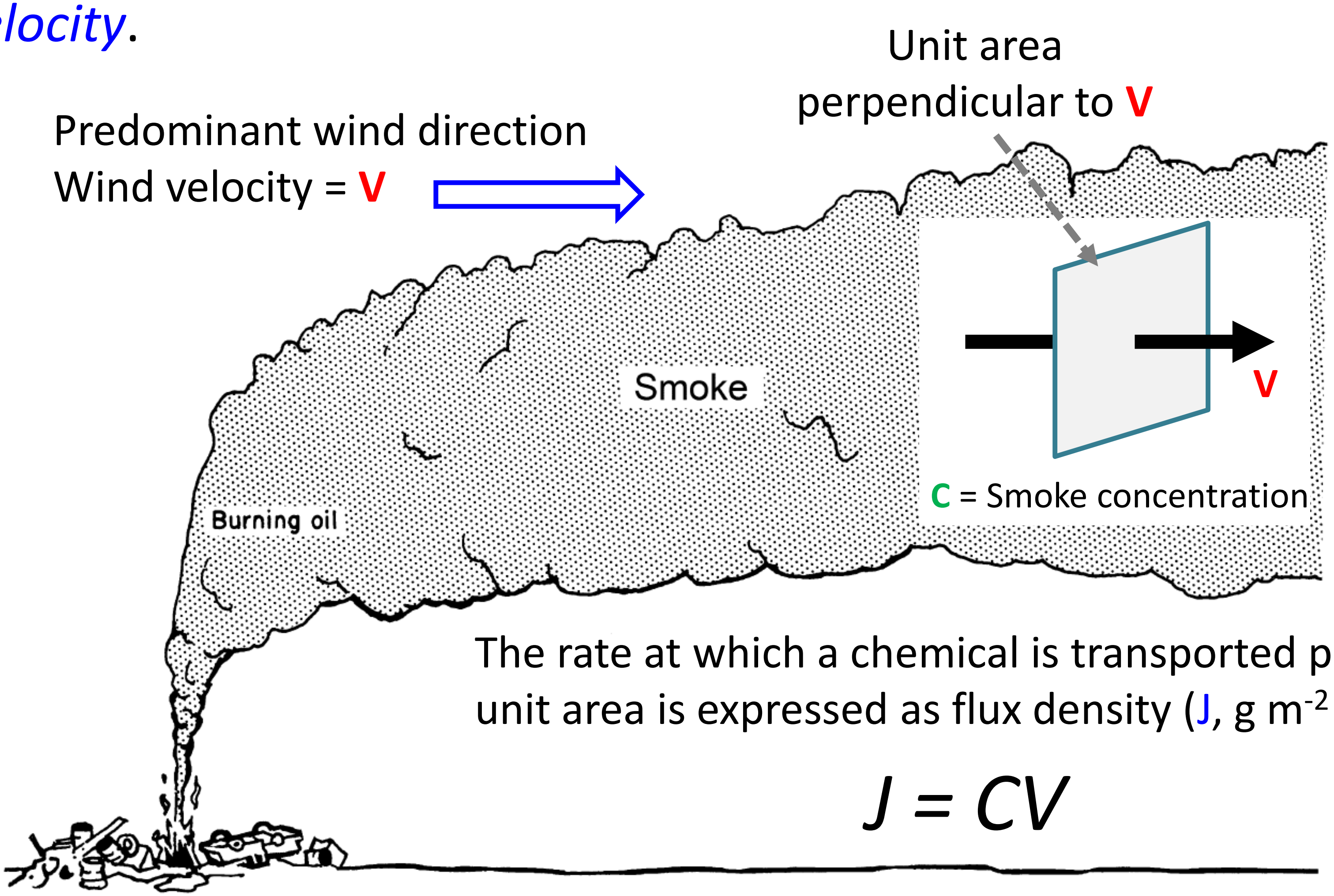
- Advection is due to *bulk, large-scale movement of fluid* (air or water), as seen in the blowing wind and flowing streams.





Advective transport – flux density

- If a chemical is introduced into flowing air or water, *the centre of mass of chemical moves by advection at the average fluid velocity*.



The rate at which a chemical is transported per unit area is expressed as flux density (J, g m^{-2} s^{-1})

$$J = CV$$

Advective transport – mass flux

- *Flux density*: Because both flux density (g m^{-2} s^{-1}) and fluid velocity have direction, this equation can also be expressed as a vector equation

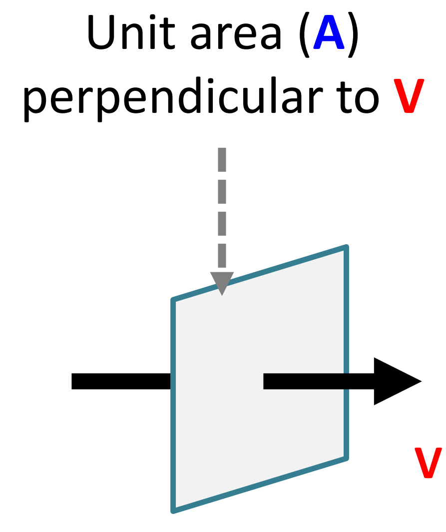
$$\vec{J} = C\vec{V}$$

- *Mass flux* : The flux density (g m^{-2} s^{-1}) can be converted to mass flux (g t^{-1}) for a given cross section area

$$m = \vec{J}A = CA\vec{V} = QC$$

where A = Cross sectional area (m^2)

Q = volumetric flow (m^{-3} s^{-1})



Example (1)

Example: Calculate the average mass flux (in kg/d) of the pesticide A passing a point in a river draining a large agricultural basin. The mean concentration of pesticide is 1.0 μg/L and the mean flow is 50 m^3/s

Example (1)

Solution:

1) Convert µg/L to kg/m³:

$$C = \frac{1.0\ \mu g}{L} \cdot \frac{1000\ L}{1\ m^3} \cdot \frac{1\ \times 10^{-9}\ kg}{1\ \mu g} = 1\ \times 10^{-6} \frac{kg}{m^3}$$

2) Convert m³/s to m³/d:

$$Q = \frac{50\ m^3}{s} \cdot \frac{(24)(60)(60)s}{1\ day} = 4.32\ \times 10^6 \frac{m^3}{day}$$

3) Estimate the average mass flux of pesticide A:

$$Mass\ flux = QC = \left(4.32\ \times 10^6 \frac{m^3}{day}\right)\left(1\ \times 10^{-6} \frac{kg}{m^3}\right) = 4.32 \frac{kg}{day}$$

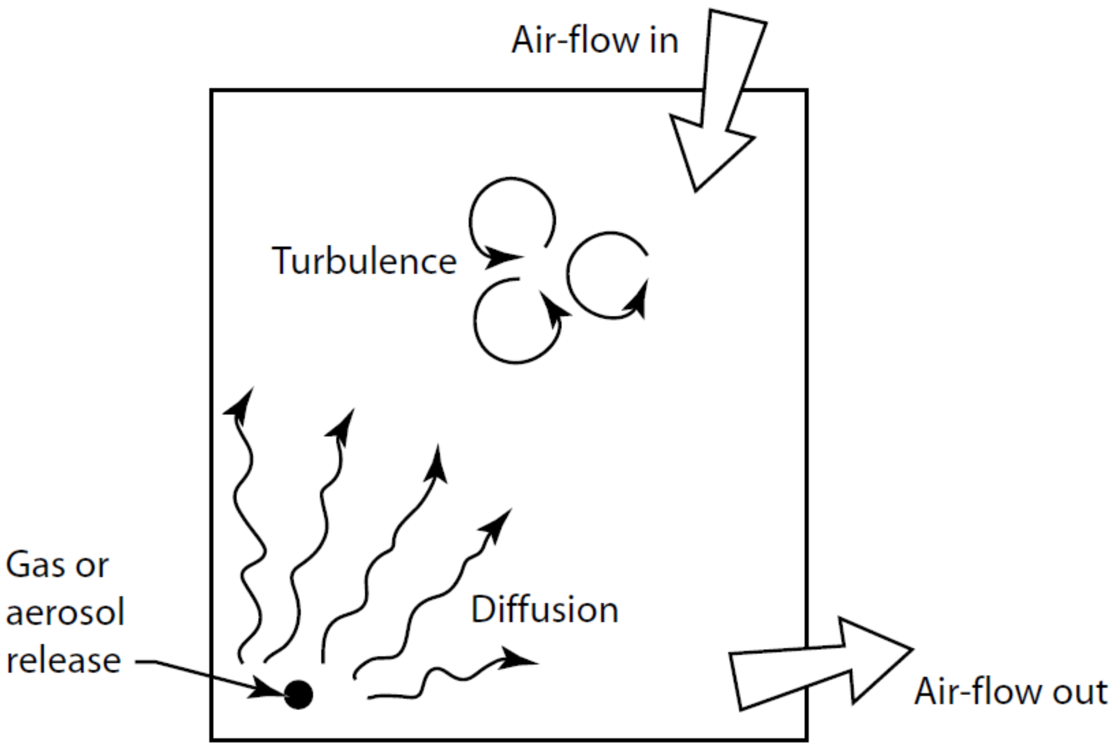
https://youtu.be/3nx4Xxtpl-0

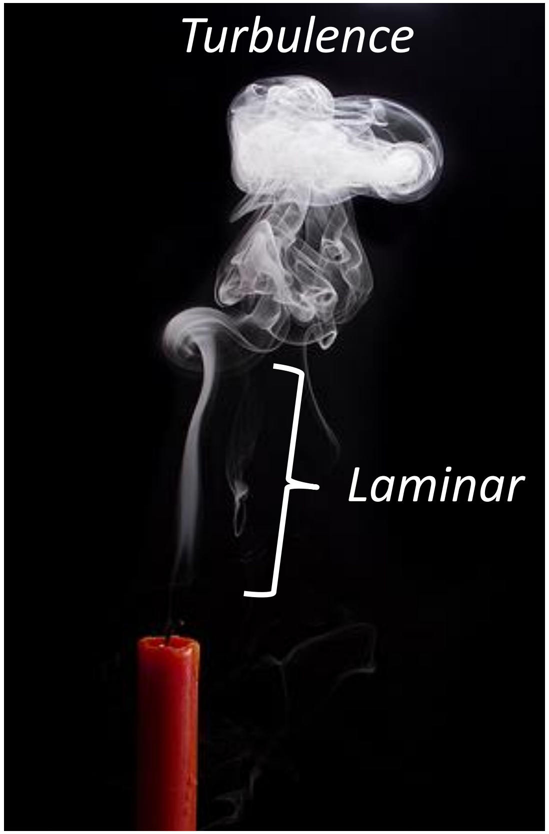
Diffusion

1. *Turbulent/eddy diffusion*: from random turbulence/eddies
2. *Molecular diffusion*: from random molecular motion

Both diffusion mechanisms are commonly observed in air and water

For example: Indoor environment





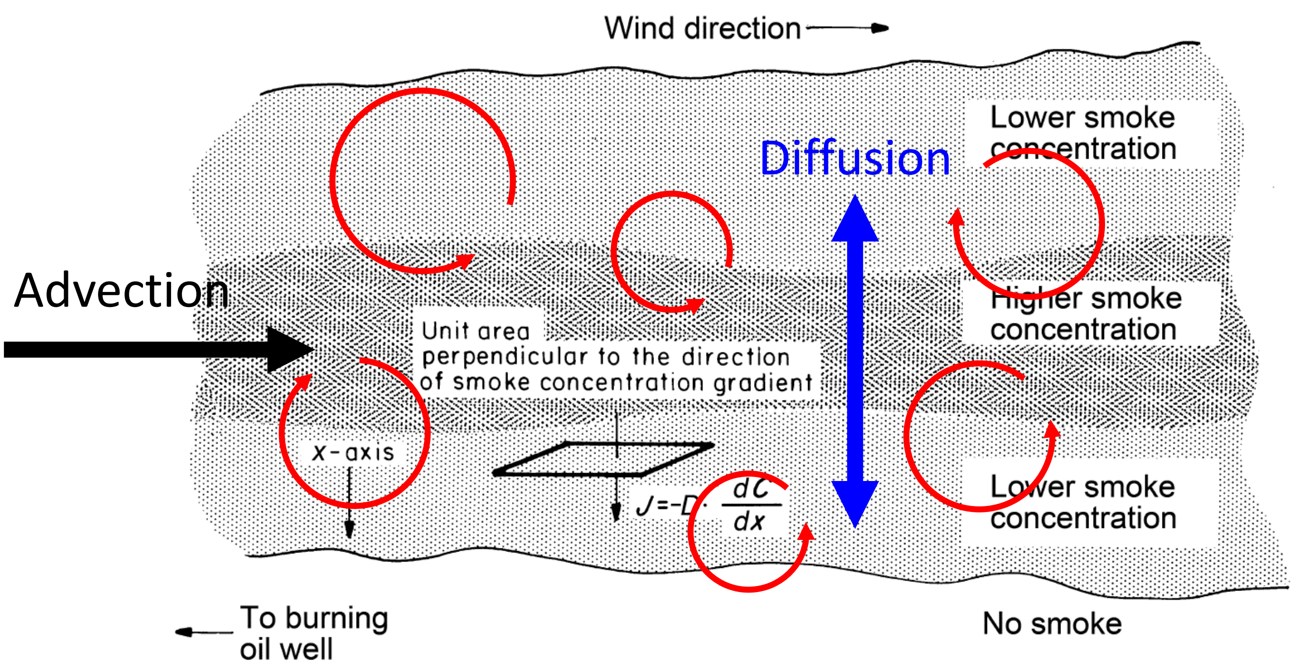
Turbulent diffusion - Fick's law

- Fick's first law is typically used to describe the flux density (J, g m^{-2} s^{-1}) of mass transported by turbulent diffusion. In one dimension, along the x-axis,

$$J = -D\left(\frac{dC}{dx}\right)$$

$$D = \text{Turbulent diffusion coefficient}$$

$$\frac{dC}{dx} = \text{concentration gradient along the x} - \text{axis}$$



For three-dimension,

$$\vec{J} = -D\vec{\nabla}C$$

$\vec{\nabla}$ = Gradient operator (i.e. the vector for differential operator)

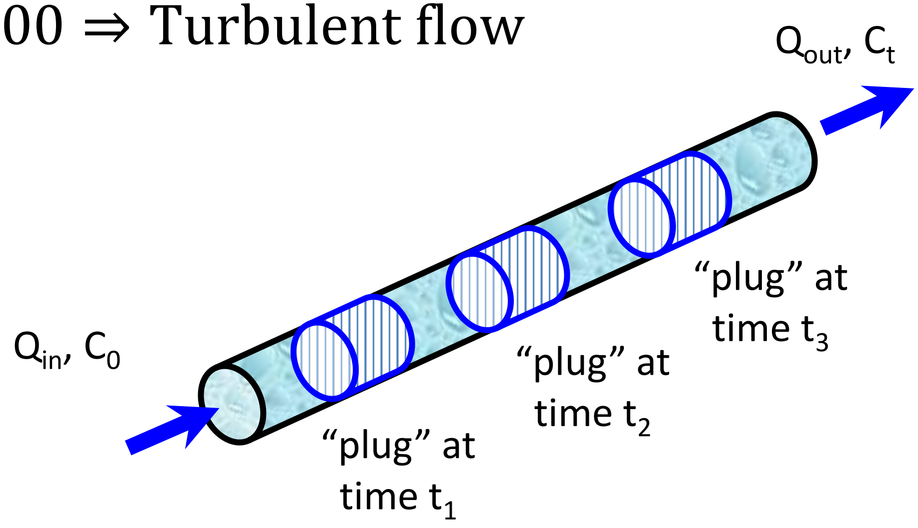
Turbulence – Reynolds number (1)

- Turbulent diffusion coefficient *depends on the properties of the fluid flow, rather than on the properties of the pollutant molecules*.
- Turbulence is *only present at flow velocities above a critical level*, and the degree of turbulence is correlated with velocity (Reynolds number, Re).

