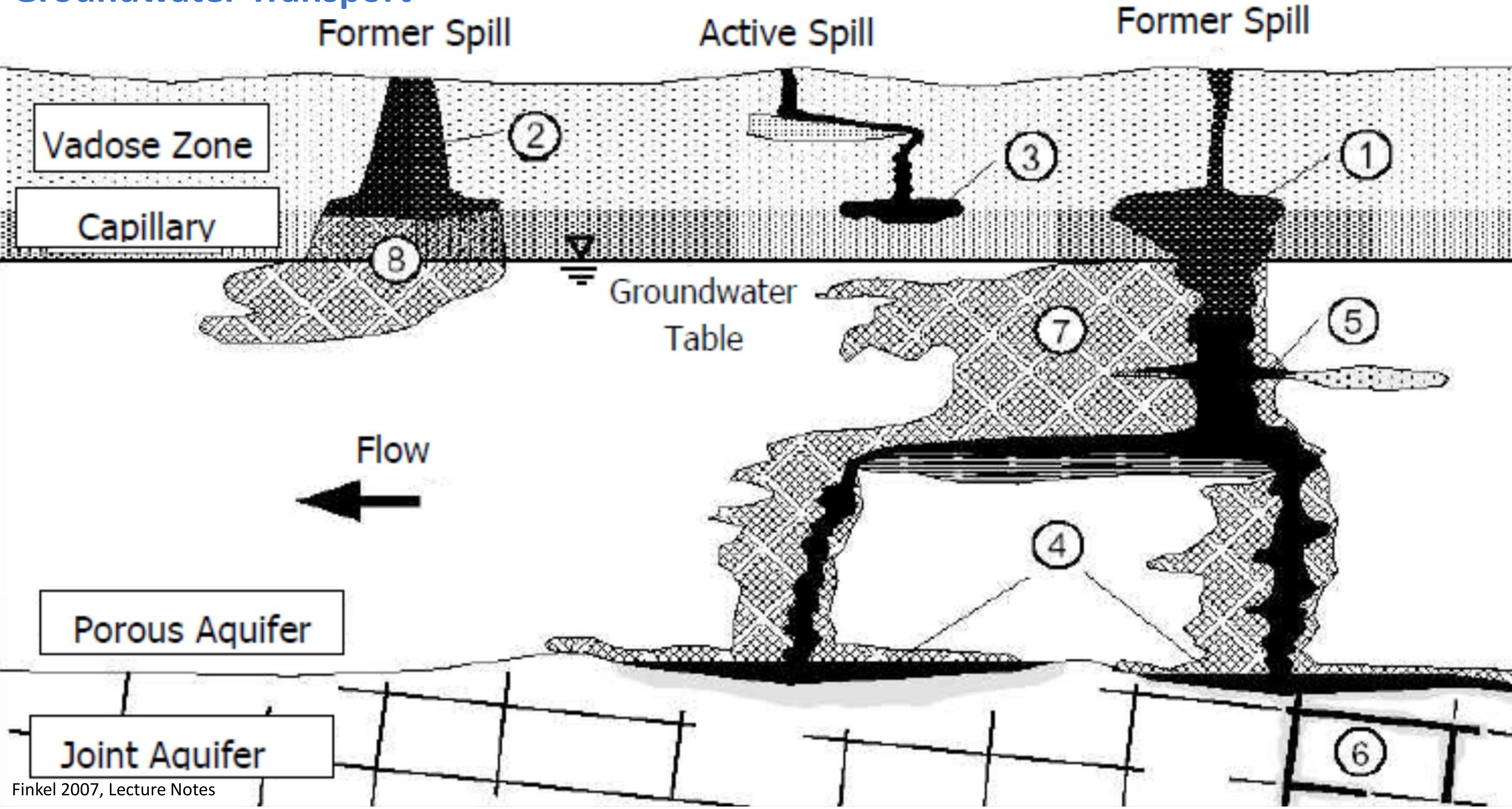
Main Transport Processes

Groundwater Transport



Finkel 2007, Lecture Notes

Main Transport Processes

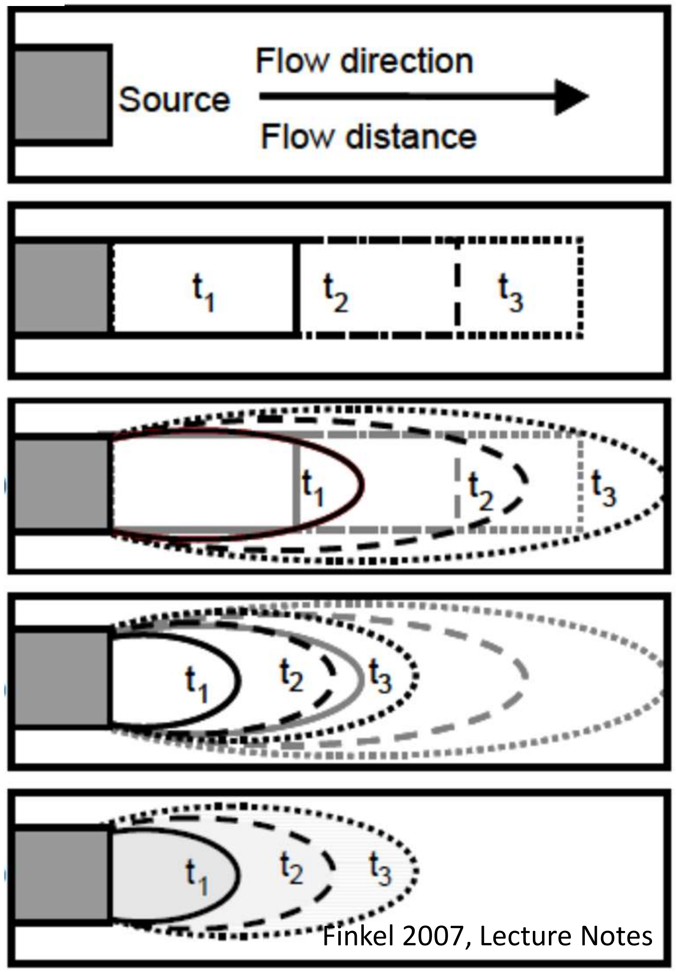
$$\nabla = \begin{bmatrix} \frac{\partial}{\partial x_1} \\ \frac{\partial}{\partial x_2} \\ \frac{\partial}{\partial x_3} \end{bmatrix}$$

$$\frac{\partial c}{\partial t} = -\mathbf{v}.\nabla c$$

$$\frac{\partial c}{\partial t} = -\mathbf{v}.\nabla c + \mathbf{D}\nabla^2 c$$

$$R\frac{\partial c}{\partial t} = -\mathbf{v}.\nabla c + \mathbf{D}\nabla^2 c$$

$$R\frac{\partial c}{\partial t} = -\mathbf{v}.\nabla c + \mathbf{D}\nabla^2 c + n_e r$$



Advection

Advection + Dispersion/Diffusion

Advection + Dispersion/Diffusion + Sorption

Advection + Dispersion/Diffusion + Sorption + Transformation

