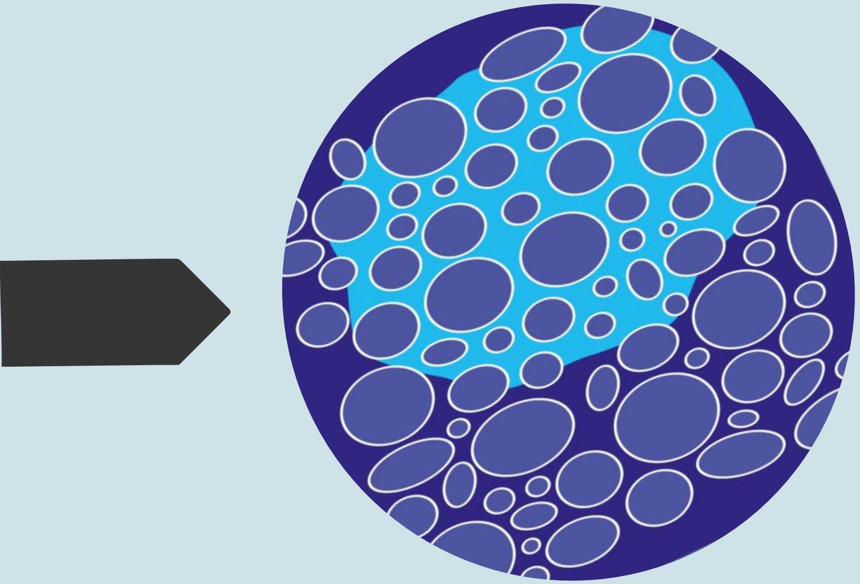


多孔介质污染迁移动力学

Contaminant Transport in Porous Media

郭芷琳

Office hour: 周三 15:00-17:00

工学院618

guozl@sustech.edu.cn

Lecture 2

- 1 Solute Transport 溶质迁移

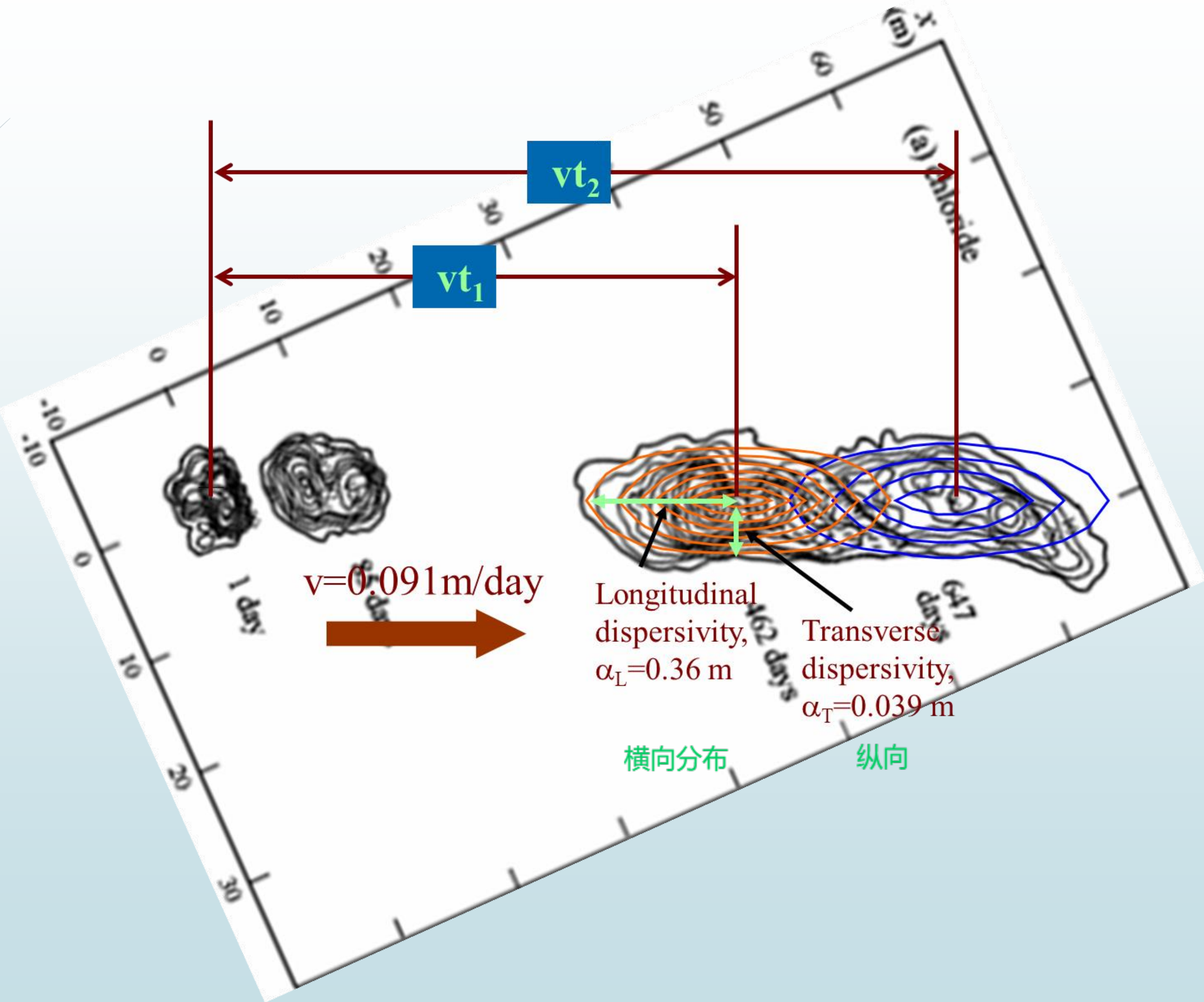
Transport Terms

- Solute – matter dissolved in fluid.
- Hydraulic residence time- mean time for water molecules to travel to a point some distance from an initial position.
- Travel time – time required for a solute molecule to travel to a point some distance from an initial position (mean travel time).

Solute Transport

Two methods of representation

1. Spatial Distribution —— Plume
   [sample many point at one time]
   provides info. on dimensions and locations of solutes
   Lagrangian Approach = “move along with solute”
   primarily 2-D and 3-D focus



vt_2
vt_1
v=0.091m/day
Longitudinal dispersivity, α_L=0.36 m
Transverse dispersivity, α_T=0.039 m
横向分布
纵向
(a) Chloride
1 day
462 days
647 days

Solute Transport

Two methods of representation

1. Temporal Distribution —— Breakthrough curves

   [sample at many times at one point]

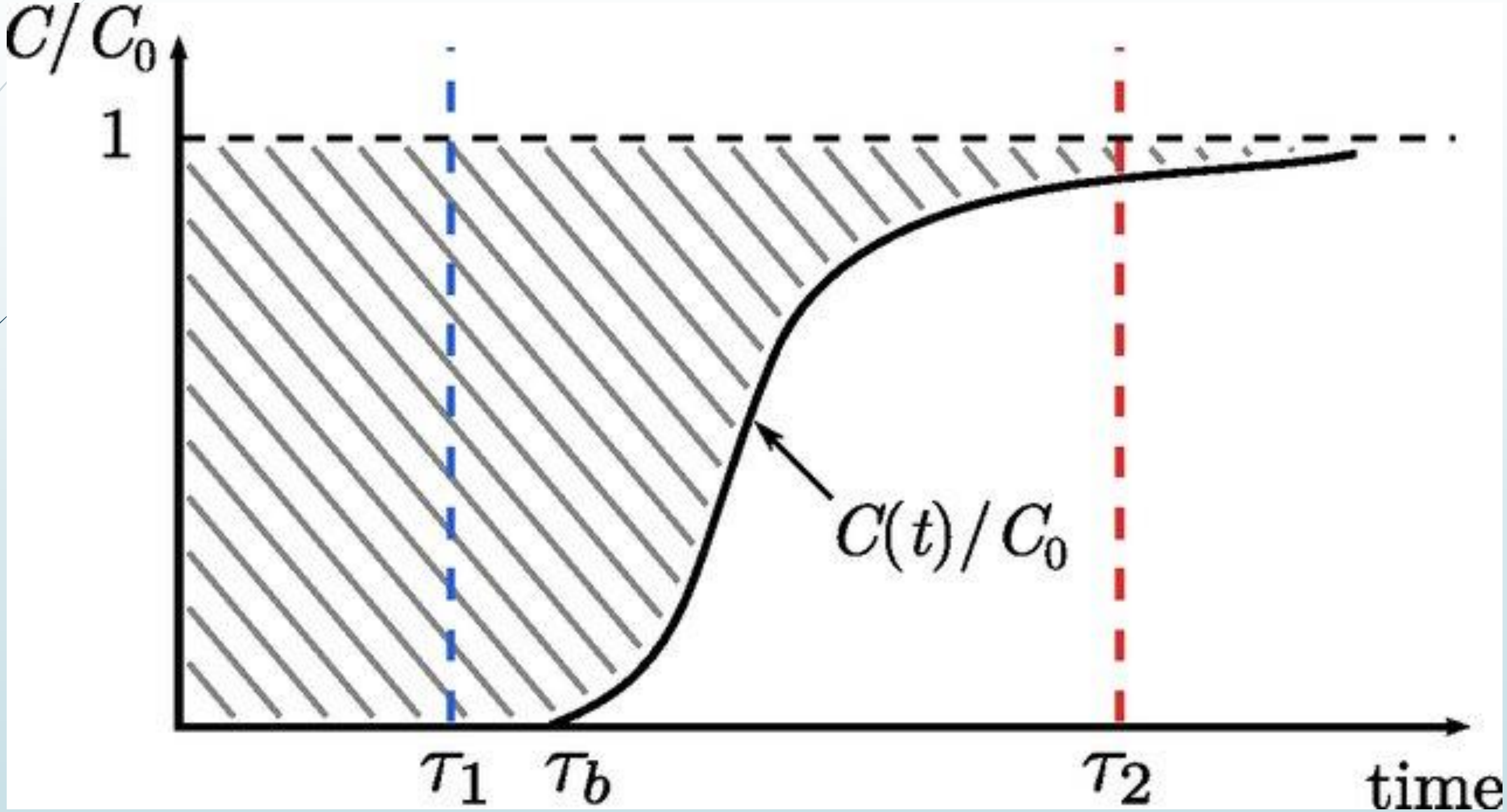
   provides info. on arrival times of solute

   Eulerian Approach = “watch solute pass by”

   primarily 1-D

Concentration Distribution

1. Spatial Distribution — Plumes — Concentration areal extent (2D) or volume map (3D) at one point in time requires sampling many locations at one time. It provides information about extent of concentration distribution, total mass, and transport behavior. It uses the Lagrangian Approach → moving with the solute during transport.
2. Temporal Distribution — Breakthrough curves (BTC) — Concentration variability through time as observed at one location. It can be samples collected over time at one downgradient monitoring well or effluent concentrations observed from a laboratory column or extraction well. It provides information about solute transport arrival time or travel time, and it uses the Eulerian Approach → fixed location monitoring the solute as it passes by.


C/C_0
1
$C(t)/C_0$
τ_1
τ_b
τ_2
time

Solute Transport Characteristics

1. Total Mass-- Zeroth Moment

    Nonreactive solutes = mass in solution

    Reactive solutes mass in all rel. phases

    Provides mass balance

2. Center of Mass-- [Mean; First Moment]

    Describes mean position of solute mass

    Center of mass vs. time velocity

3. Spread-- [Standard deviation; Second Moment]

    Describes spread of solute mass

4. Asymmetry-- [Third Moment]

    Describes degree of symmetry of solute distribution(e.g., "bell shaped"?)

These are used for both plumes (spatial moments) and breakthrough curves (temporal moments)

Moment Analysis

- Moment analysis can be used for both spatial (C varies in x)and temporal (C varies in t) solute concentration distributions.
- 1D Spatial Moments:
- Absolute
- nth (general) =

$$M_n = \int C x^n dx \cong \sum \bar{C} x^n \Delta x$$

- 0th (total mass) =
- 1st (center of mass) =
- 2nd (spread of plume) =

Moment Analysis

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- 1D Spatial Moments:
- Absolute
- nth (general) = $$M_n = \int C x^n dx \cong \sum \overline{C} x^n \Delta x$$
- 0th (total mass) = $$M_0 = \int C dx \cong \sum \overline{C} \Delta x$$
- 1st (center of mass) = $$M_1 = \int C x dx \cong \sum \overline{C} x \Delta x$$
- 2nd (spread of plume) = $$M_2 = \int C x^2 dx \cong \sum \overline{C} x^2 \Delta x$$

Moment Analysis

- Moment analysis can be used for both spatial (C varies in x)and temporal (C varies in t) solute concentration distributions.
- 1D Spatial Moments:
- nth (general) = $$M_n = \int Cx^n dx \cong \sum \bar{C} x^n \Delta x$$
- 0th (total mass) = $$M_0 = \int C dx \cong \sum \bar{C} \Delta x$$
- 1st (center of mass) = $$M_1 = \int Cx dx \cong \sum \bar{C} x \Delta x$$
- 2nd (spread of plume) = $$M_2 = \int Cx^2 dx \cong \sum \bar{C} x^2 \Delta x$$
- M_0 = the total mass in the system
- M_1Normal = mean location of the plume (center of mass location)
- M_2Central = spread of concentration away from the center of mass
- Moment accuracy decreases with increasing order, but the 3rd moment is asymmetry.