For example: a pipeline or a plug flow reactor (no longitudinal mixing but complete latitudinal mixing)

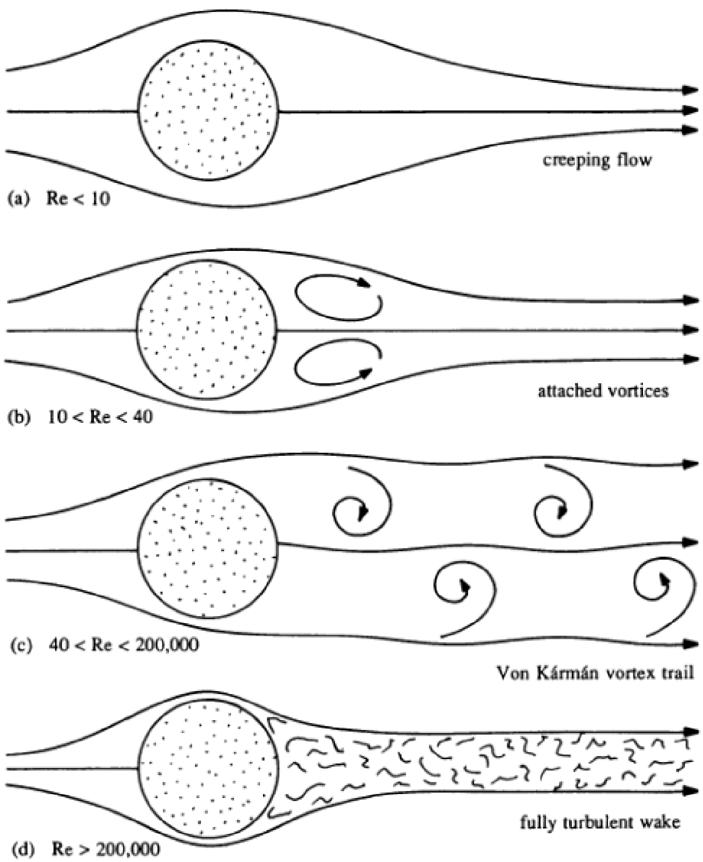
$$Re = \frac{\rho v d}{\mu} \quad \text{if Re} > 4000 \Rightarrow \text{Turbulent flow}$$

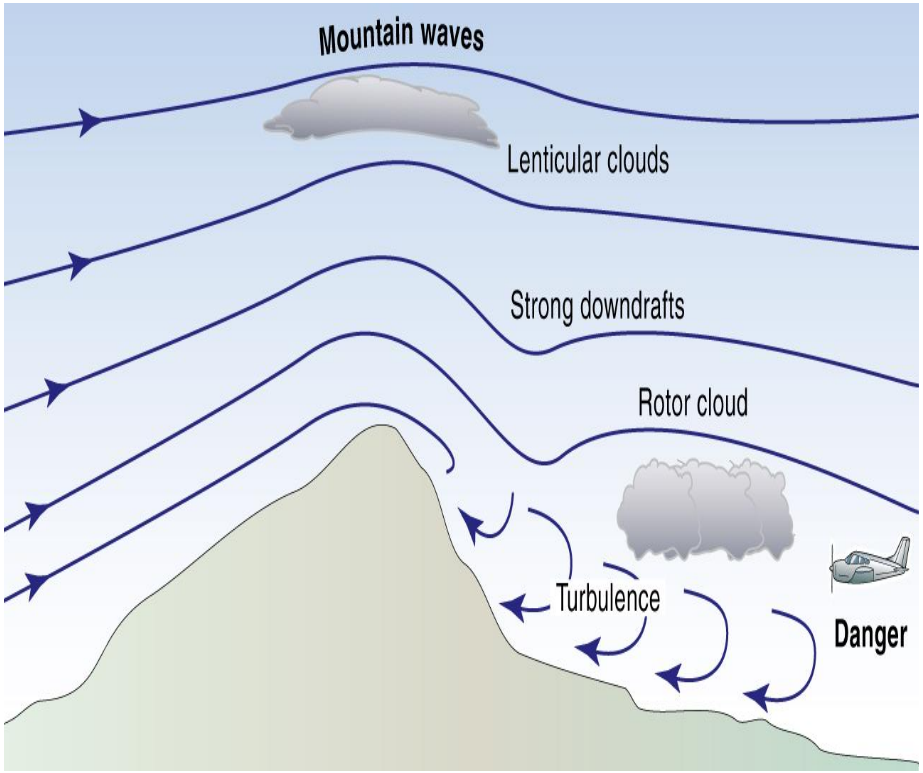
Where ρ = Density of fluid
v = velocity of fluid
d = diameter of pipe/reactor
μ = viscosity of fluid



Turbulence – Reynolds number (2)

- The degree of turbulence depends on the material over which the flow is occurring, so that flow over bumpy surfaces will be more turbulent than flow over a smooth surface, and the increased turbulence will cause more rapid mixing.

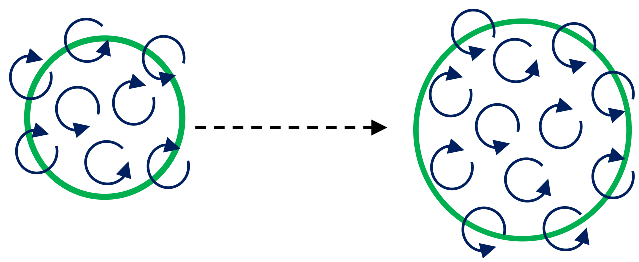




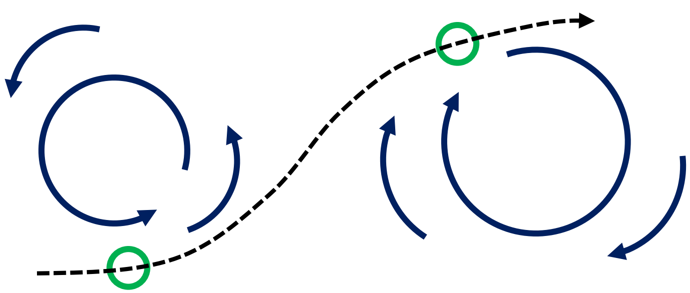
Scales of turbulence

- Turbulence diffusion coefficient depends on the scale of turbulence.

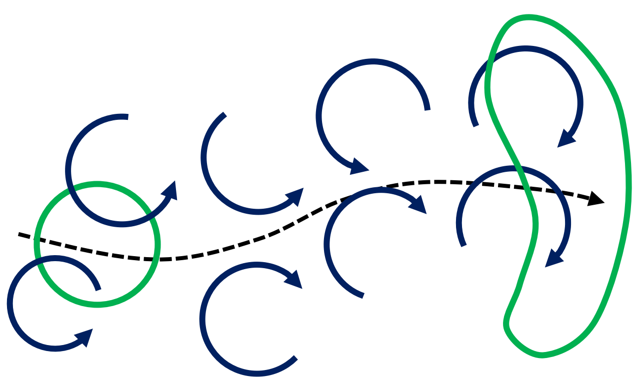
Mixing of an isolated puff of pollutant in a turbulence: $J = -D\left(\frac{dC}{dx}\right)$



The size of the *puff >> turbulent eddies*. Turbulent diffusion is slow.



The size of the *puff << turbulent eddies*. The entire puff is moved along with the fluid eddies (advection).



The size of the *puff* $\approx$ *turbulent eddies*, and the puff is rapidly stretched out and mixed with the surrounding fluid. The turbulence diffusion coefficient would be rather large.

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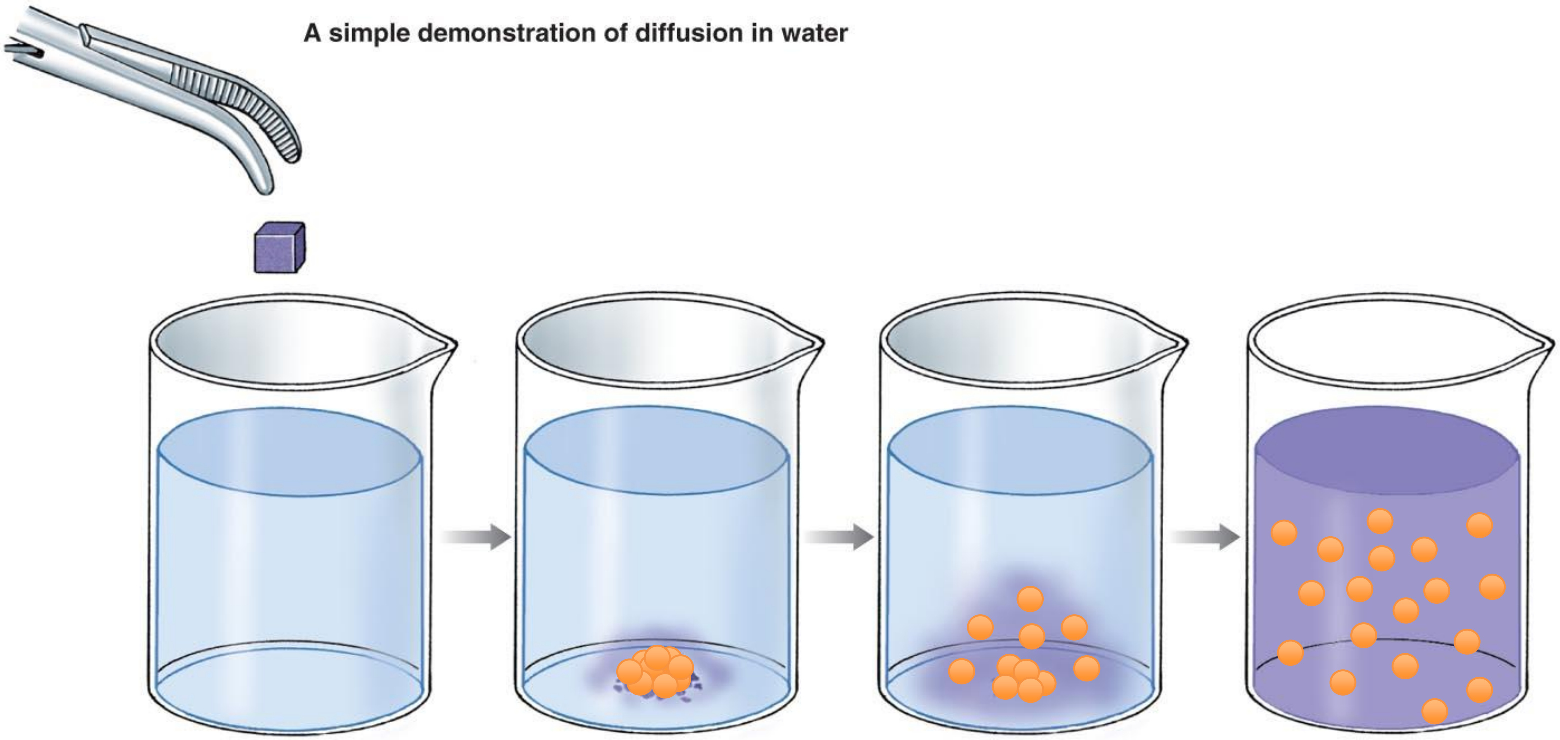
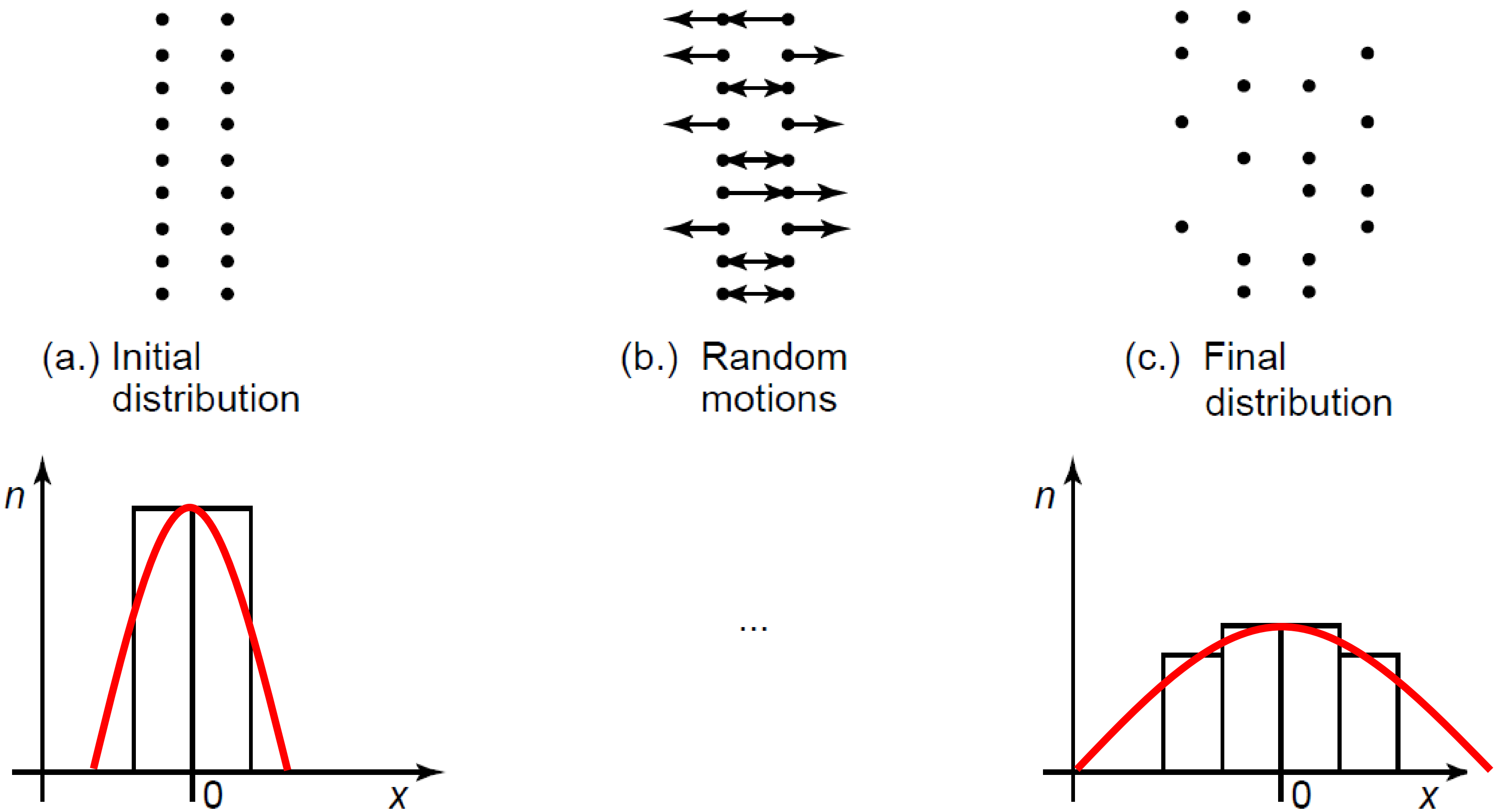
Molecular diffusion