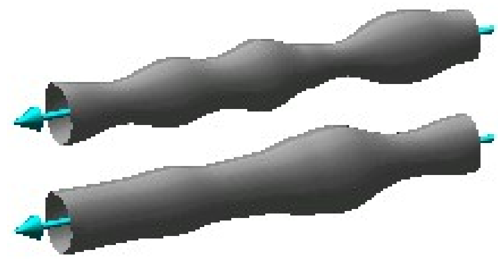
Before we proceed what are: (1) seepage velocity *v* [L/T] , (2) dispersion coefficient **D** [L^2/T] and (3) (3) Specific reaction rate r [M/L^3T] of chemical transformations, (4) retardation factor R [-] ?

Seepage velocity [L/T]

Seepage velocity v_p [L/T]: Velocity experienced by a water particle along its true trajectory.

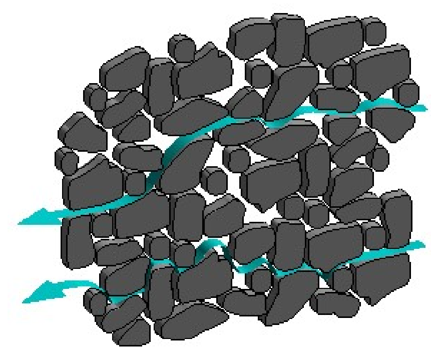
Darcy velocity (Specific discharge) q [L/T]: Groundwater discharge per unit cross-section area $q=dQ/dA$

Seepage velocity v [L/T]: Length of a streamline section divided by the time needed to distance $v=\Delta s/\Delta t \approx q/n_e$



Average linear velocity

Hornberger et al 1998



True velocities

Hornberger et al 1998

Before we proceed: What is effective porosity n_e ?