Moment Analysis

- *Normalized* (always divide by 0th moment M_0)

- nth (general) = $$\mu_n' = \frac{M_n}{M_0} = \frac{\int C x^n dx}{\int C dx} \cong \frac{\sum \bar{C} x^n \Delta x}{\sum \bar{C} \Delta x}$$

- - an example of normal moment is plume's mean velocity (1st moment):

- *Central* (centered on the mean) = mean location of the plume (center of mass location)

- nth (general) $$\mu_n = \frac{\int C(x-\mu_1')^n dx}{\int C dx} \cong \frac{\sum \bar{C}(x-\mu_1')^n \Delta x}{\sum \bar{C} \Delta x}$$

- -an example of central moment is statistical variance (2nd central moment)

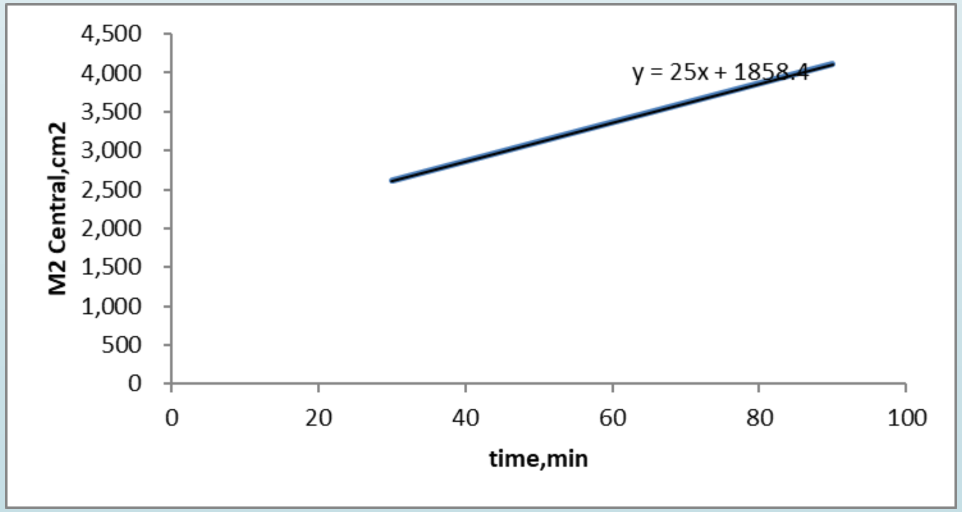
Moment Analysis

- -an example of central moment is statistical variance (2nd central moment)

$$\mu_2 = \frac{\int C(x-\mu_1')^2\,dx}{\int C\,dx} \cong \frac{\sum \overline{C}(x-\mu_1')^2\,\Delta x}{\sum \overline{C}\Delta x}$$

- Also $\mu_2 = 2Dt$ or $\frac{d\mu_2}{dt} = 2D$

- Where D is a term called a dispersion coefficient that describes the spreading of a plume, which we will discuss in detail.



Moment Analysis

- Temporal Moments:

  M_0 = the total mass transported passed monitoring location

  M_1 Normal = mean arrival time of the plume (center of mass arrival time)

  M_2 Central = variability in arrival times about the mean arrival time

  Moments may also be derived for 2D and 3D analysis.

  t(arrival) = M_1 normal

  t(travel) = t(arrival)-0.5t_0

  Pulse width = t_0 = t (stop injection)-t(start injection)

  Average injection time = [t(stop injection)-t(start injection)]/2

IDEAL SOLUTE TRANSPORT

Major Assumptions:

- Homogeneous Porous Media
- Instantaneous Mass Transfer, Reactions
- First-order Transformation

Transport Behavior--Spatial:

- First Moment: constant velocity
- Second Moment: small degree of spreading
- Third Moment: symmetrical

Transport Behavior--Temporal:

- First Moment: inflection point = first moment
- Second Moment: small degree of spreading
- Third Moment: symmetrical (no tailing)

NON-IDEAL SOLUTE TRANSPORT

Major Causes:

- Heterogeneous Porous Media
- Structured Porous Media
- Rate-Limited Mass Transfer, Reactions
- Non-Linear Partitioning
- Non-First-order Transformation
- Facilitated Transport
- Non-Uniform Gradients

Transport Behavior--Spatial:

- First Moment: non-constant velocity
- Second Moment: large degree of spreading
- Third Moment: asymmetrical

Transport Behavior-- Temporal:

- First Moment: inflection point $\neq$ first moment
- Second Moment: large degree of spreading
- Third Moment: asymmetrical (tailing)

BASIC TRANSPORT PARAMETERS

1. Normalized Concentration [C/C_0]

   C = measured concentration

   C_0 = influent or resident concentration

2. Normalized Distance [X]

   $X = x/L$

   x = distance

   L = system length

3. Normalized Time [T]

   "Hydraulic Residence Time" or "Pore Volume"

   $T = tv/L$

   t = time

   v = average pore-water velocity

   L = system length

$$HRT: T = \left[\frac{time}{residence\_time}\right] = \frac{t}{L/v} = \frac{tv}{L}$$

$$PV: T = \left[\frac{disch\arg e}{capacity}\right] = \frac{Qt}{ALn} = \frac{vnAt}{ALn} = \frac{tv}{L}$$

Processes

1. Advection: transport due to movement of fluid in response to fluid-potential gradient

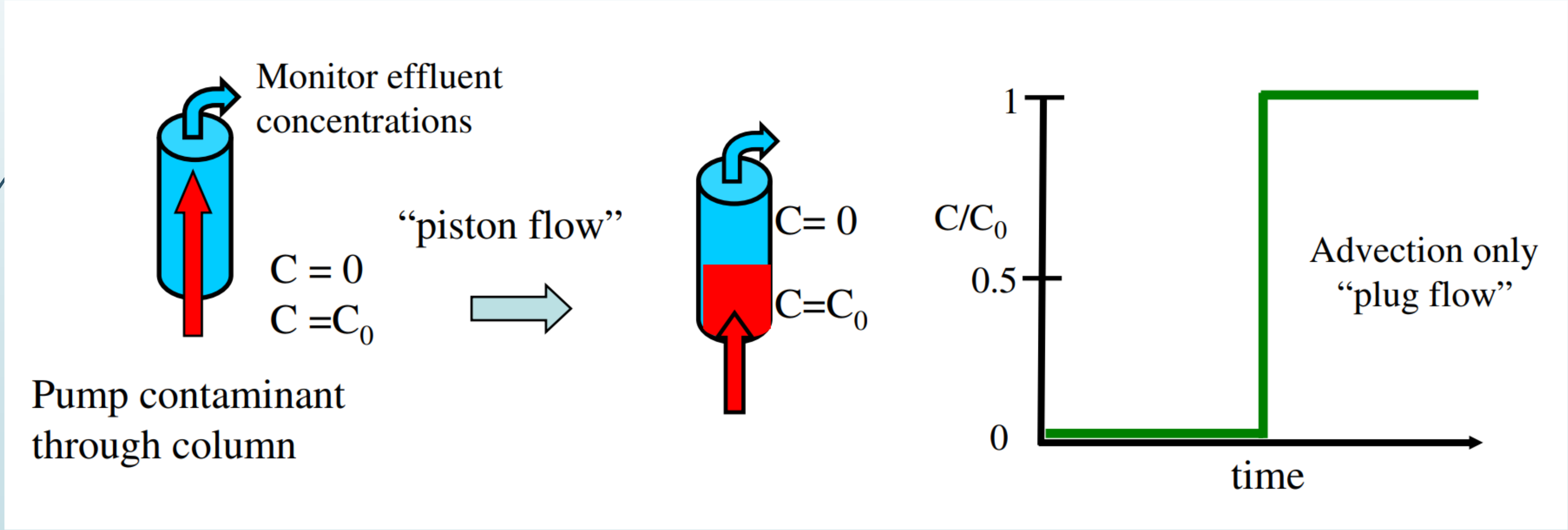
2. Dispersion or Spreading: transport due to non-uniform flow fields and Molecular diffusion

3. Reactions: Mass-transfer and transformation processes

Solute Transport – Advection Only

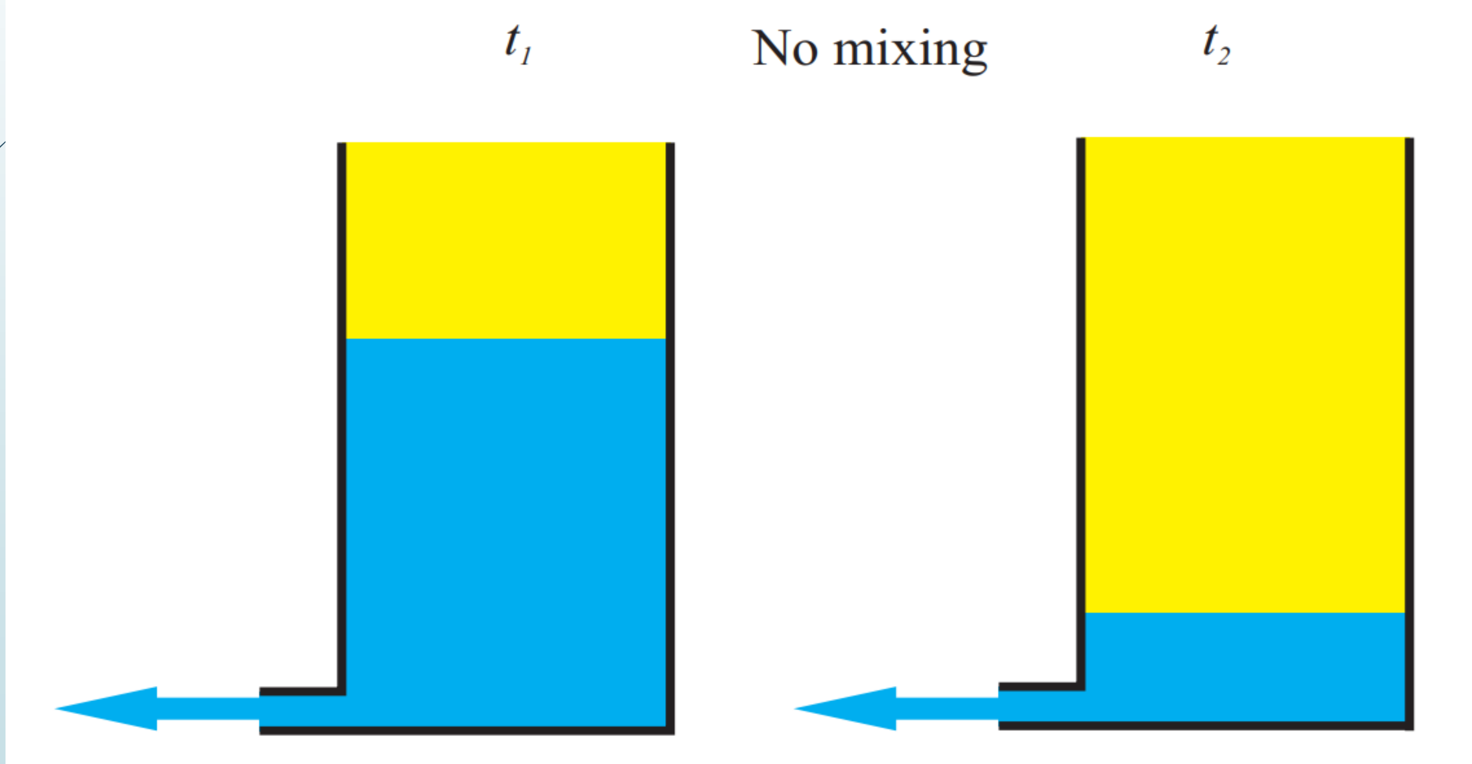
One-dimensional Column Experiments

(monitoring concentrations at one point over time)