- Even if a fluid is entirely *quiescent and without obstructions*, chemicals will still move form regions of higher concentration to regions of lower concentration due to *thermal motion of molecules*.



Molecular diffusion



Molecular diffusion - Fick's law

- Similar to turbulent diffusion, Fick's first law can be used to describe the flux density (J, g m^{-2} s^{-1}) of mass transported by molecular diffusion. In one dimension, along the x-axis,

$$J = -D\left(\frac{dC}{dx}\right)$$

$$D = \text{Molecular diffusion coefficient}$$

$$\frac{dC}{dx} = \text{concentration gradient along the x} - \text{axis}$$

$$J = -D\left(\frac{dC}{dx}\right)$$

$$D = \text{Turbulent diffusion coefficient}$$

$$\frac{dC}{dx} = \text{concentration gradient along the x} - \text{axis}$$

- Turbulent diffusion coefficient >> Molecular diffusion coefficient

Class discussion (1)

Compound	Molecular weight	Temp (^oC)	Molecular diffusion coefficient (cm^2/s)
Methanol in water	32	15	1.26×10^{-5}
Ethanol in water	46	15	1.00×10^{-5}
Acetic acid in water	60	20	1.19×10^{-5}
Ethylbenzene in water	106	20	8.10×10^{-6}
CO_2 in air	44	20	0.151

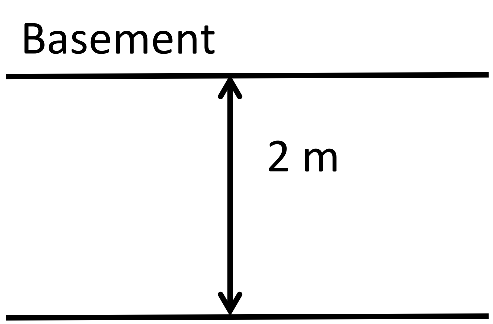
General characteristics:

- Inversely related to the *viscosity* of the medium (Molecular diffusion coefficient in liquids: ~10^{-6} to 10^{-5} cm^2/s, in gases: ~10^{-2} to 10^{-1} cm^2/s)
- Decreases as the *size and molecular weight* of the chemical increases
- Increases with an increase in ambient *temperature*

Example (2)

Example: Gasoline-contaminated groundwater has been transported under a house from a nearby gas station. Two meters below the dirt floor of the house's basement, the concentration of hydrocarbon vapors in the airspace within the soil is 3×10^{-8} g/cm^3.

Estimate the flux density of gasoline vapor transported into the basement by molecular diffusion. The diffusion coefficient for gasoline vapor in the air space within the soil is equal to 10^{-2} cm^2/s. Assume that the basement is well-ventilated, so that the concentration of gasoline in the basement is very small in comparison to the concentration in the soil.



$C = 3 \times 10^{-8}$ g/cm^3

$D = 10^{-2}$ cm^2/s

Example (2)

Solution: Treating this as a one-dimensional problem, the upward concentration gradient of vapor is approximately

$$\frac{dC}{dz} = (-3 \text{ x } 10^{-8} \text{ g/cm}^3) / 200 \text{ cm} = -1.5 \text{ x } 10^{-10} \text{ g/cm}^4$$

The flux density, calculated by using Fick's first law in Eq. (1.3), is

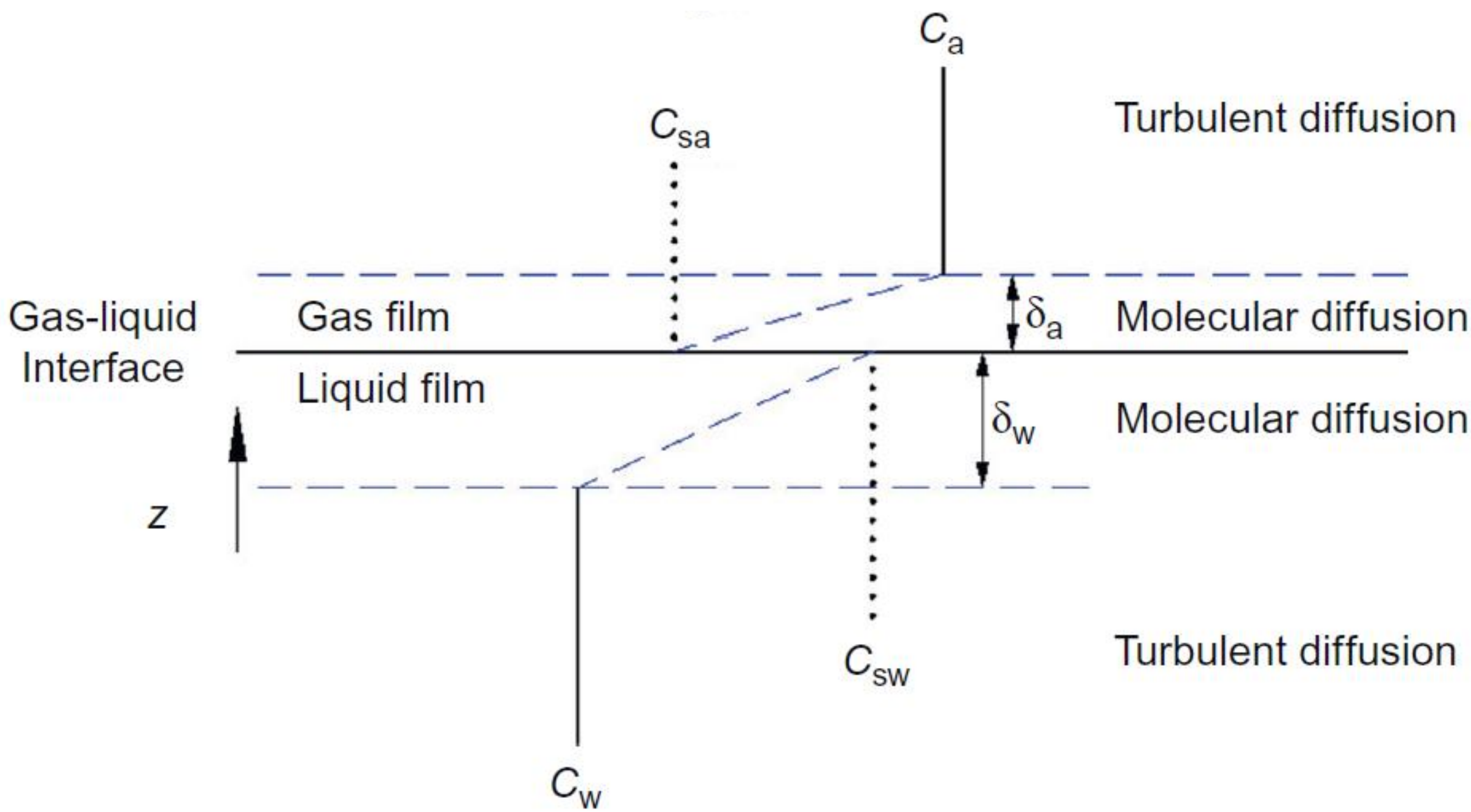
$$J = -D \cdot \frac{dC}{dz} = -(10^{-2} \text{ cm}^2/\text{sec}) (-1.5 \text{ x } 10^{-10} \text{g/cm}^4)$$
$$= 1.5 \text{ x } 10^{-12} \text{ g/ } (\text{cm}^2 \text{ sec})$$

If the basement area is 10^6 cm^2, the daily rate of vapor transport into the house is

$$(1.5 \text{ x } 10^{-12} \text{ g/cm}^2 \text{ sec}) (10^6 \text{ cm}^2) (3600 \text{ sec/hr}) (24\text{hr/ day}) = 0.13\text{g/ day}$$

Thin film model of air-water exchange

Within a few micrometers of the water-air interface*, turbulent eddies are suppressed and hence chemical transport can occur only by molecular diffusion through these stagnant layers.* Molecular diffusion through these layers is considered to be the rate-limiting step of air-water exchange.



Thin film model of air-water exchange

Water-side control ($C_a = C_{sa}$),

$$J = -D_w \frac{(C_w - C_{sw})}{\delta_w}$$

$$= -D_w \frac{(C_w - C_a/H)}{\delta_w}$$

D_w = molecular diffusion coefficient in water
H = Henry's law constant

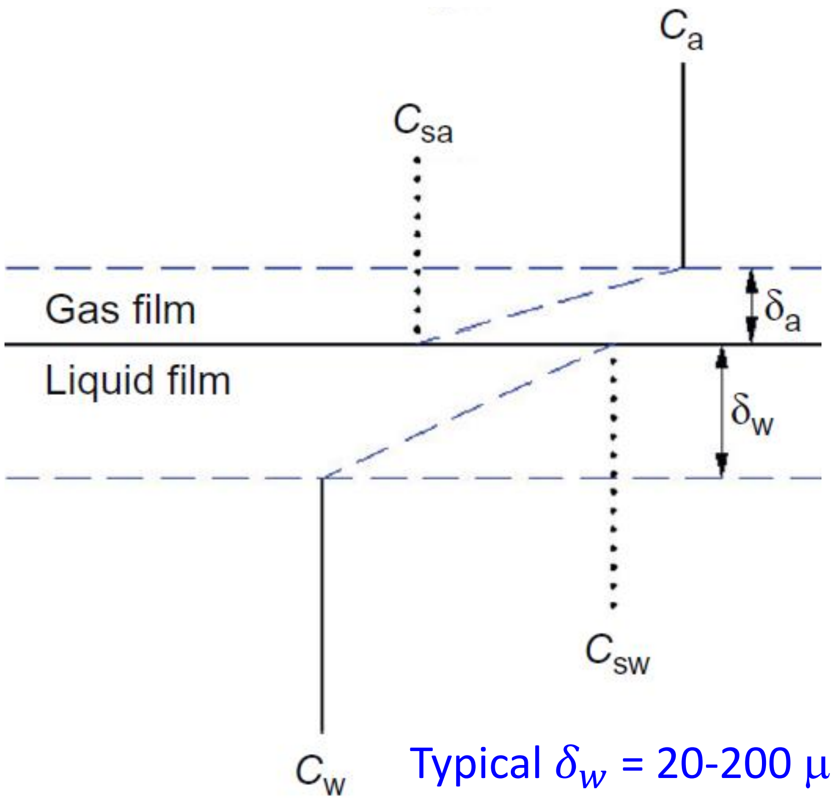
Air-side control ($C_w = C_{sw}$),

$$J = -D_a \frac{(C_{sa} - C_a)}{\delta_w}$$

$$= -D_a \frac{(C_w H - C_a)}{\delta_a}$$

D_a = molecular diffusion coefficient in air

Typical δ_a = on the order of 1 cm



Typical δ_w = 20-200 μm

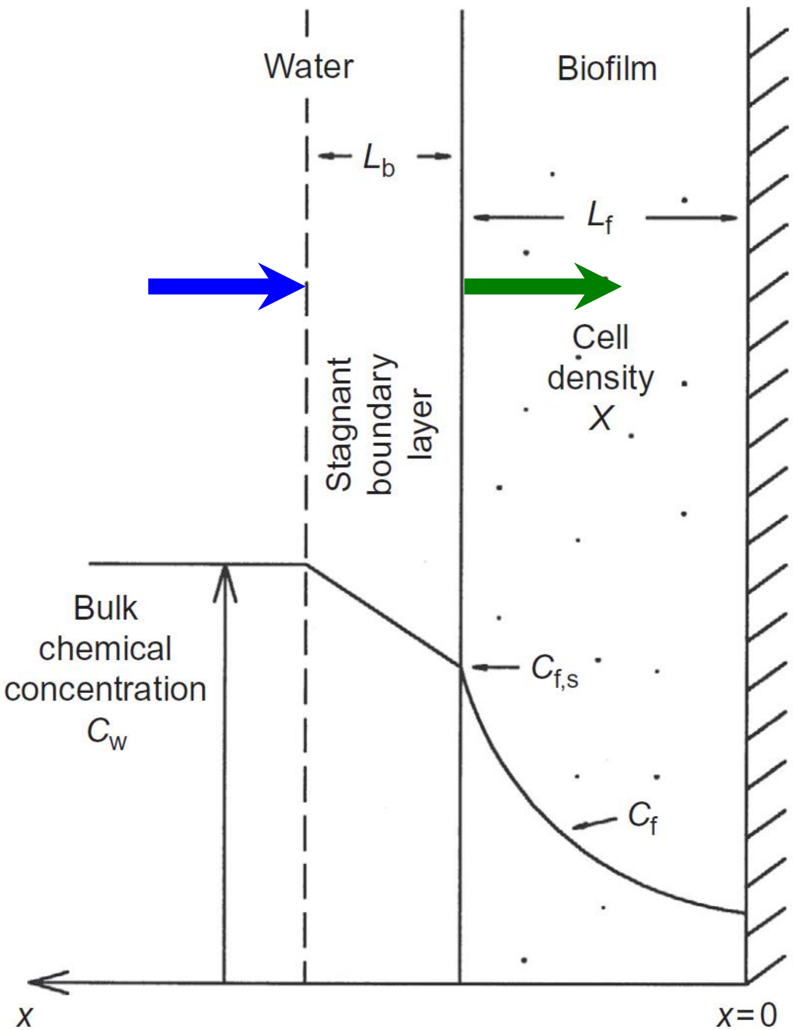
Degradation of pollutant in biofilm

Conservation of mass in the stagnant boundary layer:

