

## Physical transport of chemicals

### ♣ Mass balance expression

o Change in storage of mass

$$= \text{mass transported IN} - \text{mass transported OUT} \\ + \text{mass PRODUCED by sources} - \text{mass ELIMINATED by sinks}$$

o Rate of change in storage of mass

$$= \text{mass transport rate in} - \text{mass transport rate out} \\ + \text{mass production rate by sources} - \text{mass elimination rate by sinks}$$

(\* rate = mass per time [M/T])

☞ *If storage does not change with time the left-hand sides are zero*

---> *steady state*

### ♣ Types of mass transport

#### 1) Advection

- mainly resulting from bulk, large scale movement of a medium (e.g.) wind blows, water flows,....
- so, transported at the same velocity as the fluid
  - macroscale view; center of mass of chemical moves by advection
  - microscale view; Fickian transport occurs at the same time
- *convection*; often vertical advection (but, considered almost a similar term)
- **flux density (J)**; mass of chemical transported across an imaginary surface of unit area per unit of time

$$J = CV$$

J [M/L<sup>2</sup>T]

C [M/L<sup>3</sup>]; chemical concentration

V [L/T]; fluid velocity

- in ground water, V is the Darcy flux of water

$$J = C(nv_p)$$

n; porosity

v<sub>p</sub>; seepage (pore) velocity

#### 2) Fickian transport

o Turbulent diffusion ("eddy diffusion")

- resulting from random mixing of air or water by eddies
- carries mass in the direction of decreasing chemical concentration (e.g.) dye blob injected into a river
- important in surface water and air (**not considered in the subsurface**)
- use Fick's first law to describe

$$J = -D(dC/dx)$$

J [M/L<sup>2</sup>T]

D; turbulent diffusion coefficient

C [M/L<sup>3</sup>]; chemical concentration

x [L]; distance over which a concentration change is considered

### o (Mechanical) Dispersion

- fluctuations in the velocity field at scales smaller than advection
- ground water flow;
  - no eddies present due to its low velocity
  - but still random detours exist, causing mixing chemicals
- transport of a chemical from regions of higher to lower concentration
- use Fick's first law to describe

$$J = -D_{\text{mechanical}}(dC/dx)$$

$$J \text{ [M/L}^2\text{T]}$$

D; mechanical dispersion coefficient

C [M/L<sup>3</sup>]; chemical concentration

x [L]; distance over which a concentration change is considered

### o Molecular diffusion

- random movement of chemical due to local concentration gradient
  - lower flux density compared to other Fickian transport processes
  - use Fick's first law to describe
- $$J = -D_{\text{molecular}}(dC/dx)$$
- $$J \text{ [M/L}^2\text{T]}$$
- D; molecular diffusion coefficient
- C [M/L<sup>3</sup>]; chemical concentration
- x [L]; distance over which a concentration change is considered
- not related to turbulence (eddies) or obstructions (particles)
  - but dependent on molecular properties (primarily, size) and temperature

※ For the subsurface transport of chemical, advection, dispersion, and molecular diffusion are considered. In addition, **POROSITY** should be included.

$$J = J_{\text{adv}} + J_{\text{dis}}$$

$$\text{where } J_{\text{adv}} = C(nv_p)$$

$$J_{\text{dis}} = \{-nD(dC/dx)\} \quad (n; \text{ porosity})$$

$$D = D_{\text{mechanical}} + D_{\text{molecular}}$$

※ So far, one-dimensional situation is considered. But, in most cases, flow is **anisotropic**;

- (e.g.) flow direction vs. perpendicular to flow,
- homogeneous medium vs. heterogeneous medium,
- time