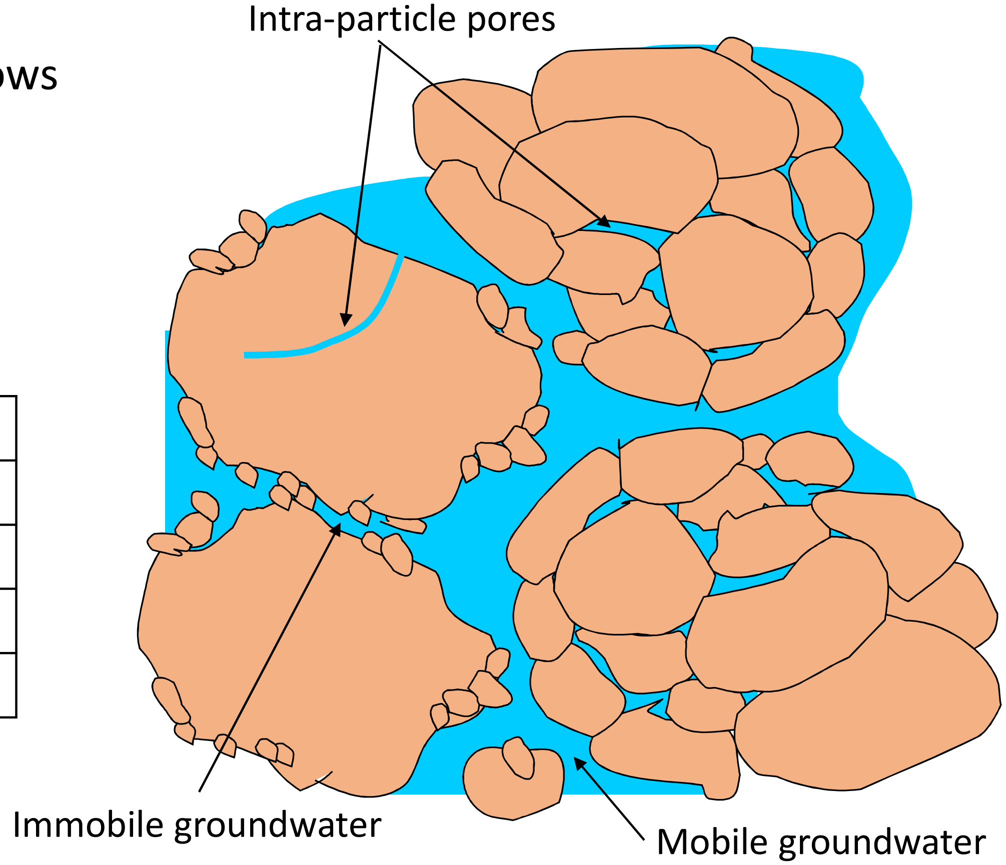
Effective porosity [-]

What is the effective porosity n_e?

It is volume of void space in which groundwater flows

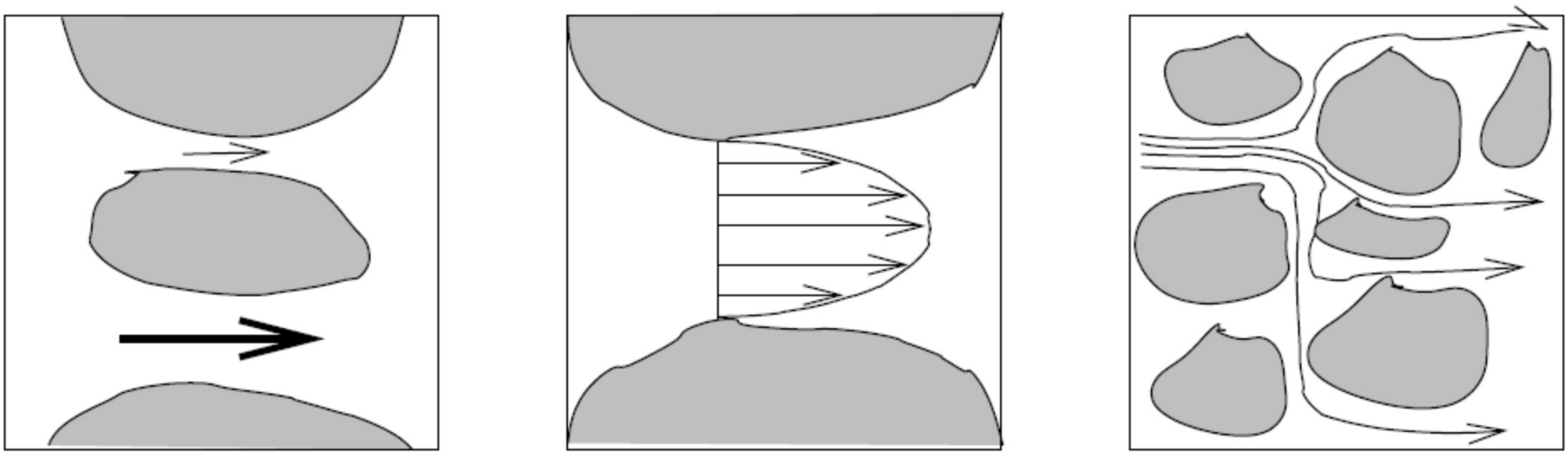
$$n = \frac{V_P}{V_P + V_S} \qquad n_e = \frac{V_E}{V_P + V_S}$$