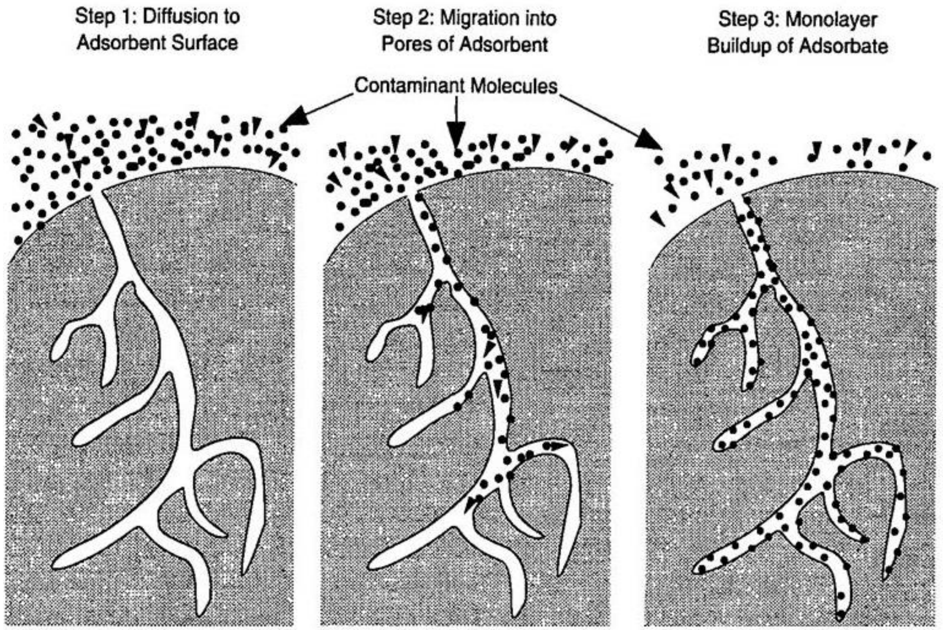
The diffusive flux into the stagnant water layer from bulk water equals the diffusive flux from the boundary layer into the biofilm.

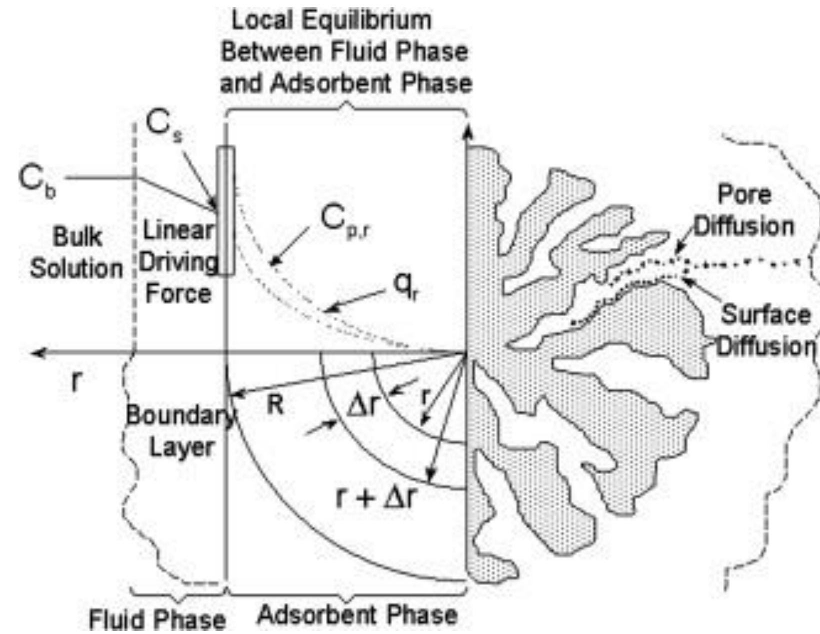
$$D_b \frac{C_w - C_{f,s}}{L_b} = D_f \left(\frac{dC_f}{dx}\right)_{\text{at biofilm surface}}$$

D_b = Molecular diffusion coefficient in the bulk water
D_f = Effective molecular diffusion coefficient in the biofilm

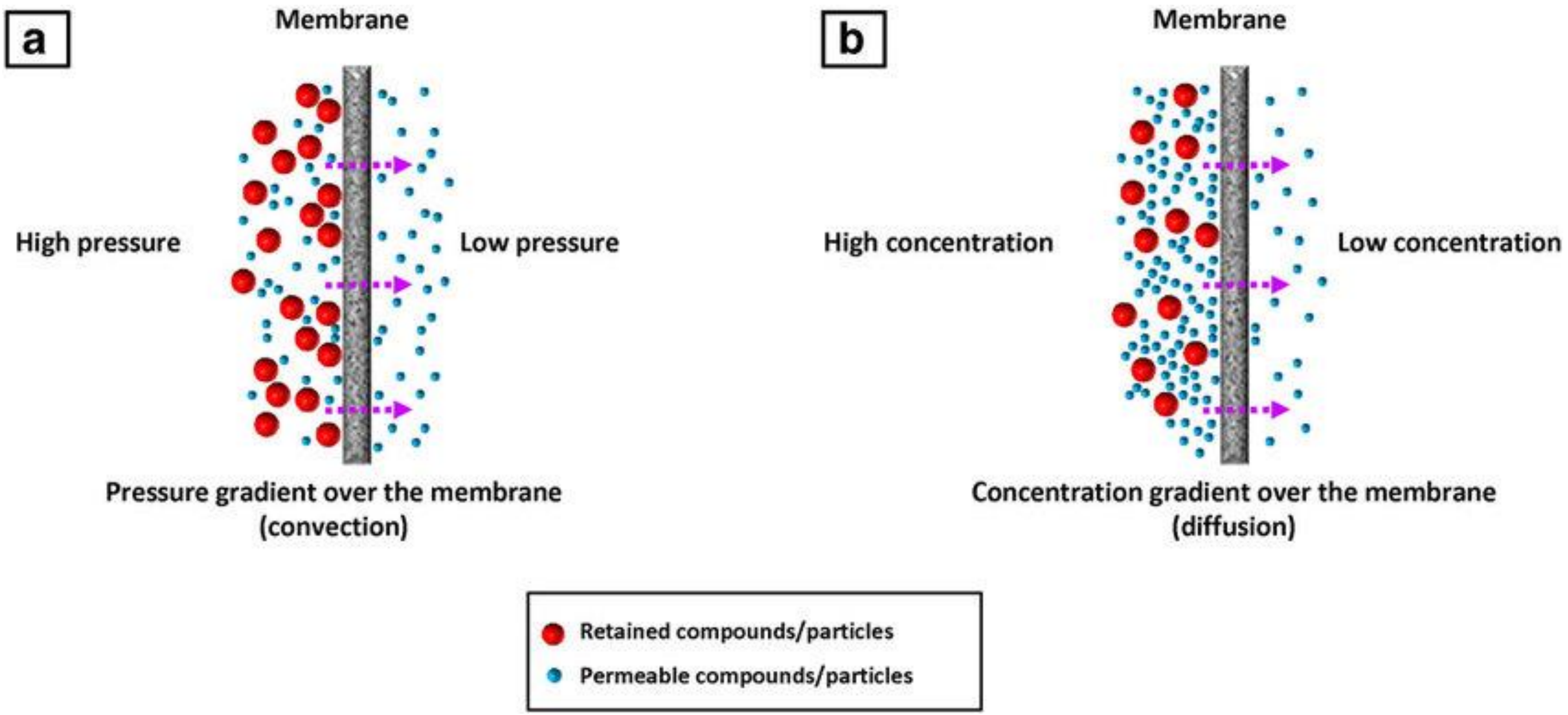


Adsorption processes





Membrane separation



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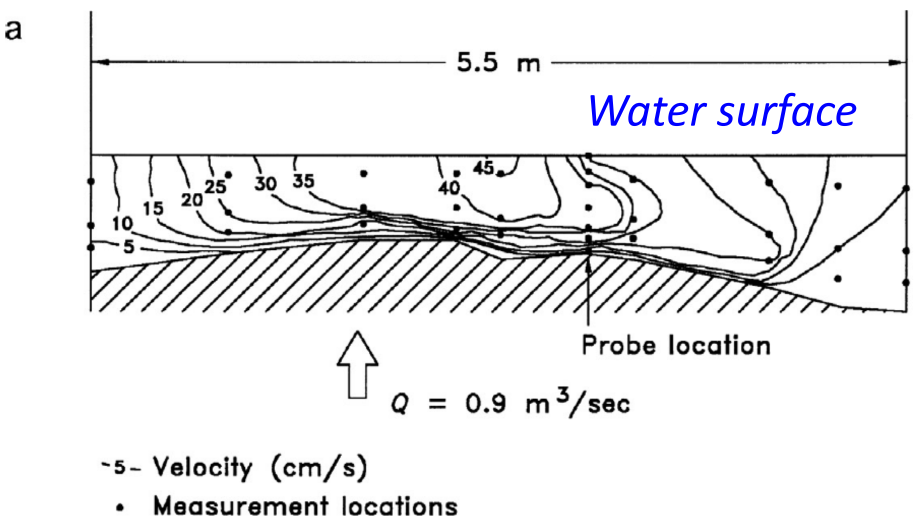
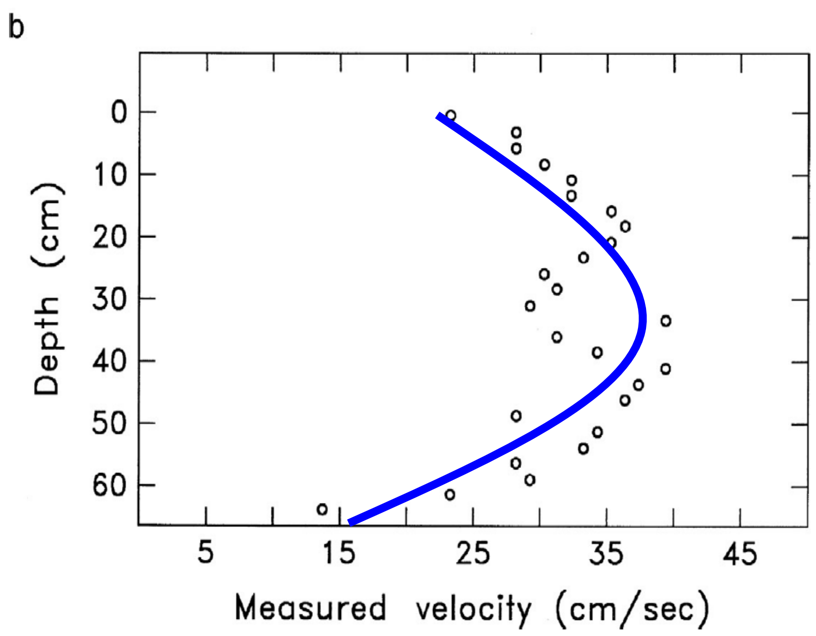
Dispersion – Velocity variations in river

Average water velocity in a river systematically increases with distance from the river bottom and sides, reaching a maximum near the river centre and usually somewhat below the water surface.