Solute Transport – Advection Only

An illustration of piston displacement without mixing



CAUSES OF DISPERSION

1. Microscopic:

Axial Diffusion {concentration gradient}

Mechanical Mixing {pore-size variations}

Boundary-Layer Mass Transfer {water films}

2. Macroscopic:

Structured Porous Media {aggregation, fractures, "macropores"}

Discontinuous Fluid Saturation

3. Megascopic:

Heterogeneous Porous Media(Hydraulic-conductivity variability}

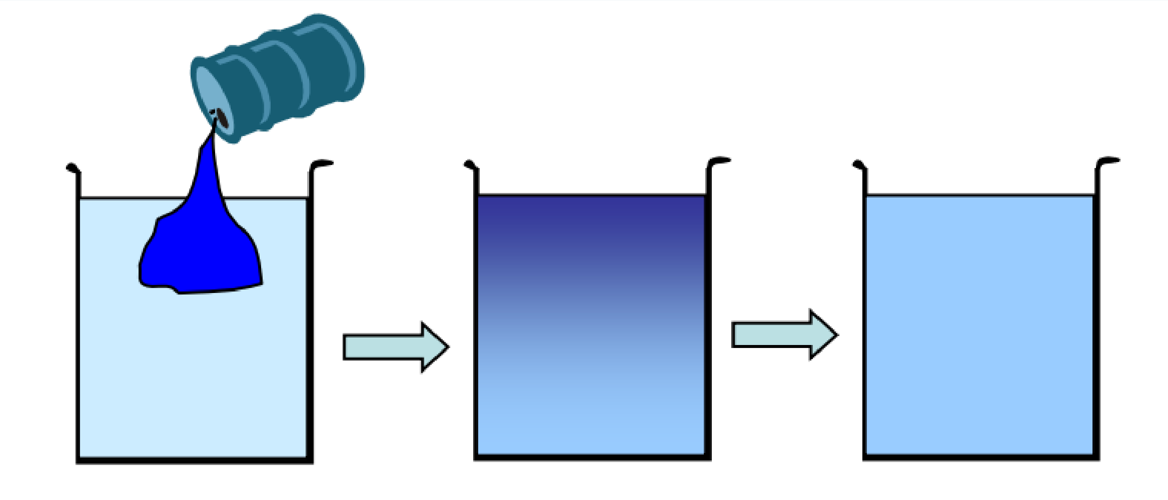
CAUSES OF DISPERSION

FACTORS INFLUENCING DEGREE OF DISPERSION

1. Porous-Media Characteristics:
   - Particle-size Distribution
   - Structure
   - Heterogeneity
2. Solute Characteristics:
   - Size
   - Reactivity
3. System Conditions:
   - Pore-Water Velocity
   - Saturation

Molecular Diffusion

- From higher to lower concentration



Net movement of solute from high concentration to low concentration domain until equilibrium is reached (uniform distribution).

Diffusion

- Random molecular motion
- Kinetic energy- $E_k = \frac{1}{2} m v^2$

    -m = mass of molecule

    -v = velocity of molecule

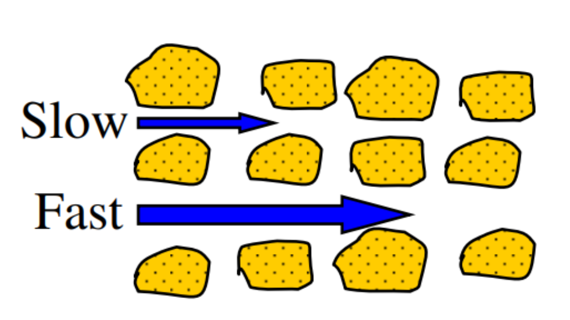
    E_k same for all solutes (given Temp)

Therefore, for larger solutes, v(and D_o)is smaller

Mechanical Mixing

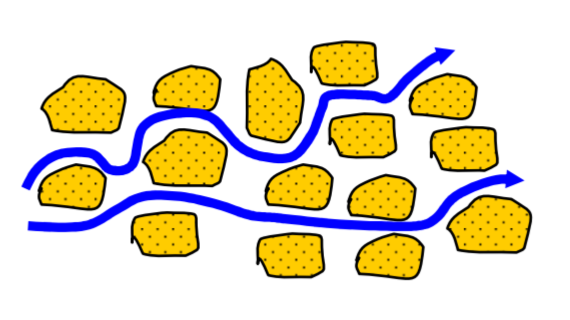
- AKA Hydrodynamic Dispersion
- For microscopic scale- due to pore-scale heterogeneity of porous medium, which leads toa spatially variable flow field, which causes ratesof advection to be spatial variable (i.e.,distribution of travel times)
- Primary axis of heterogeneity is across cross-section normal to mean direction of flow and transport

Mechanical Mixing



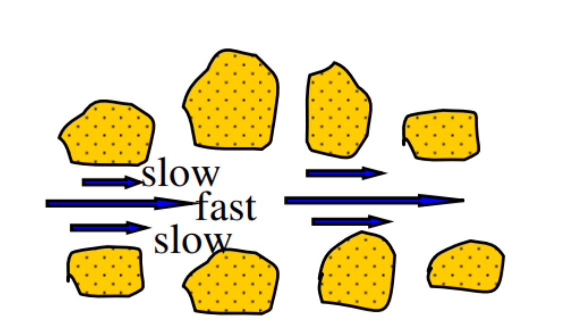
Pore Size

- larger pore diameter = higher velocities
- smaller pore diameter = lower velocities



Path Length

- long path lengths = more time to travel a given distance
- short path lengths less time to travel a given distance



Friction in Pore

more friction next to grain = slower velocity

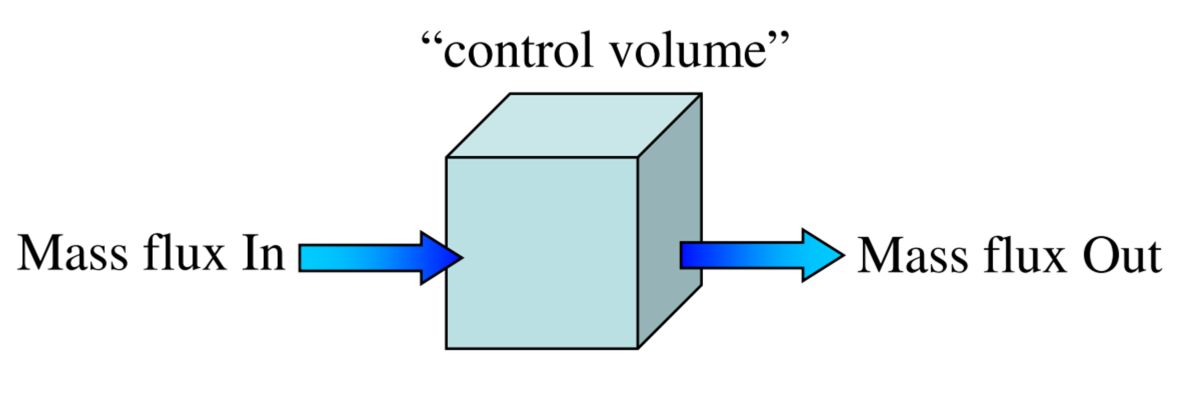
less friction in center of pore = higher velocity

Developing the Advection-Dispersion Equation

- AKA Convection-Dispersion
- Most widely used equation for solute transport
- Initial focus on physical processes-"non-reactive“ solute

Solute transport

- Continuum Approach
- Mass Balance Conducted on a Control Element



Change in Solute Mass = $\text{Mass}_{out} - \text{Mass}_{in} \pm$ Sink/Source
Mass Flux = Advection + Dispersion + Reactions
Non-reactive solute = No Reactions

Advection

- Solute Mass (M) = Fluid Volume (V) × Concentration (C)

  [C = Mass/ Fluid Volume; e.g., mg/L]
- Total Mass Flux = Fluid Discharge (Q) × C [MT^{-1}]
- Mass Flux (J_a) = QC/Area = qC [$MT^{-1}L^{-2}$]

$$\boxed{J_a = qC}$$

Dispersion

- Fick's First Law

$$\boxed{J_d = -D\theta \frac{\partial C}{\partial x}}$$

- D = Dispersion Coefficient [L^2T^{-1}; e.g., cm^2/s]
- θ = volumetric water content (porosity)

Dispersion

- Fick's Second Law

  For system where the concentration are changing with time:

$$\boxed{\frac{\partial C}{\partial t} = -D\,\frac{\partial^2 C}{\partial x^2}}$$

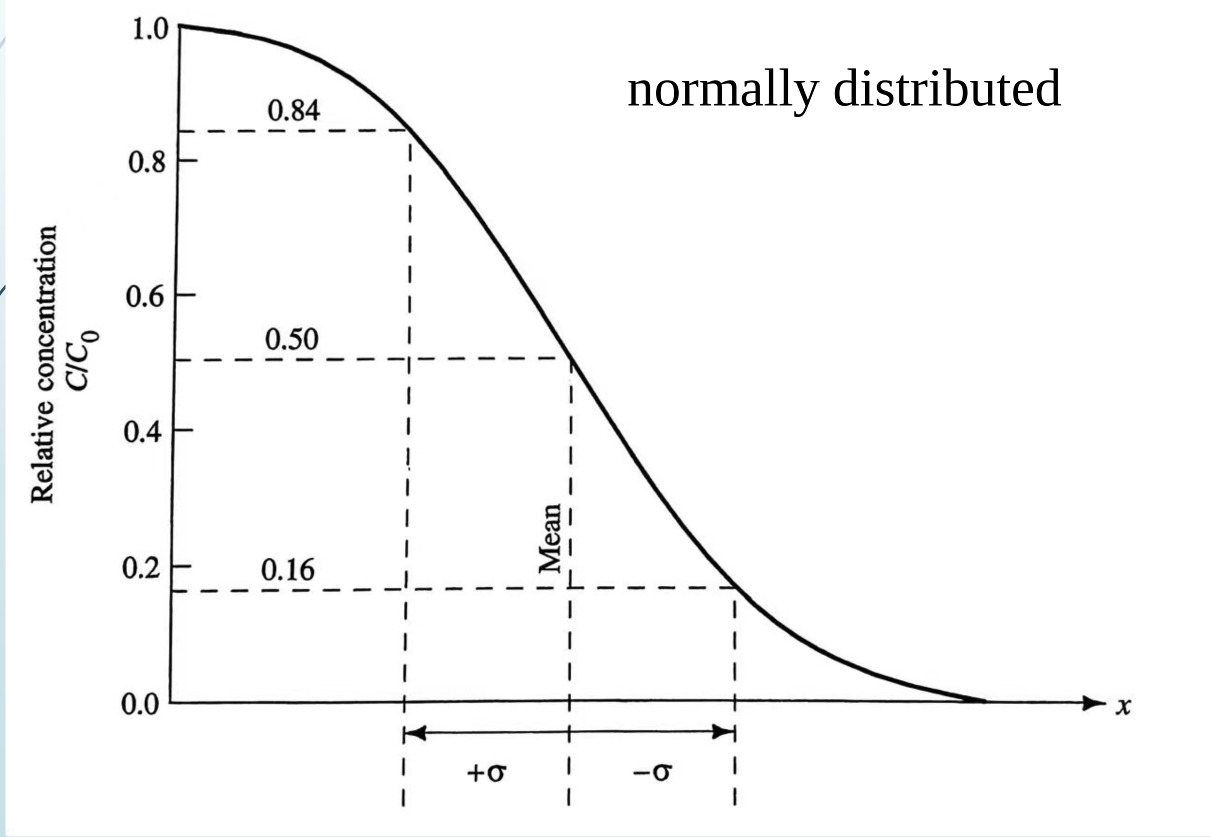
- Diffusion only, constant source C_0,

$$\boxed{C_i(x,t) = C_0 erfc\,\frac{x}{2(D_d t)^{0.5}}}$$

- C_i = the concentration at distance x from the source at time t since diffusion began
- erfc = the complementary error function

Dispersion

- Fick's Second Law



- 84% of the values will be less than the value that is one standard deviation more than the mean
- 16% of the values will be less than the value that is one standard deviation less than the mean.
- The standard deviation is the square root of the variance.