Unconsolidated Sediments	**n [%]**	**n_e [%]**
Silt	40-50	0.5-5
fine sand	40-50	10-15
Coarse sand and well sorted fine gravel	30-40	20-25
Sandy gravel	20-30	15-20



Modified from Srivastava 2014

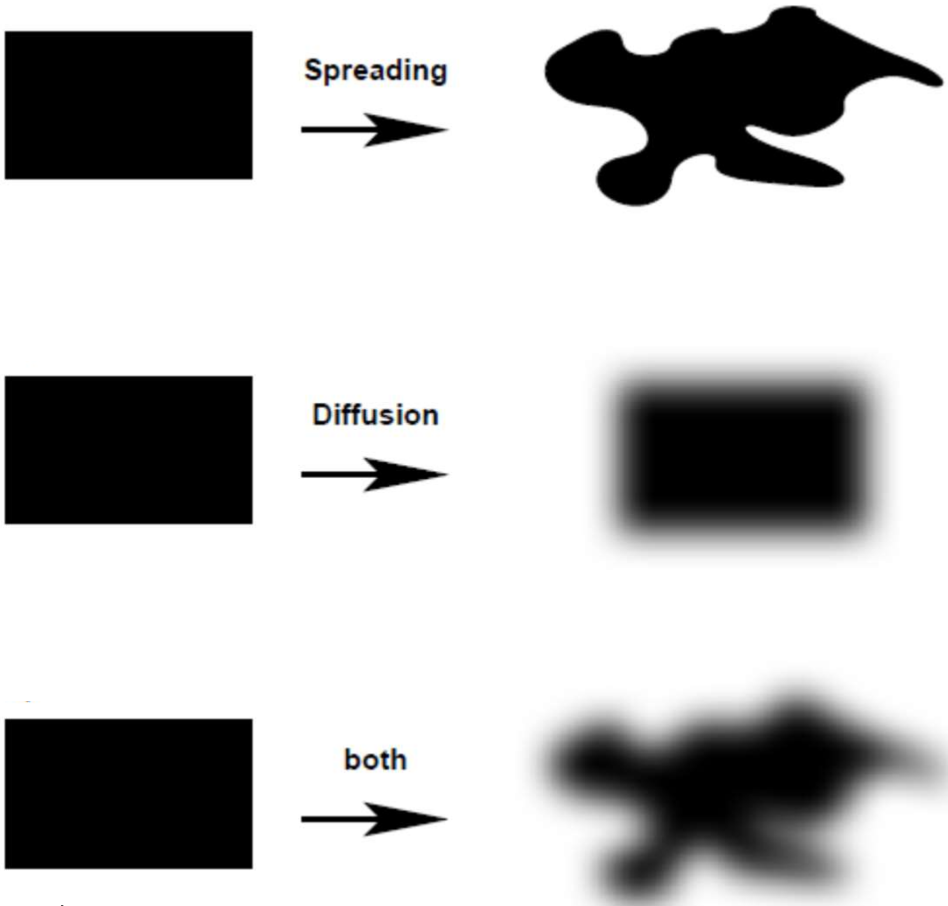
Dispersion Coefficient D [L^2/T]



Cirpka 2008, Lecture Notes

Mechanisms contributing to dispersion in porous media

Dispersion Coefficient D [L^2/T]



Cirpka 2008, Lecture Notes

$$D_l = \alpha_l v + D_e \qquad D_t = \alpha_t v + D_e$$

D_l and D_t are the longitudinal and transverse dispersion coefficient. α [L] is the dispersivity. The term αv is referred to hydrodynamic dispersion. D_e is the effective molecular diffusion coefficient.