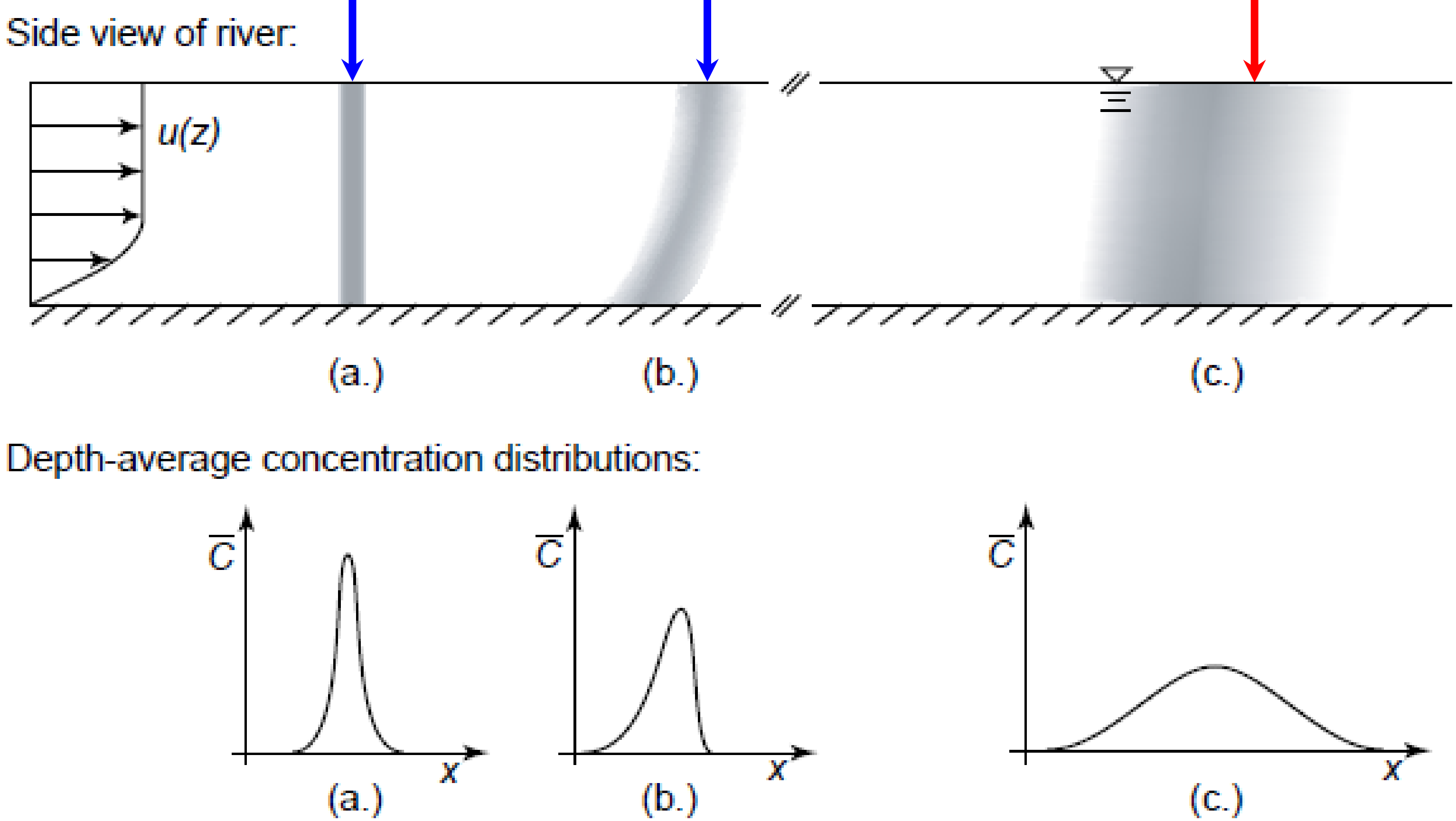


Dispersion - Longitudinal mixing in river

Injection of tracer: No vertical concentration gradients ⇨ *no net diffusive flux in vertical direction.*

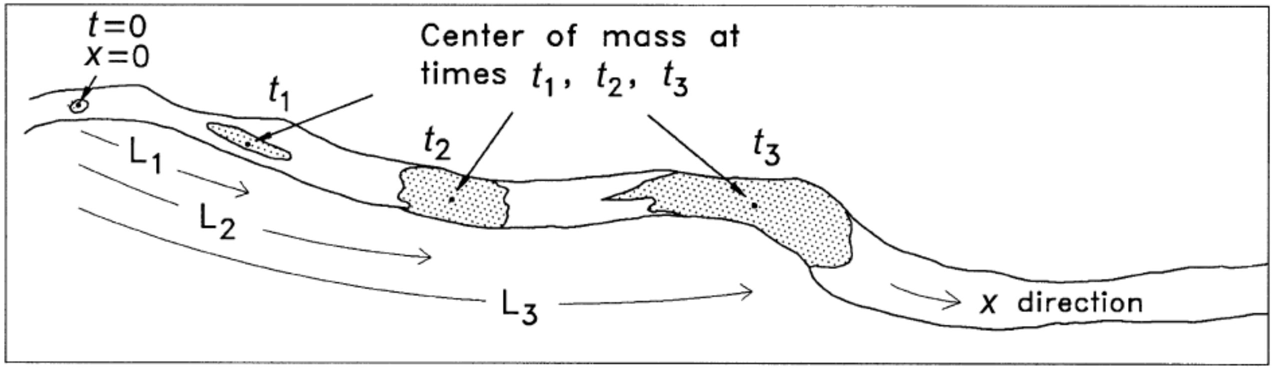
Strong vertical concentration gradients due to the different advection velocities in the shear profile ⇨ *a large net diffusive flux in the vertical.*

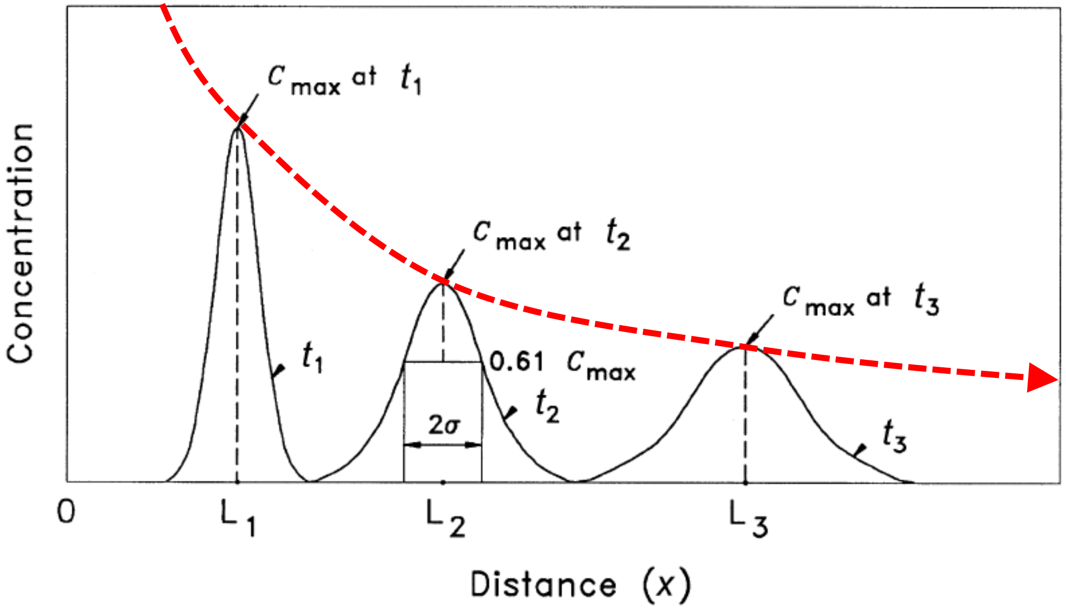
Turbulent diffusion smooths out the vertical concentration gradients. *This combined process of advection and vertical diffusion is called dispersion* (>> longitudinal turbulent diffusion).



Dispersion – Fick's law

While spreading of the chemical due to dispersion occur at the same time, the centre of mass of the chemical moves by advection at the average fluid velocity.





$$J = -D_L \left(\frac{dC}{dx} \right)$$

$$D_L = \frac{\sigma^2}{2t}$$

D_L = Longitudinal dispersion coefficient
σ^2 = spatial variance
t = time since the pulse injection

Dispersion – Gaussian distribution

$$\phi(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-x^2/2\sigma^2} \quad \text{and} \quad D_L = \frac{\sigma^2}{2t}$$

$\phi(x) = y -$ coordinate of each point on the curve
$x = x -$ coordinate of each point on the curve
$\sigma =$ Standard deviation of $\phi(x)$ about the origin
Note: $x = 0$ at the origin (peak of the curve)

$$\phi(x,t) = \frac{1}{\sqrt{2D_L t}\sqrt{2\pi}} e^{-x^2/2(2D_L t)}$$

Given that the river is flowing, the tracer's centre of mass is moving downstream at velocity V. In this coordinate system, the distance x must be replaced by (x-Vt):

$$\phi(x,t) = \frac{1}{\sqrt{2D_L t}\sqrt{2\pi}} e^{-(x-Vt)^2/2(2D_L t)}$$

The area under the curve is unity. To obtain the concentration at any time t after injection and any distance x downstream, the equation must be multiplied by Ma:

$$C(x,t) = \frac{M_a}{\sqrt{4\pi D_L t}} e^{-(x-Vt)^2/(4D_L t)}$$

For first order decay reaction (recall: $C_t = C_0 e^{-kt}$)

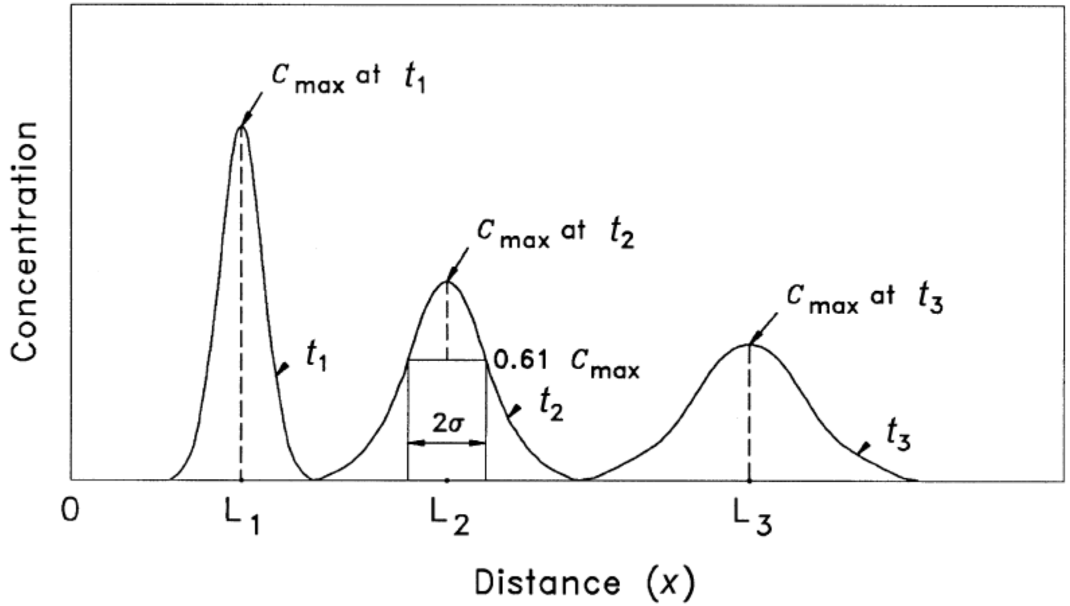
$$C(x,t) = \frac{M_a}{\sqrt{4\pi D_L t}} e^{-(x-Vt)^2/(4D_L t)} e^{-kt}$$

$$C_{max} = \frac{M_a}{\sqrt{4\pi D_L t}} e^{-kt}$$

Example (3)

Example: The t_2 profile was measured 5 hr after a pulse injection of dye. What is the average river velocity if the maximum dye concentration occurs 1025 m down the river from the pulse injection at this time?

Estimate the longitudinal dispersion coefficient for this river if the standard deviation in the longitudinal direction, σ_L, is approximately 350 m when the chemical has travelled a distance of 1975 m to L_3.



Example (3)

Solution:

$$V = \frac{L_2}{t_2} = \frac{1025\ m}{5\ hr} = 205\ m/hr$$

To estimate the dispersion coefficient, consider the concentration profile at time t_3; the peak of the profile (C_{max}) occurs at approximately 1975 m,

$$t_3 = \frac{L_3}{V} = \frac{1975\ m}{205\ hr} = 9.6\ hr$$

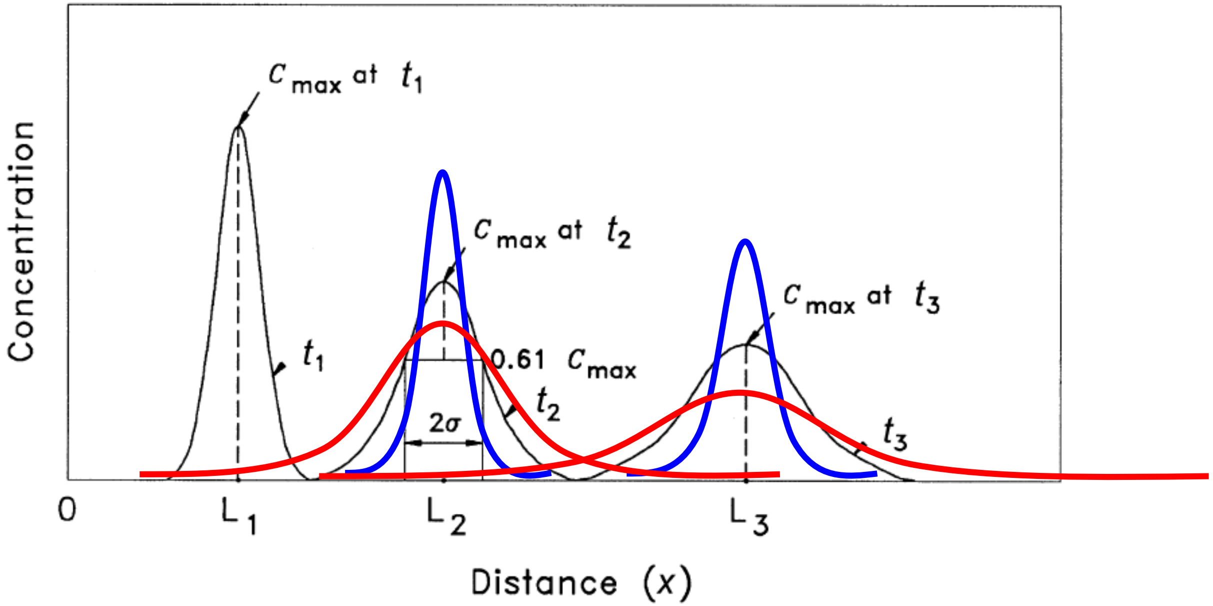
$$D_L = \frac{\sigma_L^2}{2t_3} = \frac{(350\ m)^2}{2(9.6\ hr)} \approx 6400\,\frac{m^2}{hr} \qquad \sim(10^4\,\frac{cm^2}{s})$$

Peclet number: Pe (dimensionless)

$$Pe = \frac{u^2 t}{D} = \frac{uL}{D}$$

u = mean velocity (cm/s)
L = characteristic length (cm)
D = Diffusion or dispersion coefficient (cm^2/s)
t = time (s)

- *If Pe >> 1, advection predominates*
- *If Pe << 1, dispersion (or diffusion) predominates*



Material balance in an infinitely small control volume: Advection-Dispersion-reaction equation

$$\underbrace{\text{Accumulation} = \text{inputs} - \text{outputs}}_{\text{Transport mechanisms}} + \text{reactions}$$

Transport mechanisms

(1) Advection and (2) Diffusion-dispersion (Fickian Transport)