Dispersion

$$erf(x) = \sqrt{1 - \exp\left(\frac{-4x^2}{\pi}\right)}$$

30. The error function is defined as:

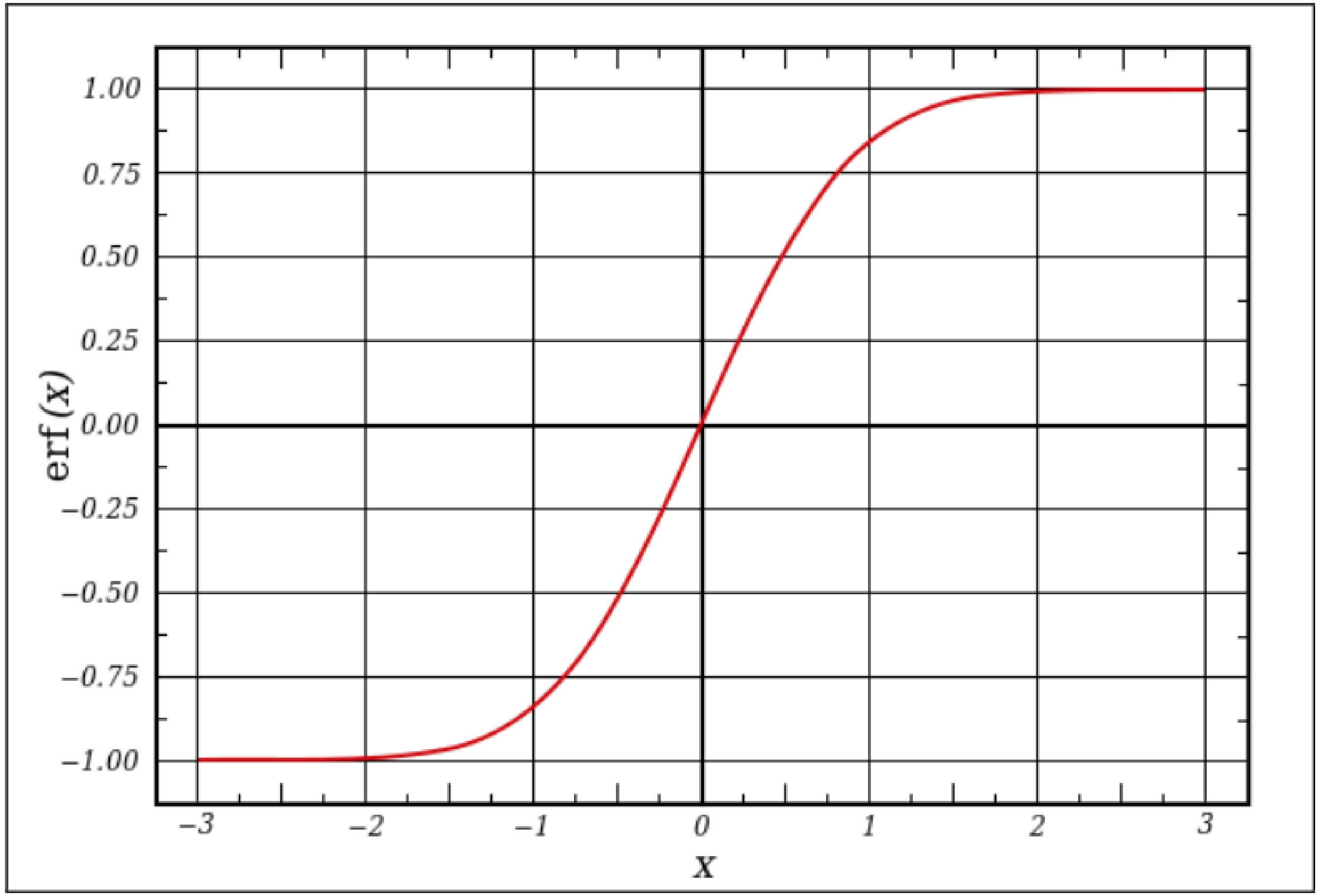
$$erf(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt$$

The complementary error function, denoted $erfc$, is defined as:

$$erfc(x) = 1 - erf(x)$$

- Draw $erf(x)$ and $erfc(x)$.
- Show that

$$erfc(x) = \frac{2}{\sqrt{\pi}} \int_x^\infty e^{-t^2} dt$$



EXAMPLE PROBLEM

Assume a D_d of $5 * 10^{-10}$ m^2/sec. Find the value of the concentration ratio, C_i/Co, at a distance of 5 m after 100 yr of diffusion.

$$\boxed{C_i(x,t) = C_0 erfc \frac{x}{2(D_d t)^{0.5}}}$$

Dispersion

- Fick's Second Law

  For system where the concentration are changing with time:

$$\boxed{\frac{\partial C}{\partial t} = -D\theta \frac{\partial^2 C}{\partial x^2}}$$

- D = Dispersion Coefficient [L^2T^{-1}; e.g., cm^2/s]
- θ = volumetric water content (porosity)

Advective-Dispersive Flux

- A-D Flux ($J_{a\text{-}d}$) = $J_a + J_d$

$$\boxed{J_{a-d} = qC - D\theta \frac{\partial C}{\partial x}}$$

Solute Transport Equation

- A-D Flux ($J_{a\text{-}d}$) = J_a + J_d

$$\frac{\partial C\theta}{\partial t} = -\frac{\partial J_{a-d}}{\partial x}$$

- Substitute

$$\frac{\partial C\theta}{\partial t} = \frac{\partial}{\partial x}\left[-qC + D\theta\frac{\partial C}{\partial x}\right]$$

- Expand Concentration and Flow Terms

$$\theta(t)\frac{\partial C}{\partial t} + C\frac{\partial \theta}{\partial t} = -q(x)\frac{\partial C}{\partial x} - C\frac{\partial q}{\partial x} + \frac{\partial}{\partial x}\left[D\theta\frac{\partial C}{\partial x}\right]$$

IDEAL CONDITIONS

- Assume Homogeneous Porous Medium [K, D = constant]

$$\theta\frac{\partial C}{\partial t} + C\frac{\partial \theta}{\partial t} = -q\frac{\partial C}{\partial x} - C\frac{\partial q}{\partial x} + D\theta\frac{\partial^2 C}{\partial x^2}$$

- For Steady State Fluid Flow and Incompressible Fluid

$$\frac{\partial \theta}{\partial t} = \frac{\partial q}{\partial x} = 0$$

- Simplify

$$\theta\frac{\partial C}{\partial t} = -q\frac{\partial C}{\partial x} + D\theta\frac{\partial^2 C}{\partial x^2}$$

- Rearrange(θ) and Substitute v=q/θ:

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

Non-Dimensional Transport Equation

- Divide by C_0, v; multiply by L:

$$\frac{\partial C/C_0}{\partial t}\frac{L}{v} = -\frac{v}{v}\frac{\partial C/C_0}{\partial x/L} + \frac{D}{vL}\frac{\partial^2 C/C_0}{\partial x^2/L^2}$$

- Substitute non-dimensional parameters:

$$\frac{\partial C*}{\partial T} = -\frac{\partial C*}{\partial X} + \frac{1}{P}\frac{\partial^2 C*}{\partial X^2}$$

- Where $C^*=C/C_0$

  X=x/L

  P=vL/D

$$T = -\frac{tv}{L}[\frac{t}{L/v}][\frac{Qt}{AL\theta} = \frac{v\theta At}{AL\theta} = \frac{vt}{L}]$$

Boundary and Initial Condition

- The initial conditions describe the values of the variable under consideration, in this case concentration, at some initial time equal to 0.
- The boundary conditions specify the interaction between thearea under investigation and its external environment.
- Three types of boundary conditions for mass transport:

  the first type : a fixed concentration (Dirichlet)

  the second type : a fixed gradient (Neumann)

  the third type : a variable flux boundary (Cauchy)

Boundary and Initial Condition

For one-dimensional flow :

$C(x, t) = C(t)$ where $C(t)$ is some known function.

For example

$C(0, t) = Co, t>0$ first-type boundary

$C(x, 0) = 0, x>0$ initial condition

$C(\infty, t) = 0, t\geq 0$ first-type boundary condition at $x = \infty$

Boundary and Initial Condition

$C(x,0)= C_i$, $x \geq 0$ initial condition with concentration of C_i

Exponential decay of the source term and pulse loading at a constant concentration for a period of time followed by another period of time with a different constant concentration.

Exponential decay for the source term : $C(0, t) = C_o e^{-it}$

Pulse loading:

$C(0, t) = C_o \qquad 0<t\leq t_0$

$C(0, t) = 0 \qquad t> t_0$

Boundary and Initial Condition

Fixed-gradient boundaries:

$$\left.\frac{dC}{dx}\right|_{x=0} = f(t) \quad \text{or} \quad \left.\frac{dC}{dx}\right|_{x=\infty} = f(t)$$

The variable-flux boundary, a third type:

$$-D\frac{\partial C}{\partial x} + v_x C = v_x C(t)$$

C(t) is a known concentration function

A common fixed-gradient condition:

$$\left.\left(-D\frac{\partial C}{\partial x} + v_x C\right)\right|_{x=0} = C_0$$

Analytical Solution

- One-Dimensional Step Change in Concentration (First Type Boundary)

Initial condition C(x, 0) = 0, x > 0

Boundary condition C(0, t) = Co, t ≥ 0

C(∞, t) = 0, t≥0

Solution: $$C = \frac{C_0}{2}\left[erfc\left(\frac{L - v_x t}{2\sqrt{D_L t}}\right) + \exp\left(\frac{v_x t}{D_L}\right) erfc\left(\frac{L + v_x t}{2\sqrt{D_L t}}\right)\right]$$

in dimensionless form:

$$C_R(t_R, P_e) = 0.5\left\{erfc\left[\left(\frac{P_e}{4t_R}\right)^{1/2} \cdot (1 - t_R)\right] + \exp(P_e)\, erfc\left[\left(\frac{P_e}{4t_R}\right)^{1/2} \cdot (1 + t_R)\right]\right\}$$

Analytical Solution

- One-Dimensional Continuous injection into a Flow Field

(Second Type Boundary)

Initial condition C(x, 0) = 0, -∞ < x < +∞

Boundary condition $\int_{-\infty}^{+\infty} n_e C(x,t)dx = C_0 n_e v_x t, t \geq 0$

C(∞, t) = 0, t≥0

Solution:

$$C = \frac{C_0}{2}\left[erfc\left(\frac{L - v_x t}{2\sqrt{D_L t}}\right) - \exp\left(\frac{v_x t}{D_L}\right) erfc\left(\frac{L + v_x t}{2\sqrt{D_L t}}\right)\right]$$

in dimensionless form:

$$C_R(t_R, P_e) = 0.5\left\{erfc\left[\left(\frac{P_e}{4t_R}\right)^{1/2} \cdot (1 - t_R)\right] - \exp(P_e) erfc\left[\left(\frac{P_e}{4t_R}\right)^{1/2} \cdot (1 + t_R)\right]\right\}$$

Analytical Solution

- A solution for Third-Type Boundary Condition given by van Genuchten (1981)

Initial condition $C(x, 0) = 0$

Boundary condition $\left.\left(-D\frac{\partial C}{\partial x}+v_x C\right)\right|_{x=0} = v_x C_0$ $\left.\frac{dC}{dx}\right|_{x=\infty} = f(t)$

Solution:

$$C = \frac{C_0}{2}\left[\begin{array}{l} erfc\left(\frac{L-v_x t}{2\sqrt{D_L t}}\right)+\left(\frac{v_x{}^2 t}{\pi D_L}\right)^{1/2}\exp\left[-\frac{(L-v_x t)^2}{4D_L t}\right] \\ -\frac{1}{2}\left(1+\frac{v_x t}{D_L}+\frac{v_x^2 t}{D_L}\right)\exp\left(\frac{v_x t}{D_L}\right)erfc\left(\frac{L-v_x t}{2\sqrt{D_L t}}\right)\end{array}\right]$$

Sauty(1980)gives and approximation: $C = \frac{C_0}{2}\left[erfc\left(\frac{L-v_x t}{2\sqrt{D_L t}}\right)\right]$

Analytical Solution

- One-Dimensional Slug Injection into a Flow Field

  If a slug of contamination is instantaneously injected into a uniform, 1D flow filed, it will pass through the aquifer as a pulse with a peak concentration C_{max} at t_{max}