The dispersion coefficient tensor **D** can for any arbitrarily oriented ***v***

$$\mathbf{D} = \frac{\mathbf{v}\mathbf{v}^T}{\|\mathbf{v}\|}(\alpha_l - \alpha_t) + \mathbf{I}(D_e + \alpha_t \|\mathbf{v}\|)$$

Specific Reaction Rate r [M/L^{3}T] of Chemical Transformations

Reactions leading to the chemical transformation of the compounds:

(1) Equilibrium Reactions: in which the concentrations (activities) of the products and educts (original compounds) are in a fixed ratio. The equilibrium can be calculated from thermodynamic properties of the compounds involved. The mathematical description of equilibrium reactions is by (systems of algebraic equations.

In the mathematical description of reactive solute transport, the transformation rates *r* [M/L^{3}T] appear as source and sink terms of the involved compounds.

$$R\frac{\partial c}{\partial t} = -v\frac{\partial c}{\partial x} + D\frac{\partial^2 c}{\partial x^2} + r_w + \frac{(1-n_e)}{n_e}r_s$$

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(5) Catalyzed Reactions: require a catalyst which reacts with the original compounds in an initial step but is recovered in a later step. A catalyst is not consumed in the net reaction, although it is involved in intermediate steps. Most biotransformations are catalytic (here the catalysts are called enzymes). The transformation rates of catalytic reactions are often proportional to the amount of the catalyst.

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Exercise 1: Breakthrough Curve

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$$\frac{\partial c}{\partial t} = -v\frac{\partial c}{\partial x} + D\frac{\partial^2 c}{\partial x^2}$$

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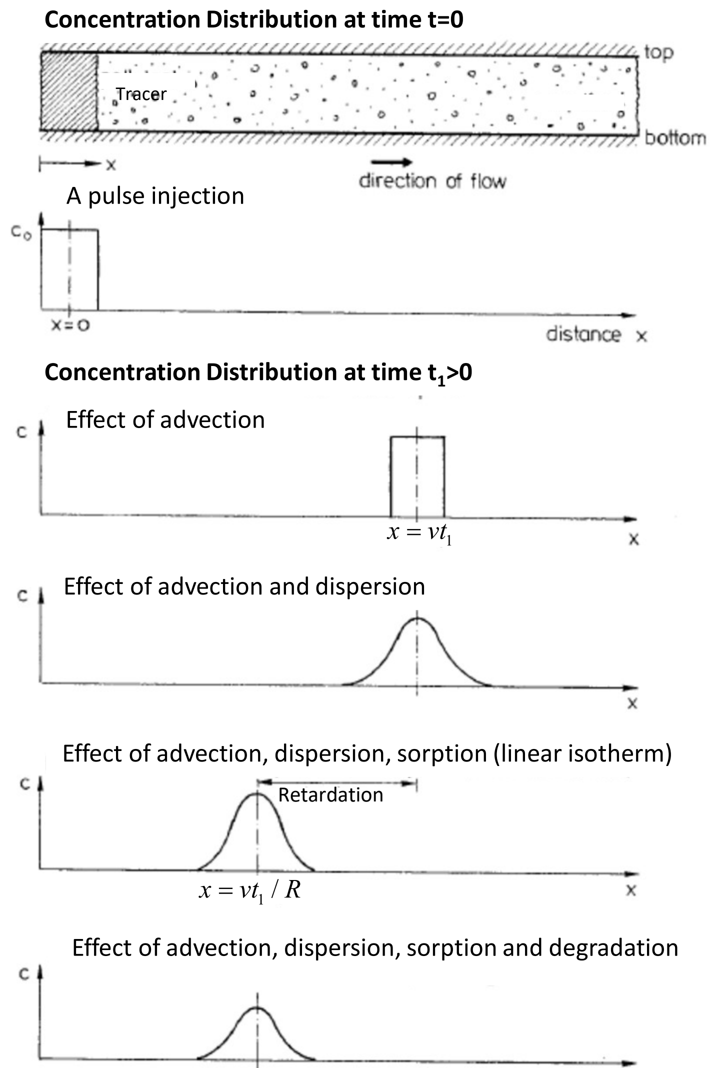

Finkel 2007, Lecture Notes