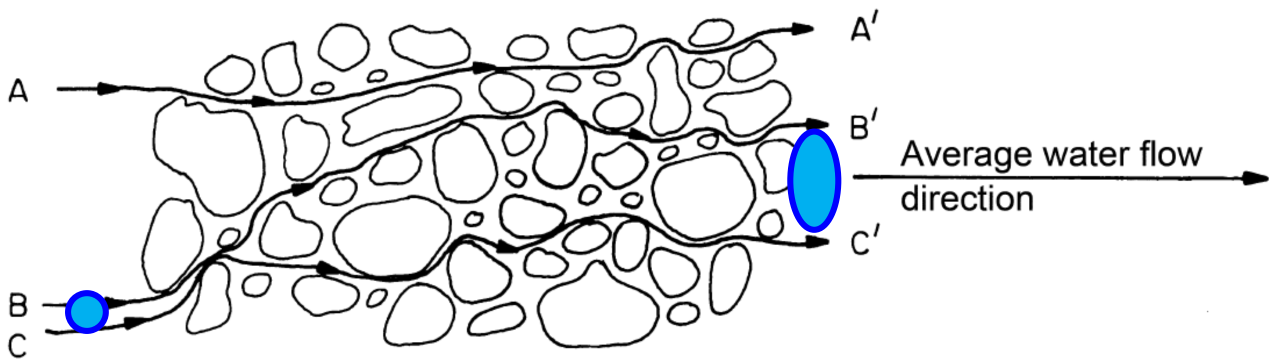
1-D
$$\frac{dC}{dt} = -V\frac{dC}{dx} + \frac{d}{dx}\left(D\frac{dC}{dx}\right) + r$$

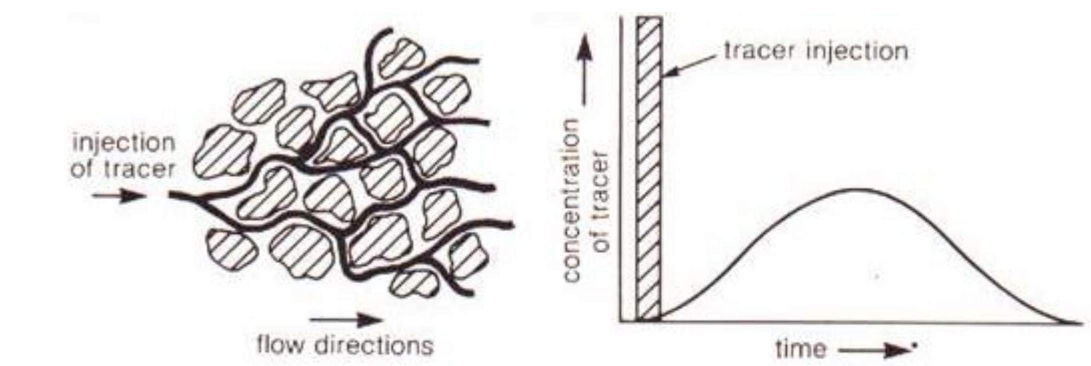
where V = fluid velocity and D = diffusion or dispersion coefficient

3-D
$$\frac{dC}{dt} = -V\,\nabla C + \nabla D(\nabla C) + r$$

Mechanical dispersion

- In the groundwater environment, mixing normally is not dominated by turbulence, as it is in most surface waters.
- Mechanical dispersion is the result of variations in the flow pathways taken by different fluid parcels that originate in the nearby locations.





Mechanical dispersion - Fick's law

- Mechanical dispersion can be treated mathematically in the same way that turbulent diffusion and dispersion in surface water are treated, by applying Fick's first law.

$$J = -D\left(\frac{dC}{dx}\right)$$

$D = Mechanical\ dispersion\ coefficient$

$\frac{dC}{dx} = concentration\ gradient\ along\ the\ x - axis$

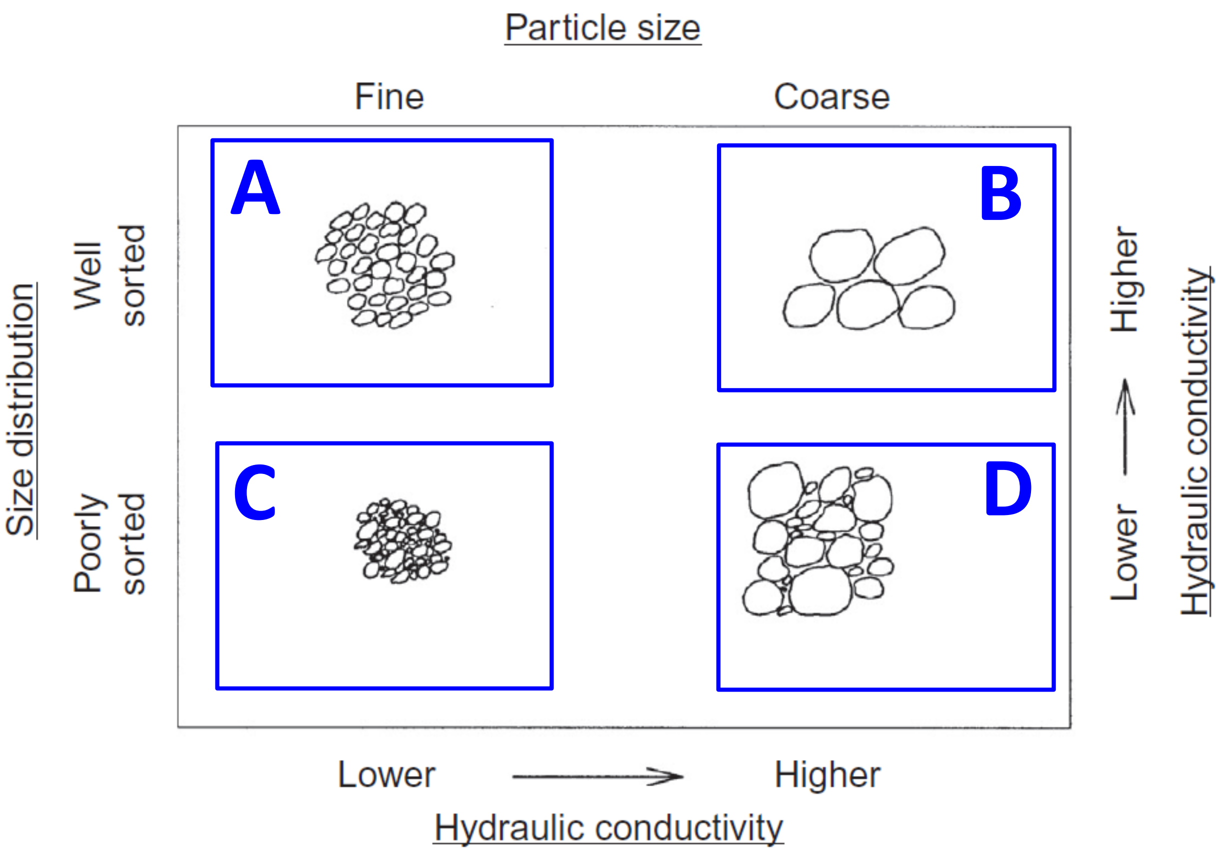
$$D = \alpha\ v$$

where α is the dispersivity of the aquifer, *approximately equal to the median grain diameter* of the aquifer solids;

v is the seepage velocity, the apparent velocity through the bulk of the porous medium .

In-Class Poll (3)

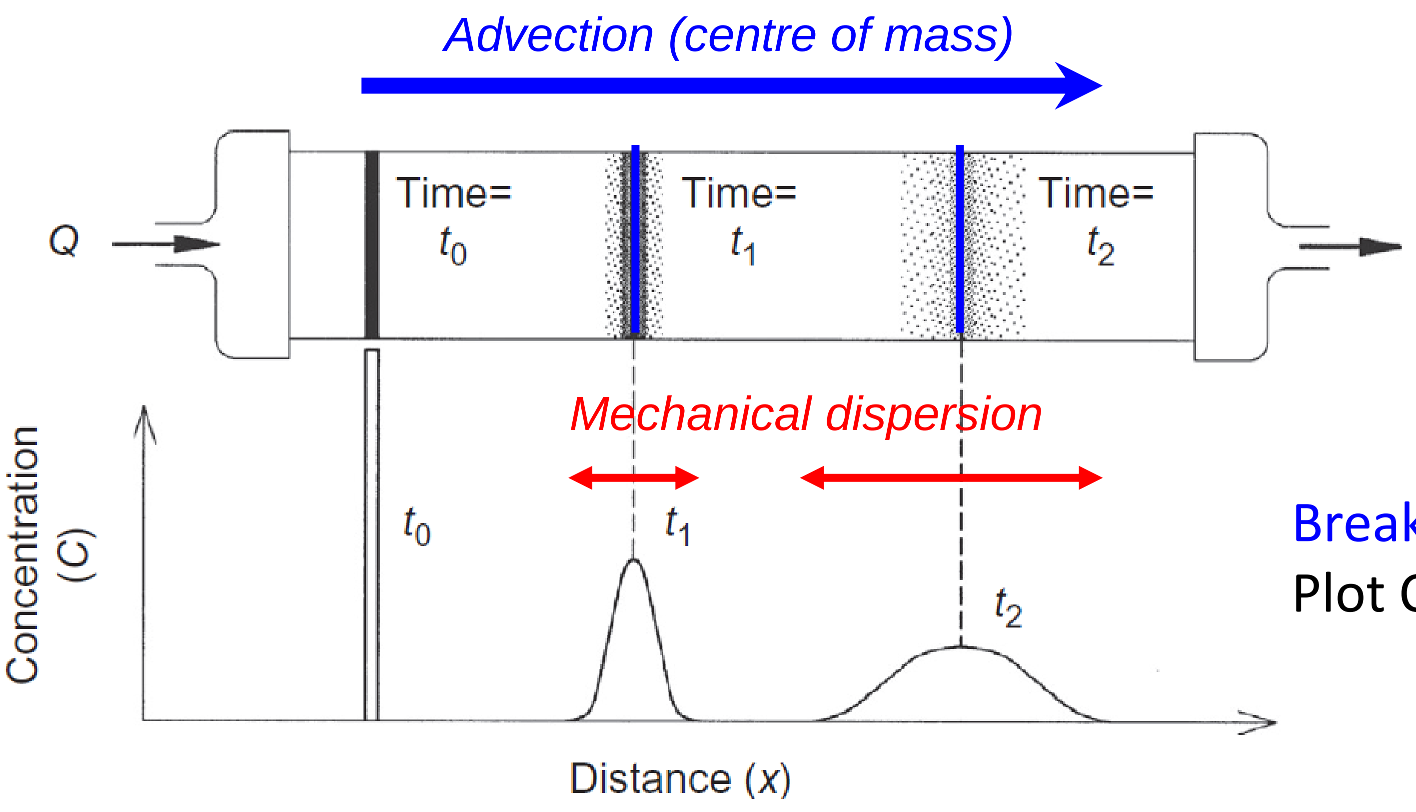
- Which type of porous medium likely gives the largest degree of mechanical dispersion?



Macrodispersion: Variations in the properties of the porous media, resulting in mixing.

1-D Dispersion in a Column (a pulse injection)

Dispersion can be demonstrated in laboratory studies in which water moves at a known seepage velocity, v, through porous media. An ideal chemical tracer (a salt or dye that has minimal sorption to particles and negligible decay), is initially injected at the upstream.



Breakthrough curve:

Plot C vs. t

1-D Dispersion in a Column (a pulse injection)

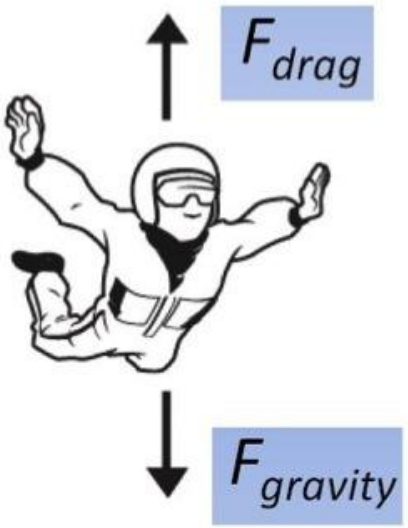
$$C(x,t) = \frac{M_a}{\boldsymbol{n}\sqrt{4\pi D_L t}} e^{-(x-Vt)^2/(4D_L t)} \quad \Rightarrow \quad C_{max}(x,t) = \frac{M_a}{\mathbf{n}\sqrt{4\pi D_L t}}$$

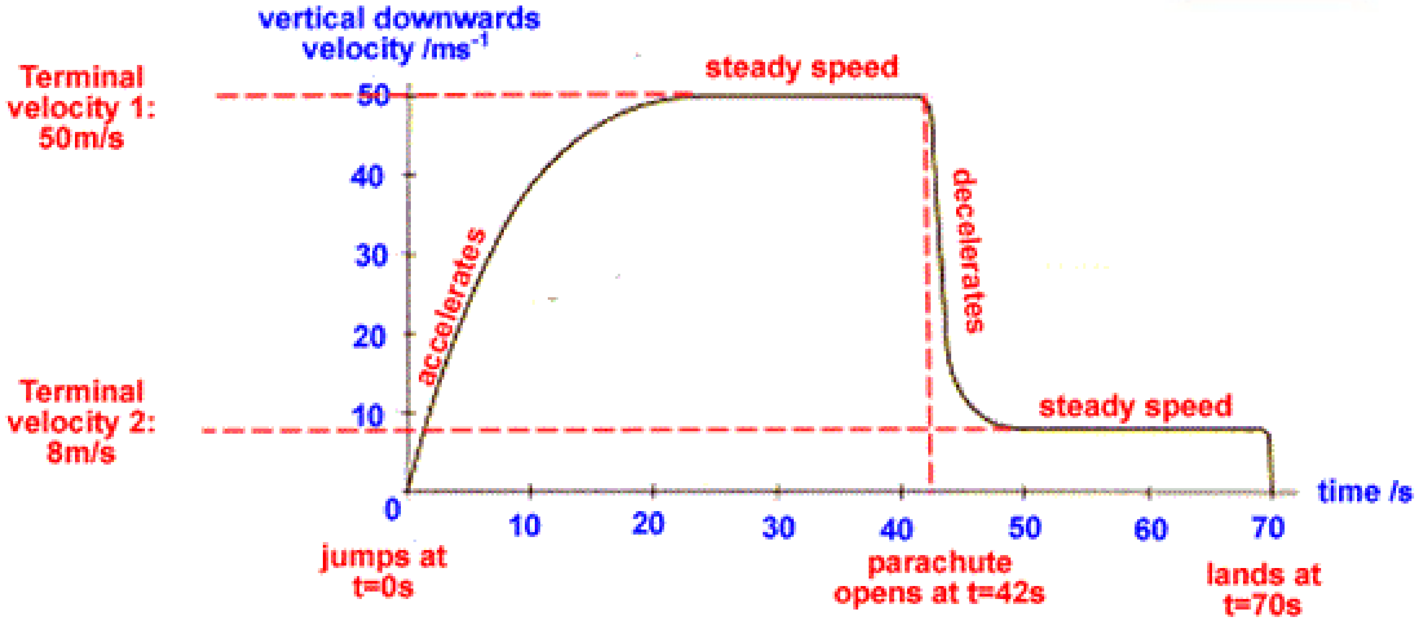
$$n = \text{porosity of medium}$$

$$C(x,t) = \frac{M_a}{\mathbf{n}\sqrt{4\pi D_L t}} e^{-(x-Vt)^2/(4D_L t)} \quad \text{and} \quad D_L = \alpha\, v$$