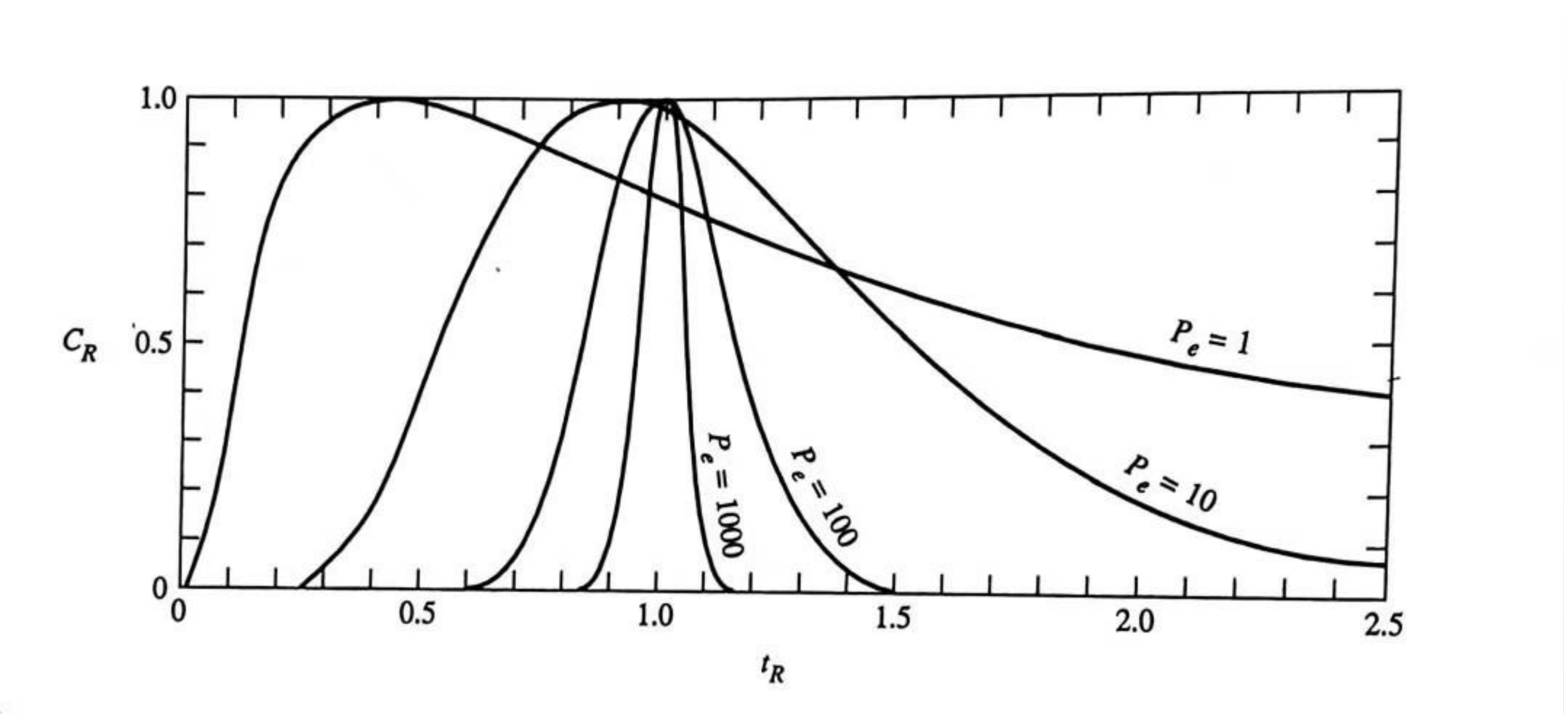
Solution (Sauty 1980): $$C_R(t_R, P_e) = \frac{E}{(t_R)^{1/2}} \exp\left(-\frac{P_e}{4t_R}(1-t_R)^2\right)$$

with $$E = (t_{R\max})^{1/2} \cdot \exp\left(\frac{P_e}{4t_{R\max}}(1-t_{R\max})^2\right)$$

where $t_{R\max} = (1+P_e^{-2})^{1/2} - P_e^{-1}$ (dimensionless time peak occurs)

$$t_{R\max} = (1+P_e^{-2})^{1/2} - P_e^{-1}$$

Analytical Solution

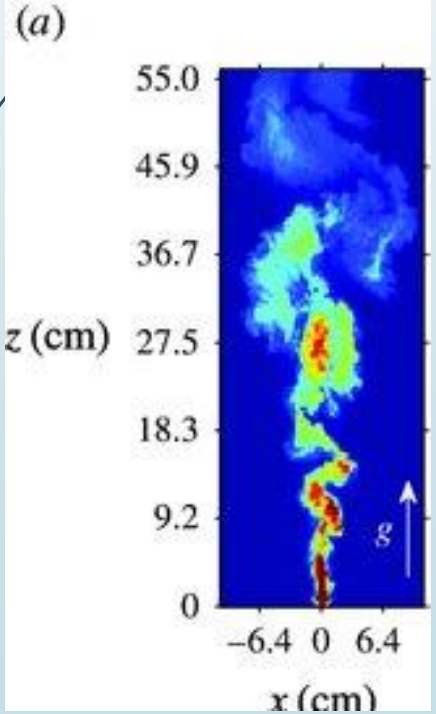


$C_R(C/C_{max})$ for a slug injected into a uniform one-dimensional flow field plotted against dimensionless time, t_R, for several Peclet numbers. it can be seen that the time for the peak concentration (Cmax) to occur increases with the Peclet number, up to a limit of t_R 1. Breakthrough becomes more symmetric with increasing Pe.

Analytical Solution

- Continuous Injection into a Uniform 2D Flow Field

  If a tracer is continuously injected into a uniform flow field from a single point that fully penetrates the aquifer, a two-dimensional plume will form.



It will spread along the axis of flow due to longitudinal dispersion and nor-mal to the axis of flow due to transverse dispersion.

This is the type of contamination that would spread from the use of an injection well, which would be a point source.

Analytical Solution

- One-Dimensional Slug Injection into a Flow Field

  The well is located at the origin (x=0, y=0), and there is a uniform flow velocity at a rate v_x, parallel to the x axis. There is a continuous injection at the origin, of a solute with a concentration Co at a rate Q over the aquifer thickness, b.

  Solution for unit injection : $C(x,y,t)=\frac{1}{4\pi t(D_L D_T)^{1/2}}\exp\left(-\frac{(x-v_x t)^2}{4D_L t}-\frac{y^2}{4D_T t}\right)$

  (Bear, 1972; Fried, 1975)

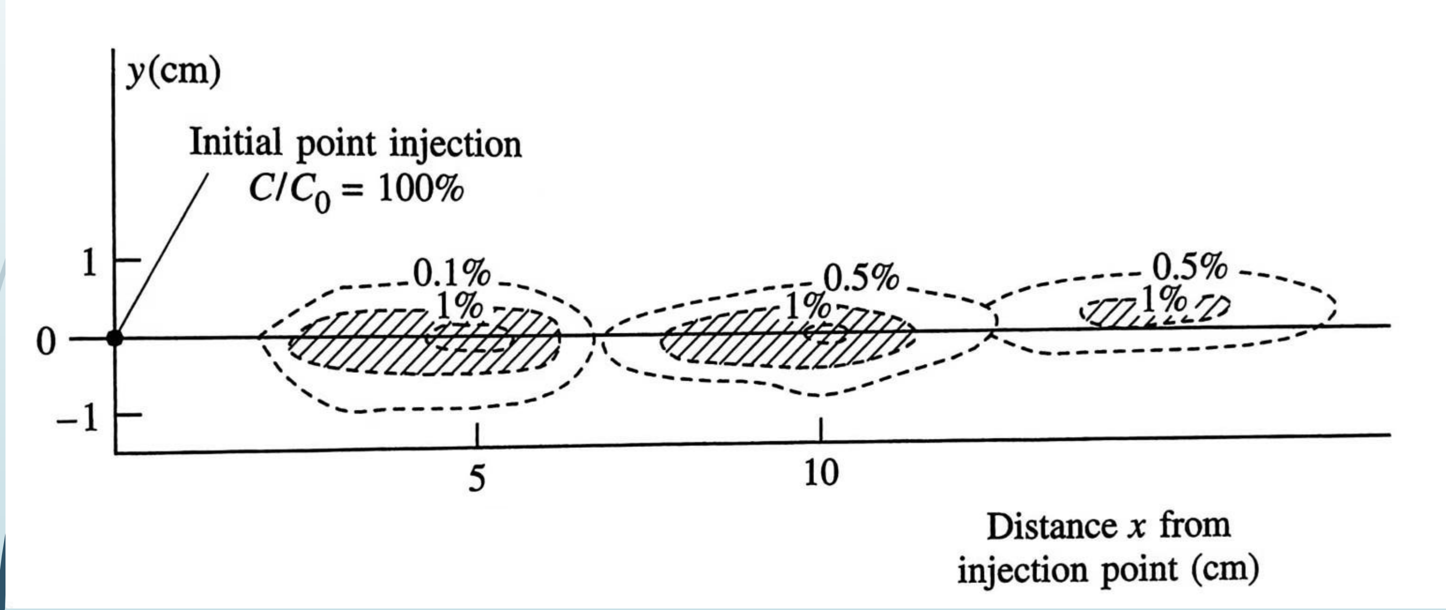
  Solution- injection rate $C_0(Q/b)$: $C(x,y,t)=\frac{C_0(Q/b)dt}{4\pi t(D_L D_T)^{1/2}}\exp\left(-\frac{(x-v_x t)^2}{4D_L t}-\frac{y^2}{4D_T t}\right)$

  Steady state when time approaches infinity

$$C(x,y)=\frac{C_0(Q/b)}{4\pi(D_L D_T)^{1/2}}\exp\left(\frac{v_x x}{2D_L}\right)K_0\left[\left(\frac{v_x{}^2}{4D_L}\left(\frac{x^2}{D_L}-\frac{y^2}{D_T}\right)\right)^{1/2}\right]$$

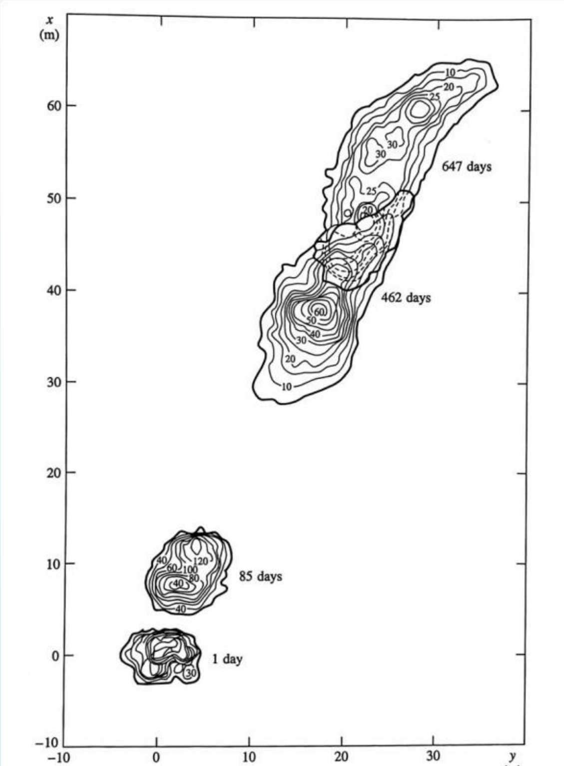
Analytical Solution

- a slug of contamination is injected over the full thickness of a two-dimensional uniform flow field in a short period of time, it will move in the direction of flow and spread with time.



the pattern of contamination at three increments that result from a one-time spill

Bear (1961)



The spread of a plume of chloride that was injected into an aquifer as a part of a large-scale field test (Mackay et al. 1986)

Analytical Solution

- If a tracer with concentration Co is injected into a two-dimension-al flow field over an area A at a point (xo, yo), the concentration at a point (x, y), at time t after the injection is