$$C_{max}(x) = \frac{M_a}{\mathbf{n}\sqrt{4\pi\alpha x}}$$

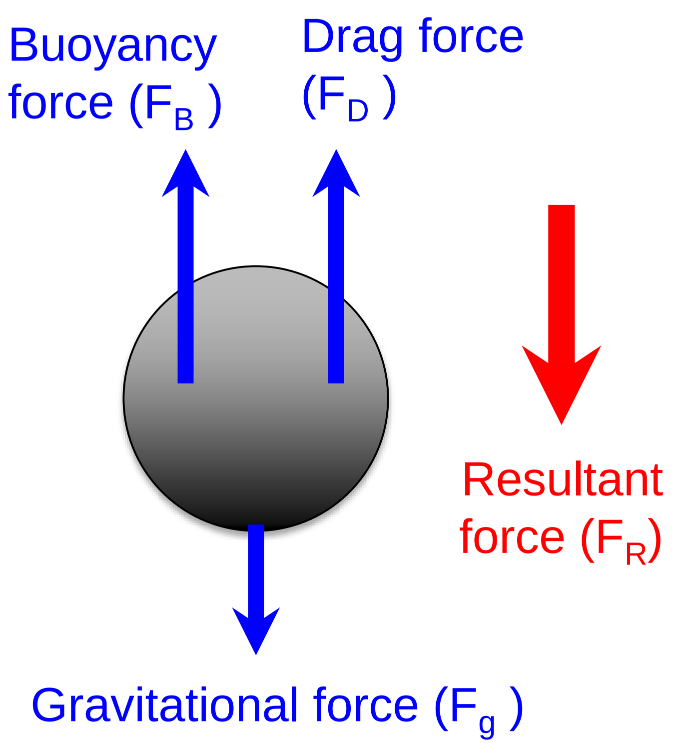
In-Class Poll (4) - Skydiving



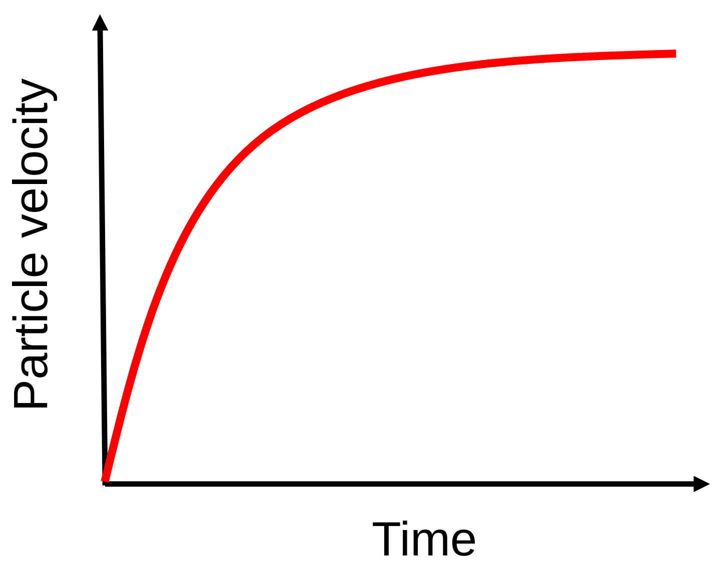


Movement of a particle – Stoke's Law

The movement of a particle in a fluid can be determined by a balance of the viscous drag forces resisting the particle movement with gravitational or other forces which cause the movement. The solution to this balance of forces in the specific problem of particle settling under gravity is known as Stoke's Law.



By force balance: $F_R = F_g - F_B - F_D$



Terminal velocity of a particle

$$F_R = F_g - F_B - F_D$$

$$F_R = m_p \frac{du}{dt}, \quad F_g = \rho_p g \frac{\pi D_p^3}{6}, \quad F_B = \rho_f g \frac{\pi D_p^3}{6}$$

$$m_p \frac{du}{dt} = \rho_p g \frac{\pi D_p^3}{6} - \rho_f g \frac{\pi D_p^3}{6} - F_D$$

$$F_D = \frac{(\rho_p - \rho_f) g \pi D_p^3}{6}$$

Experimentally, it has been found that

$$F_D = \frac{C_D \pi D_p^2 \rho_f u^2}{8}$$

where C_D is the coefficient of drag or friction (dimensionless), u is the particle velocity

Experimentally, C_D is a function of the Reynolds number, Re:

$$C_D = \frac{b}{Re^n}$$

$$Re = \frac{u D_p \rho_f}{\mu}$$

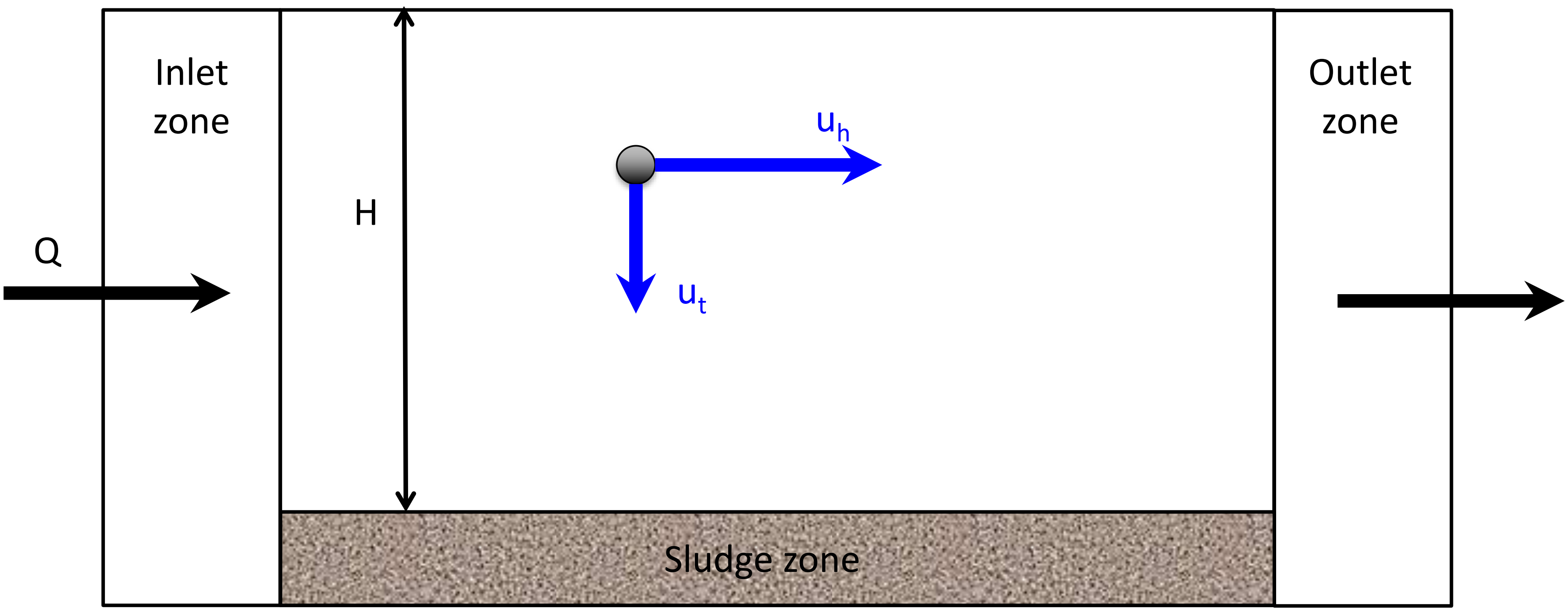
where μ is the viscosity of the medium.

For the laminar flow conditions (Stokes' law region: Re <1-2, → n=1, b=24),

$$C_D = \frac{24}{Re} = \frac{24\mu}{\rho u D_p}$$

Terminal velocity, $\mathbf{u_t} = \frac{(\boldsymbol{\rho_p} - \boldsymbol{\rho_f}) \mathbf{g} \mathbf{D_p^2}}{\mathbf{18\mu}}$

Sedimentation



Retention time, t_r = Volume of reactor/total flow = V/Q

Example (4)

Example: Calculate the settling velocity of two spherical particles of diameter (a) 0.1 mm and (b) 0.001 mm in still water at a temperature of 20°C. The density of the particles is 2645 kg/m^3.

Assume laminar flow conditions. A common retention time for sedimentation tanks is 2 h. Will these particles settle to the bottom of a 3.5-m-deep tank in that time?

$\rho_{20°C\ water} = 998\ kg/m^3$

$\mu_{20°C\ water} = 1.00 \times 10^{-3}\ kg/m\cdot s$

Example (4)

Solution: $\rho_p = 2645\ kg/m^3$

(a) $$u_t = \left(2645\,\frac{kg}{m^3} - 998\,\frac{kg}{m^3}\right) 9.81\ m/s^2 \left(\frac{(0.1 \text{ x } 10^{-3})^2 m^2}{18 \text{ x } 1.00 \text{ x } 10^{-3}\ kg/\,m \cdot s}\right)$$

$= 9.0 \text{ x } 10^{-3}\ m/s = 9.0\ mm/s$

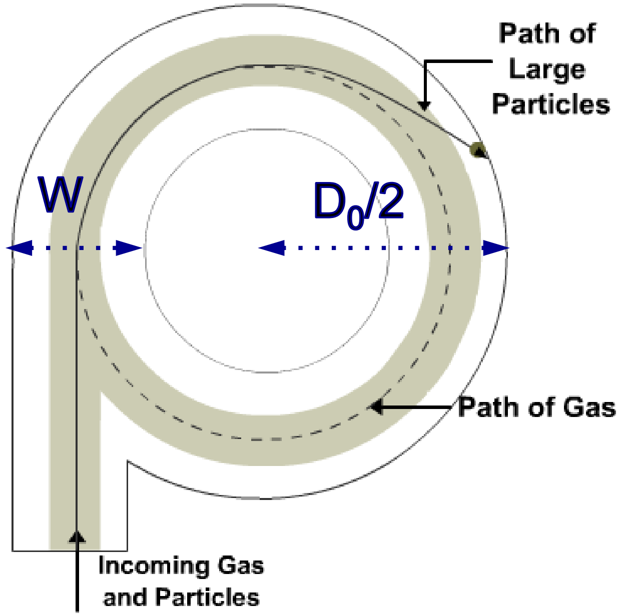
So the time to settle 3.5 m = $3.5/9.0 \text{ x } 10^{-3}$ = 390 s = 6.5 min << 2h. This settling rate is certainly practical for particle removal by sedimentation.

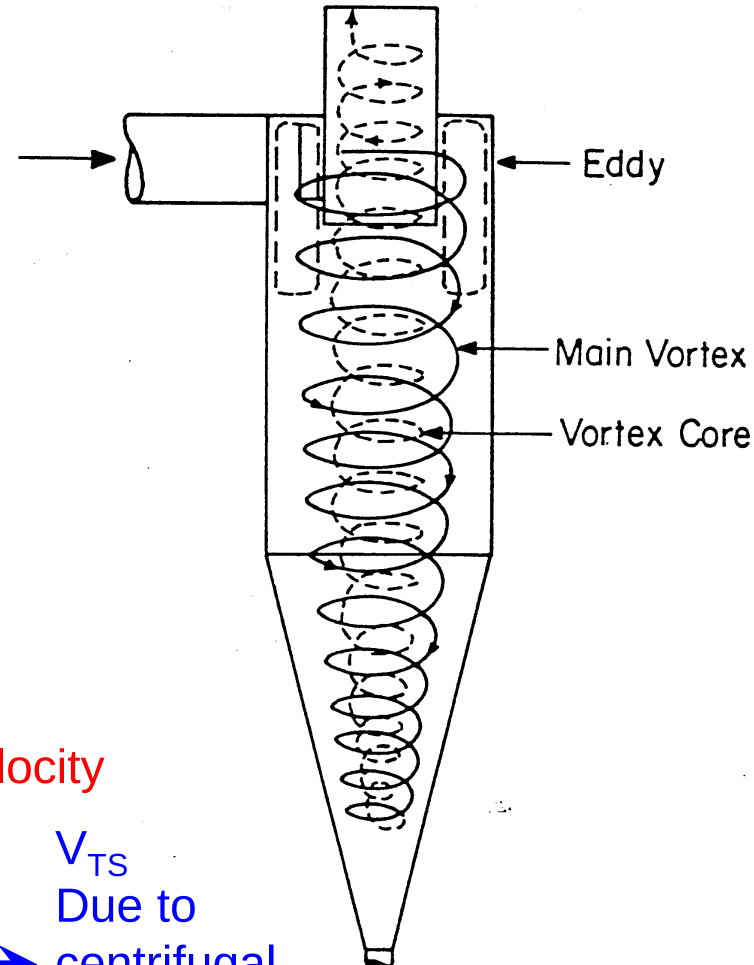
(b) $u_t = 9.0 \text{ x } 10^{-7}\ m/s = 9.0 \text{ x } 10^{-4}\ mm/s$

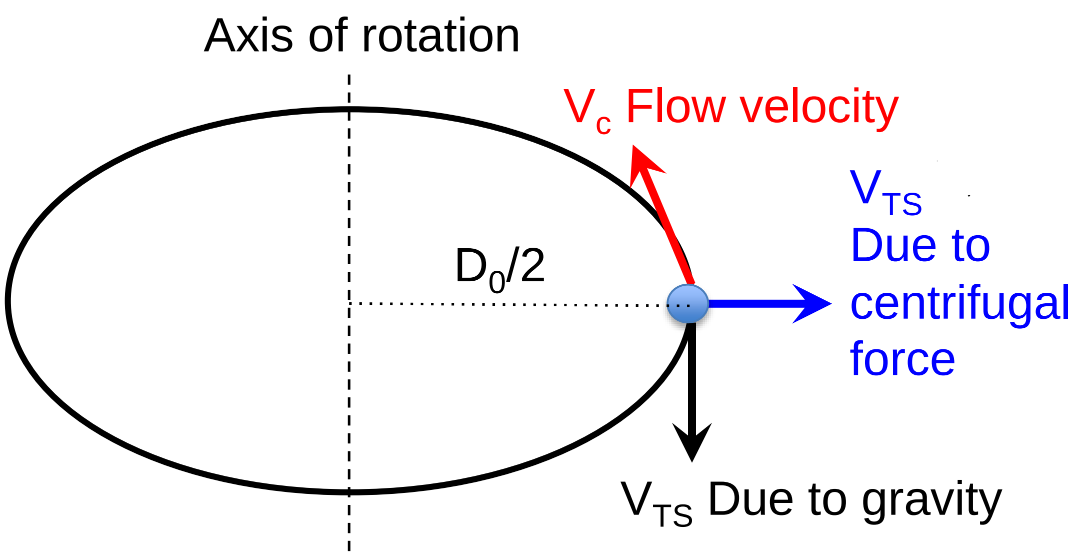
So the time to settle 3.5 m = $390 \text{ x } 10^4$ s = 1083 h.

The settling rate is much too slow for particle removal by sedimentation alone, so coagulation/flocculation must be employed to increase the particle size and thus achieve greater settling velocity

Cyclone separator







Cyclone separator

Time: 8:00 – 10:30
(https://youtu.be/bGc6Z7vwHC4)

Sampling inlet of atmospheric PM

Teflon© Coated Aluminum Cyclones

URG's complete collection of aluminum cyclone inlets are Teflon© coated, a patented process that minimizes the losses of reactive gases such as HNO_3 and NH_3 to the internal surfaces of the cyclone. Below is a selection of the Teflon© coated cyclones that URG offers.

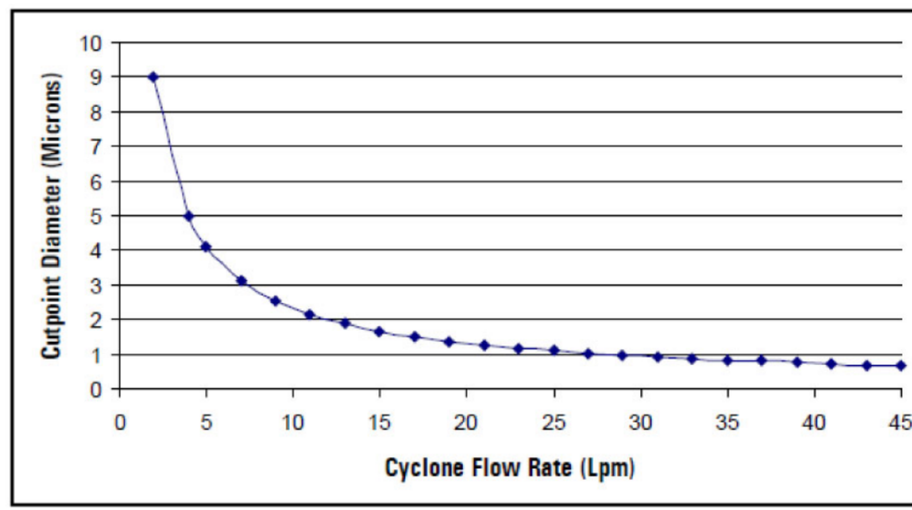
URG-2000-30EN *10Lpm Flow Rate, 2.5µm Cutpoint*

Inlet: 5/8" OD 90 Degree Arm

Outlet: #30 Male Thread

Specifications

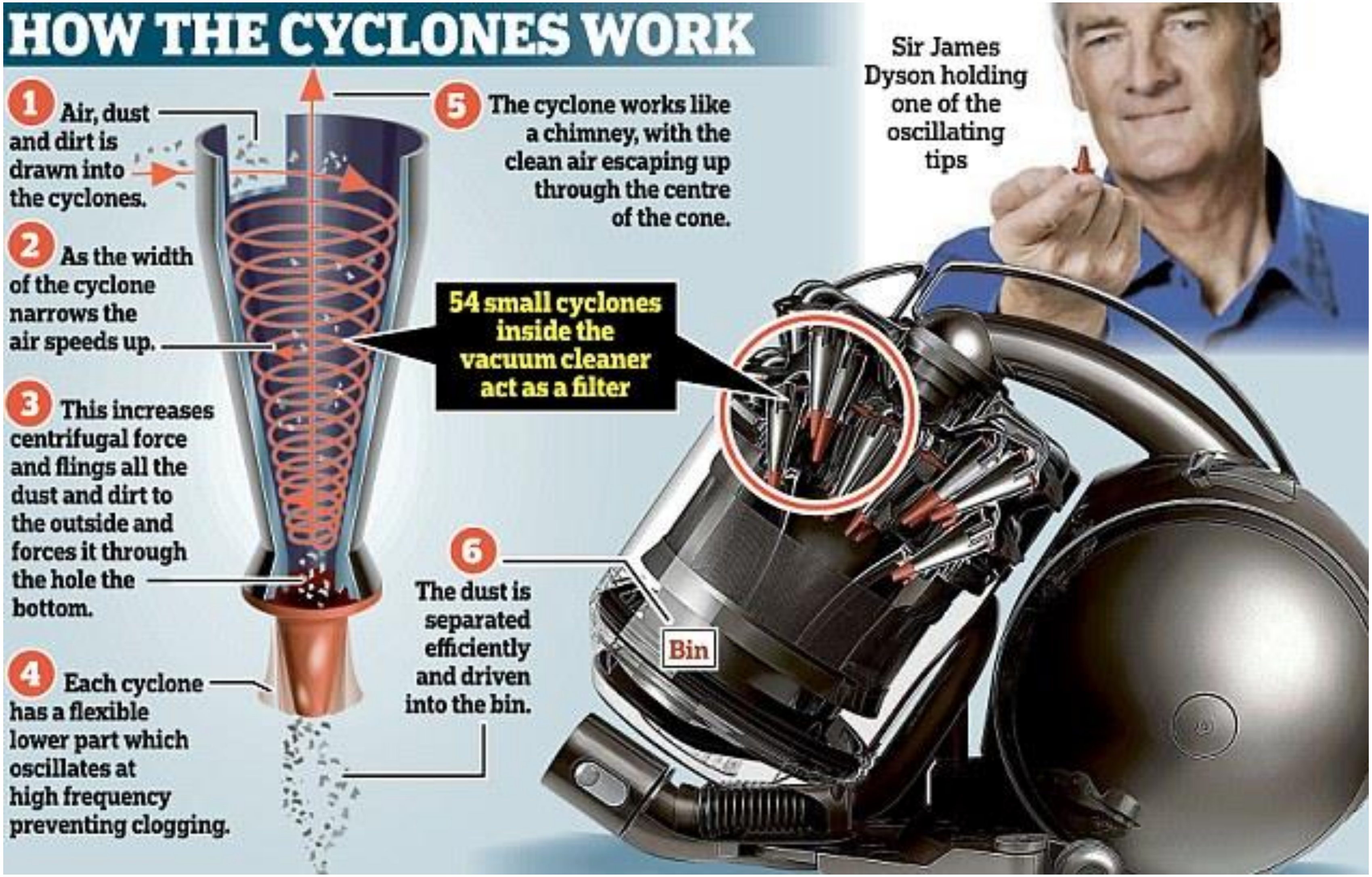
- Teflon© Coated Aluminum
- 10Lpm Flow Rate, 2.5µm Cutpoint
- Dimensions: 6 1/4" x 5 7/8" x 1 1/4" (15.9 x 14.9 x 3.2 cm)
- Weight: 0.5 lb (0.2 kg)
- Available with 90 Degree Arm (shown, URG-2000-30ENYA) and Straight Arm



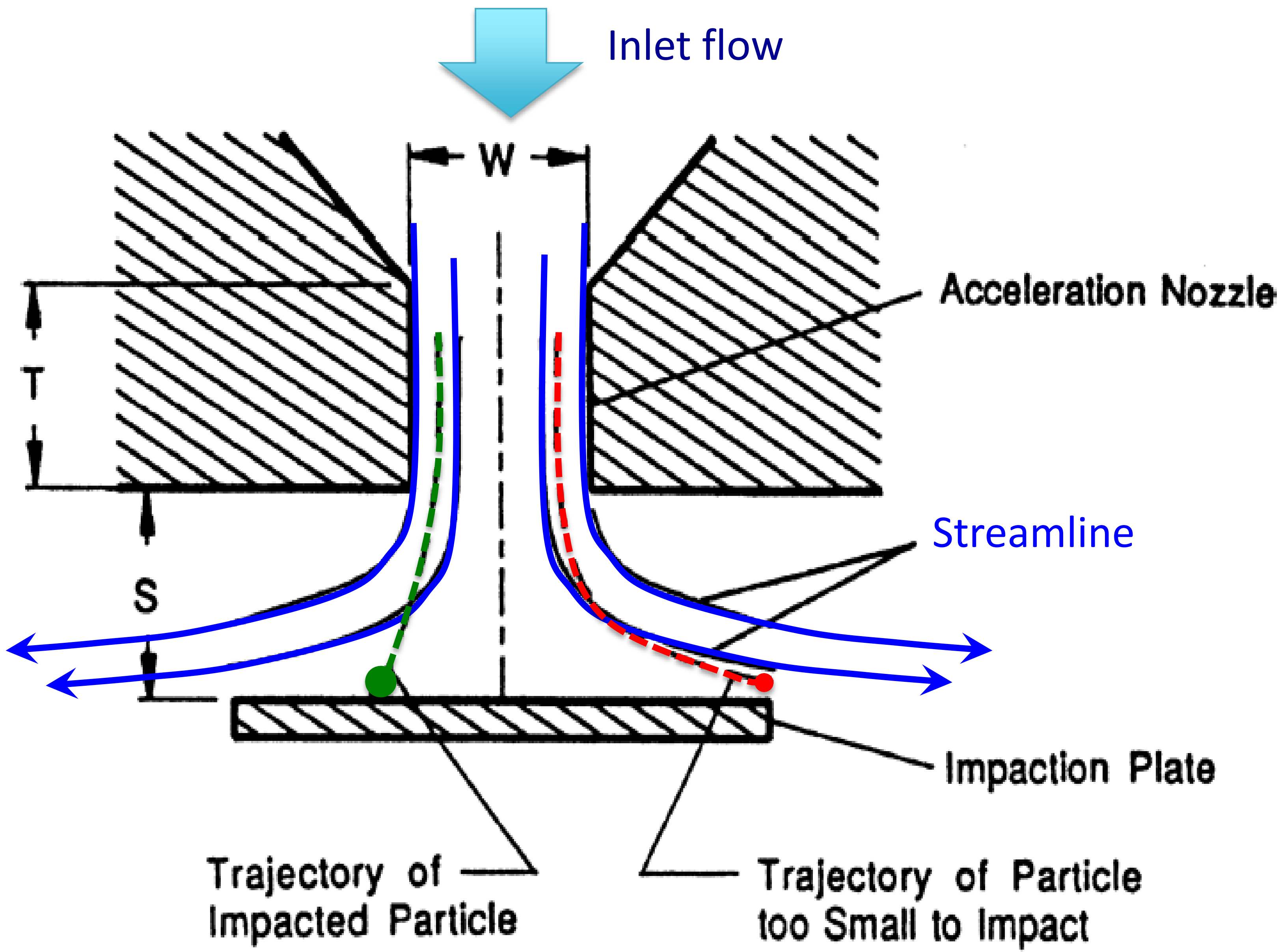
http://www.urgcorp.com/index.php/products/inlets/teflon-coated-aluminum-cyclones

Industrial application - emission control

Home application – Vacuum cleaner



Impactor: Curvilinear motion of particles



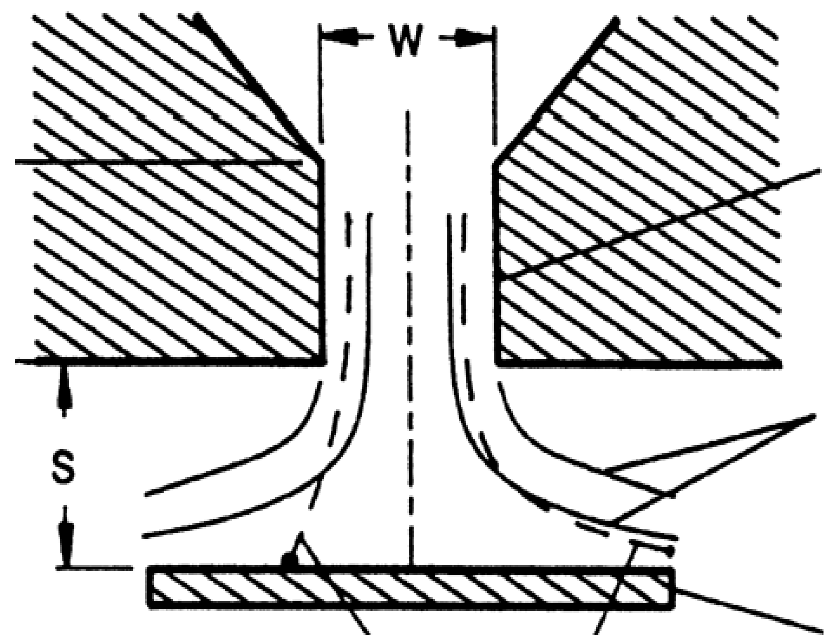
Stoke number (Stk): Inertial impaction

Stokes number (Stk) is the ratio of the stopping distance (S) of a particle to a characteristic dimension of the obstacle.

Stk >> 1, particles continue moving in a straight line when the gas turns;
Stk << 1, particles follow the gas streamlines perfectly and make the turn.

For an inertial impactor:

$$Stk = \frac{S}{W/2} = \frac{\tau U}{W/2} = \frac{\rho_p d_p^2 U C_c}{9 \eta W}$$



where τ = relaxation time
ρ_p = particle density,
d_p = particle diameter,
U = flow velocity,
η = air viscosity,
W = nozzle diameter
C_c = slip correction factor

Multiple stages impactor