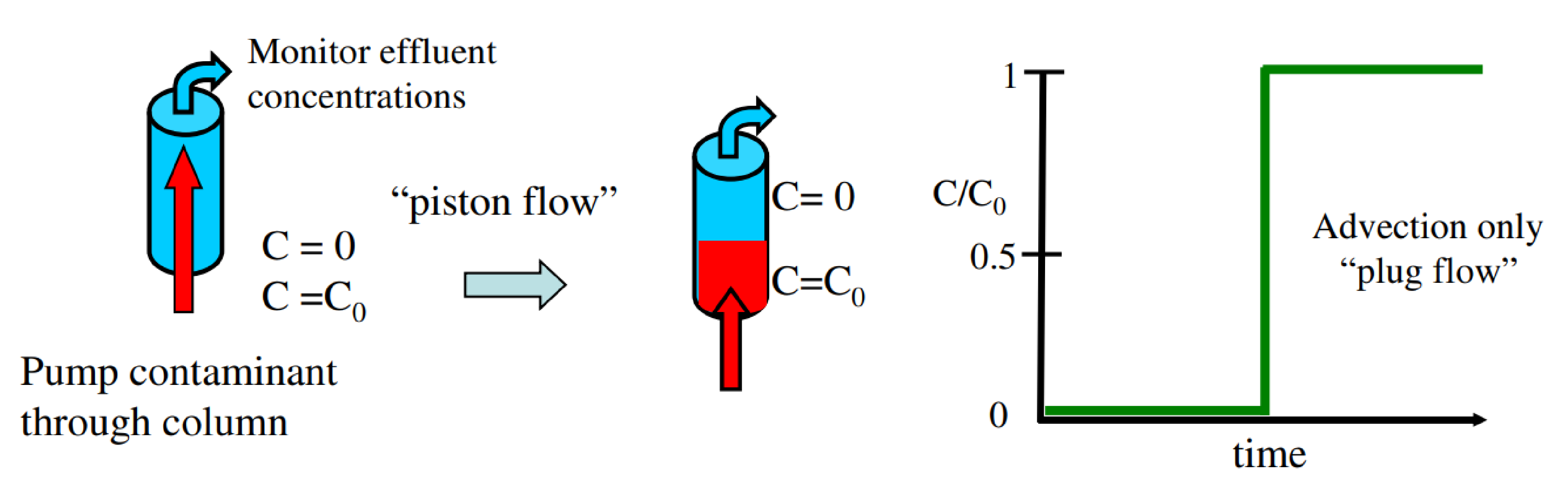
$$C(x,y,t) = \frac{C_0 A}{4\pi t (D_L D_T)^{1/2}} \exp\left(-\frac{((x-x_0)-v_x t)^2}{4D_L t} - \frac{(y-y_0{}^2}{4D_T t} \right)$$

Solute Transport – Advection Only

One-dimensional Column Experiments

(monitoring concentrations at one point over time)

$$\boxed{\frac{\partial C}{\partial t} = -v\frac{\partial C}{\partial x}}$$



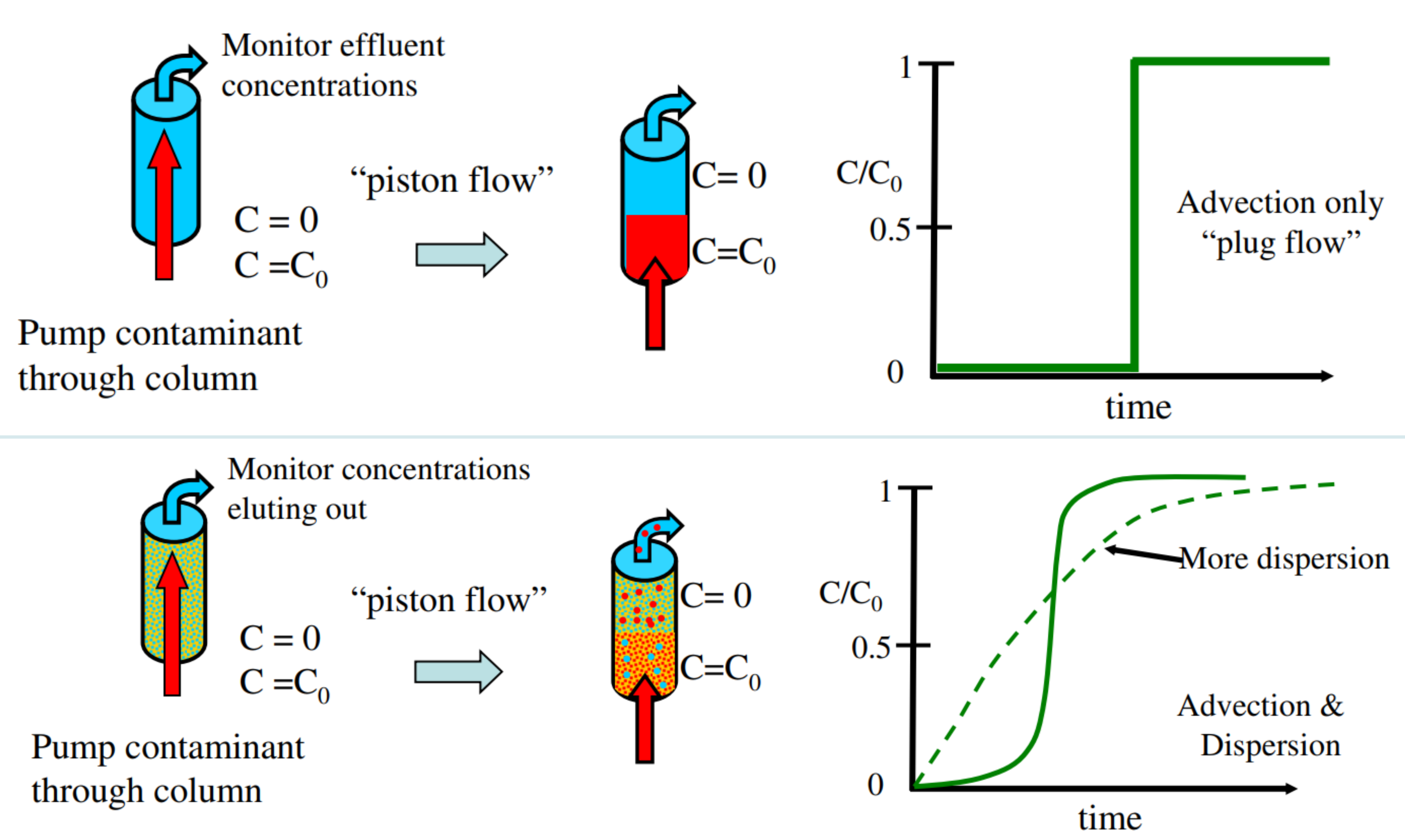
Advection

- Dissolved nitrate in a concentration of 18.0 mg/L is being advected with flowing groundwater at a velocity of 0.331 m/day in an aquifer with a porosity of 0.225. Groundwater from the aquifer discharges into a stream. What is the mass flux of nitrate into the stream if the aquifer is 1.80 m thick and 123 m wide where it discharges into the stream?
  - Q= J_a*Area

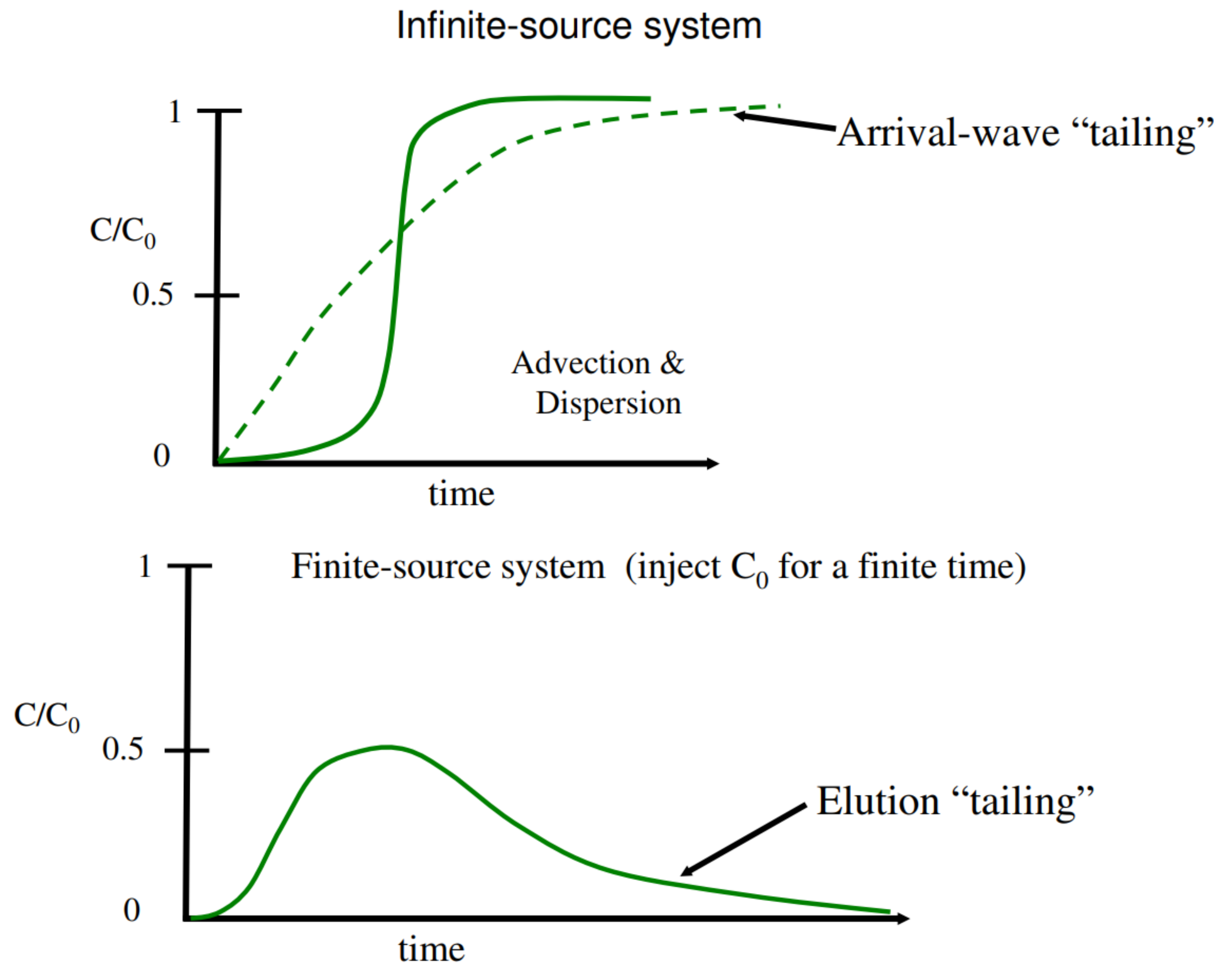
$$\boxed{J_a = qC}$$

Impact of Dispersion on Transport

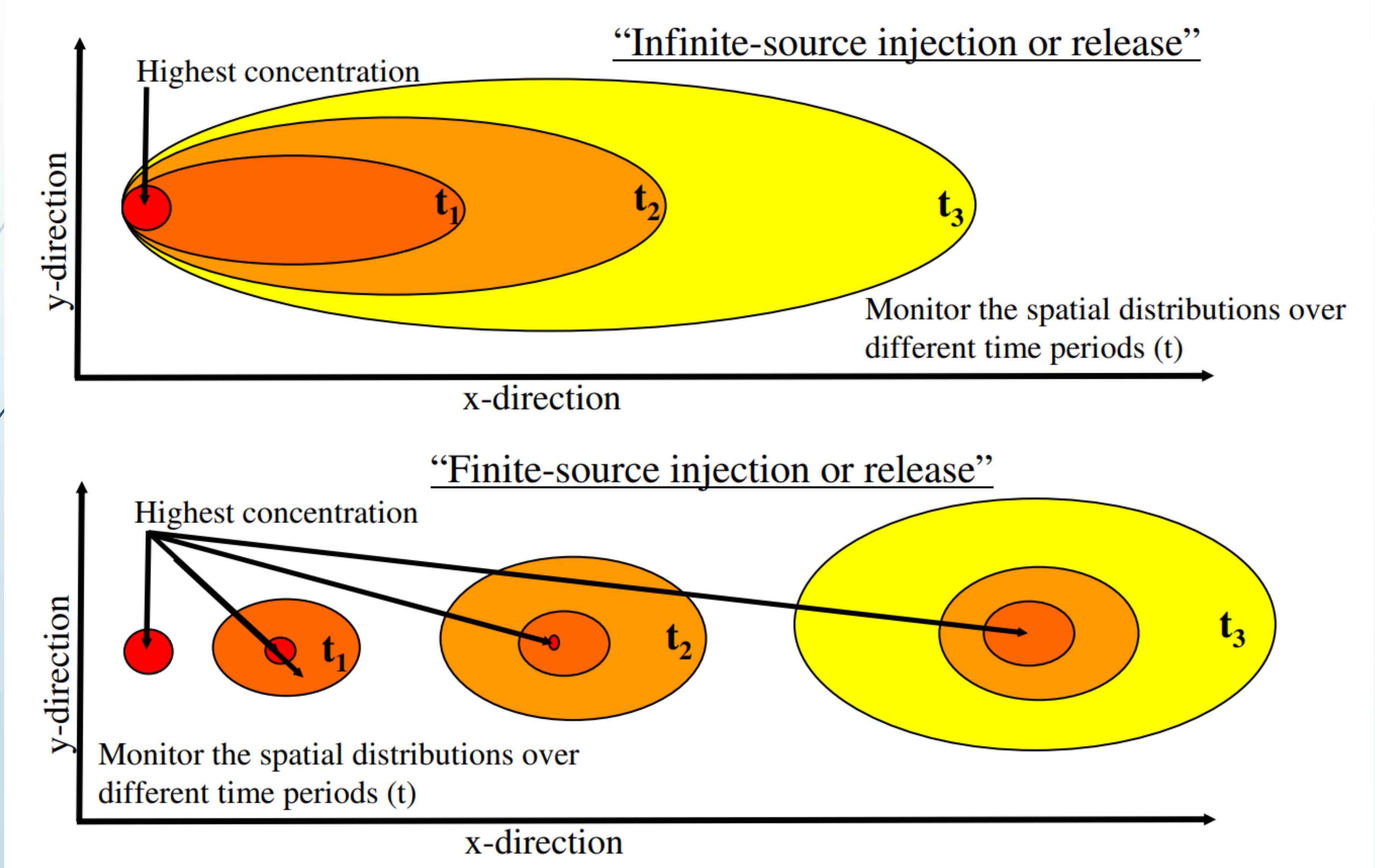
One-dimensional Column Experiments (monitoring concentrations at one point over time)



Arrival wave v.s. Elution wave v.s. full BTC



Two-dimensional Contaminant “Plumes” (map view)



Dispersion Coefficient

Dispersion Coefficient (D) Components = axial (molecular) diffusion and mechanical mixing

$$D = \frac{D_o}{\tau} + \alpha_L v^n$$

Dispersion Coefficient

Diffusion coefficient in porous medium:

$$D_d = \frac{D_o}{\tau}$$

D_o = Diffusion coefficient in bulk fluid [~10^{-5}cm^2/s in water]

τ = Tortuosity factor (>1)——— typically 1.3-2

Note: some use the form $D_d = D_o * \tau$, in this case $\tau < 1$

Dispersion Coefficient

Mechanical Mixing

$$D_m = \alpha_L v^n$$

alpha = Dispersivity (cm)

v = Pore water velocity (cm/s)

n = Dimensionless empirical parameter (typically equals 1)

Peclet Number

Peclet number (P) = (vL)/D

The non-dimensional ratio of characteristic time of dispersion (L^2/D) and characteristic time of advection(L/v)

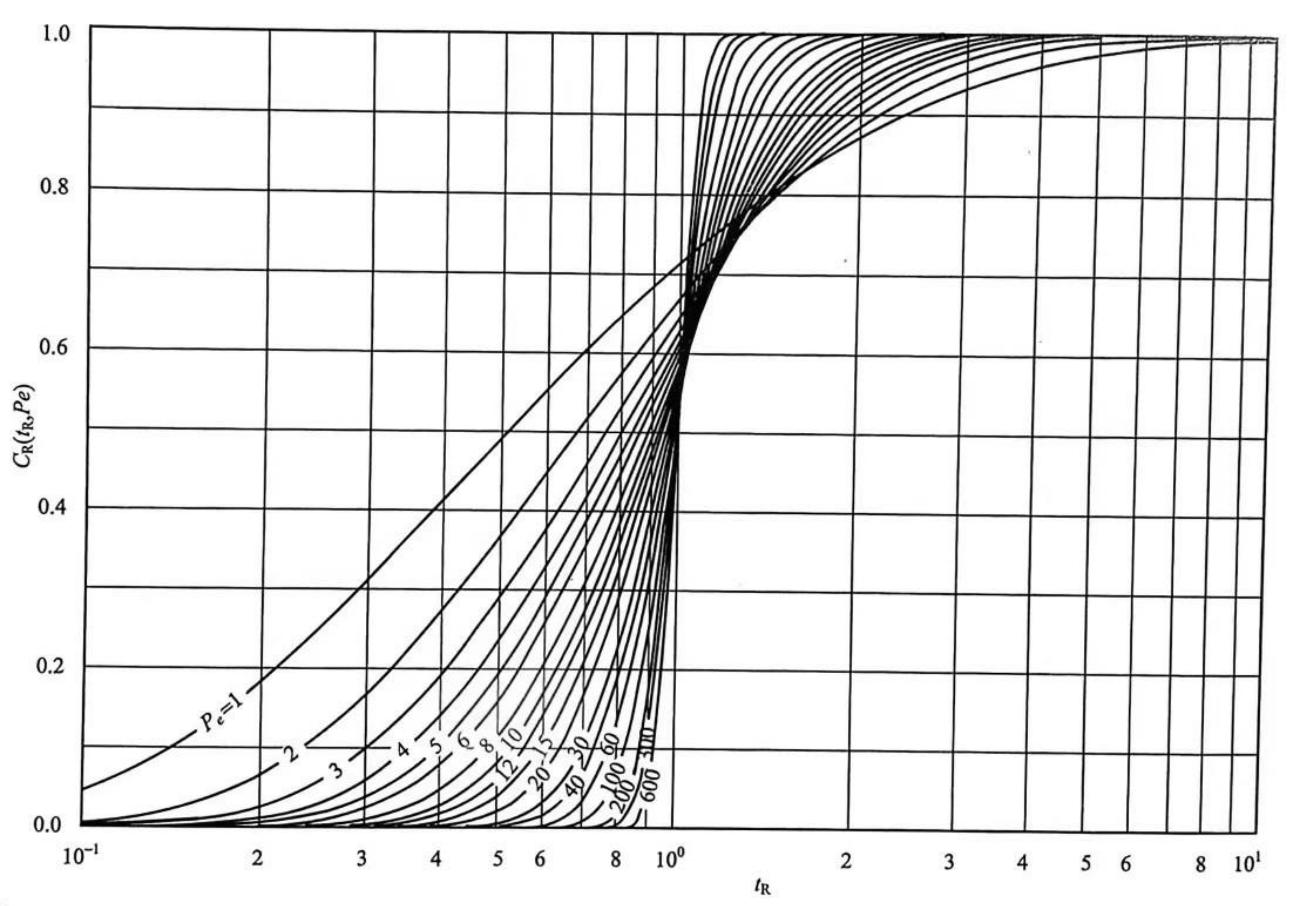
If diffusion can be neglected … $D = \alpha_L v$

And … $P = vL/D = vL/\alpha_L v = L/\alpha_L$

Value of P controls the magnitude of spreading

BRENNER SOLUTION

[Nonreactive and conservative solutes]



Dispersivity

Dispersivity is a key property used to characterize spreading component of transport

Range of Lab values: 0.01-1 cm

Magnitude of dispersivity characterizes-

length of "mixing zone“ for spatial distributions

travel-time distribution for temporal distributions

Dispersivity

Factors Influencing Dispersivity at the Microscopic Scale:

1. grain size distribution pore size distribution

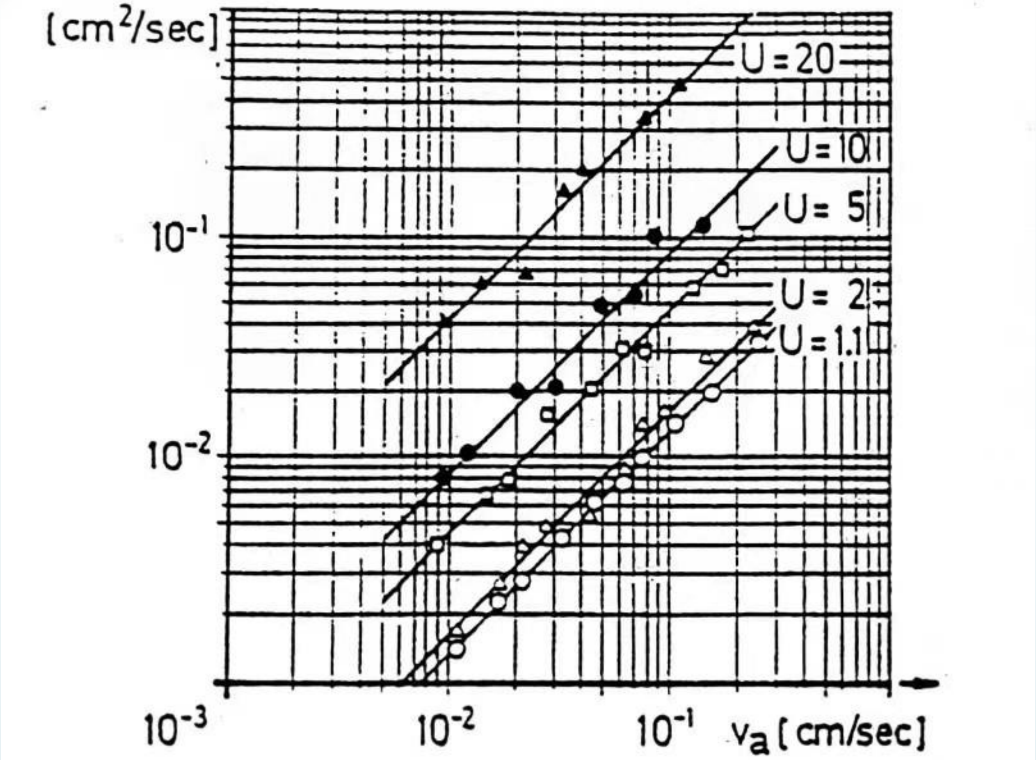
   (pore size is related to grain size)

   uniformity coefficient is a measure of the grain-size distribution

   (larger U= larger distribution... poorly sorted… well graded)

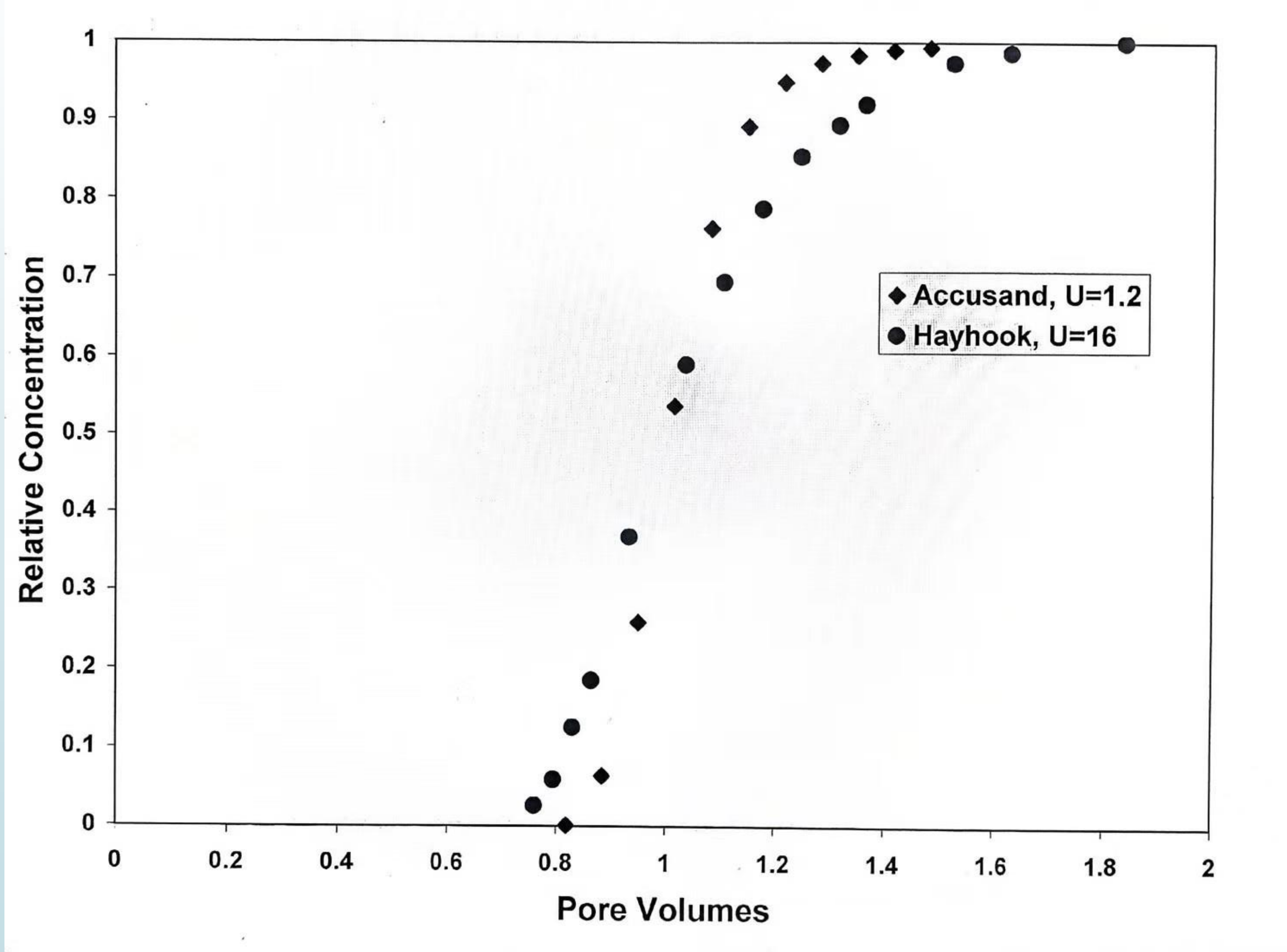
2. roughness or angularity of grains

Dispersivity

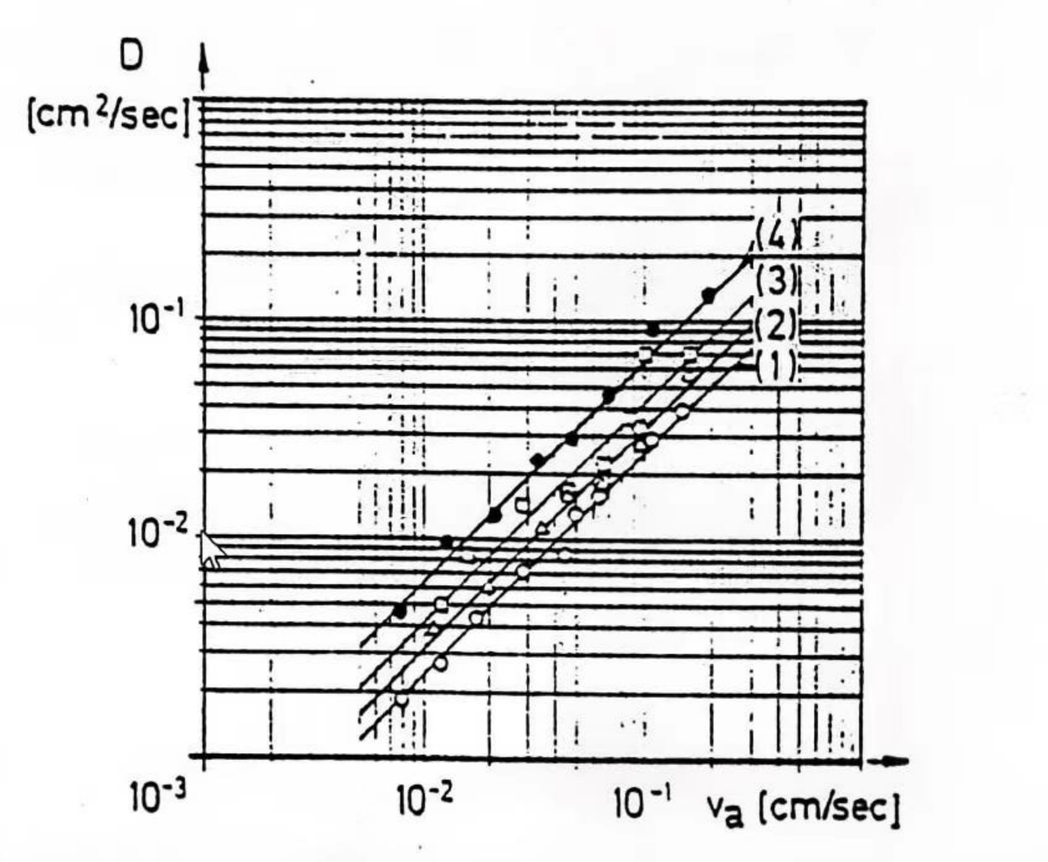


Longitudinal dispersion coefficient D in relation to distance velocity v_a for sands of effective grain diameter d_{50} = 1.0 mm with different uniformity coefficients U of grain-size distribution: total porosities: n = 0. 39 for U = 1. 1; n = 0. 33 for U = 2; n = 0. 31 for U =5; n = 0.29 for U = 10; n = 0. 28 for U = 20

Dispersivity

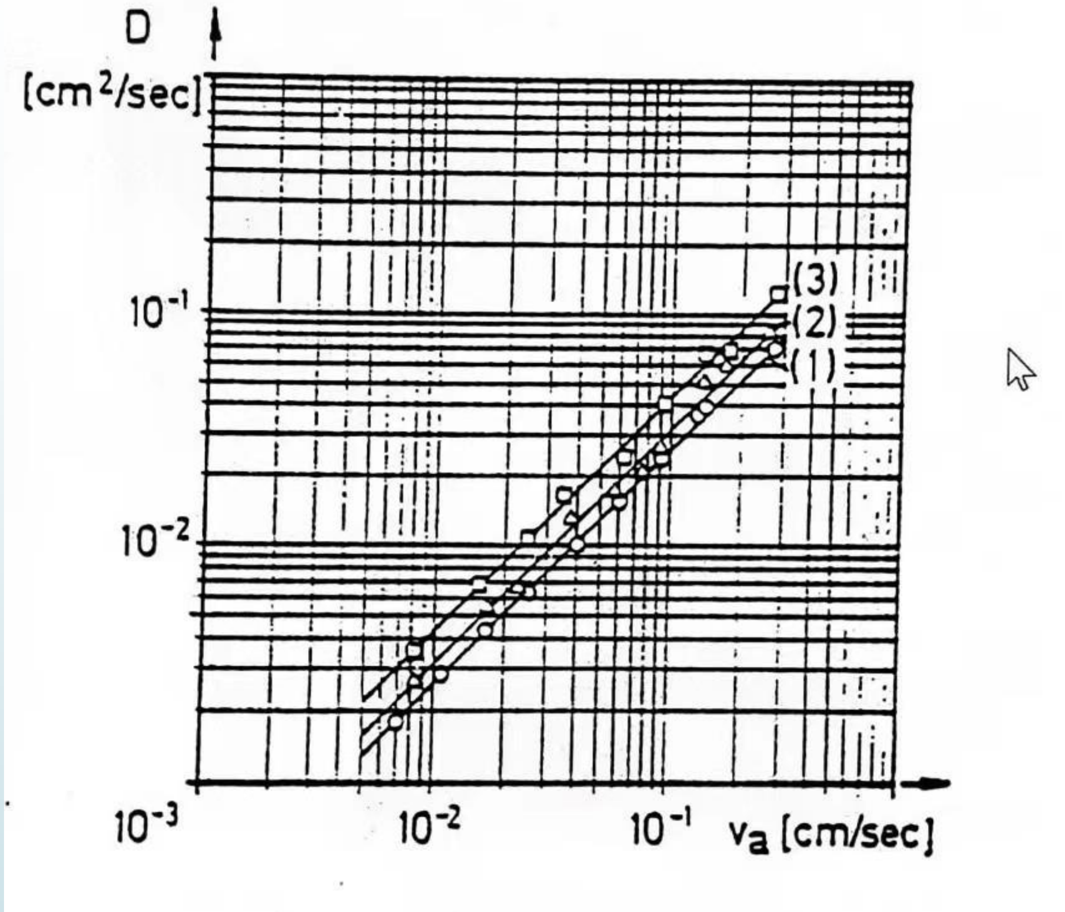


Dispersivity



Longitudinal dispersion coefficient D in relation to distance velocity v_a for sands with a grain size of 0.9 -1.12 mm (U = 1. 1) with varying roughness and angularity of grains: (1) completely rounded (spheres),n=0.37;(2) well rounded (filter sand), n =0.38; (3) averagely rounded, n =0. 39;(4) entirely angular(chip material), n=0.42.

Dispersivity



Longitudinal dispersion coefficient D in relation to distance velocity v_a for porous media of grainsizes 2 -3 mm(U≈1. 5) with different grain shapes: (1) spherical shape, n=0. 36; (2) lenticular shape, n=0.32; (3) cylindrical shape, n=0.33.

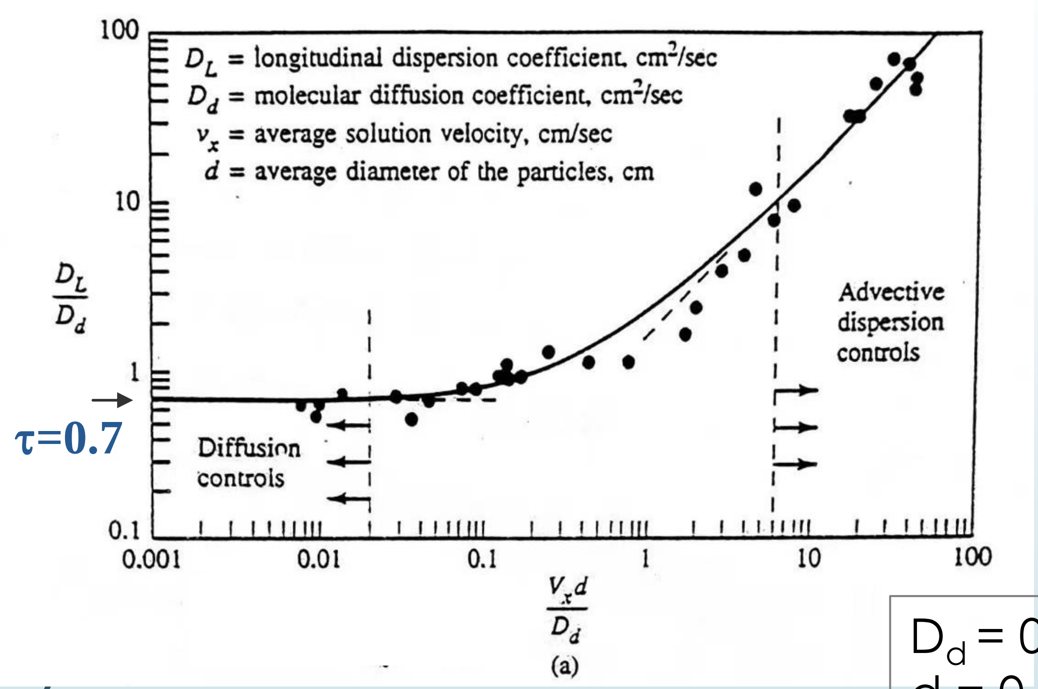
Mechanical Mixing vs Diffusion

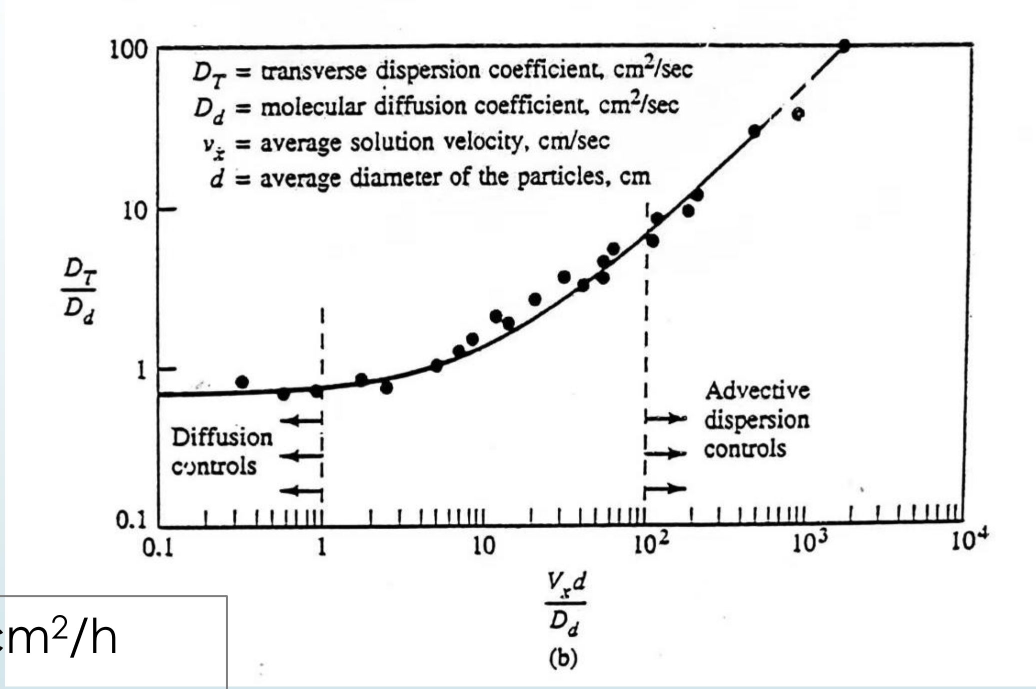
- Diffusion always occurs

  -when is it significant

- Mechanical mixing occurs only when $v>0$

Mechanical Mixing vs Diffusion





$D_d = 0.09 cm^2/h$
$d = 0.1cm$

- Graph of dimensionless dispersion coefficients versus Peclet number, $P = v_x d/D_d$ (a)D_L/D_d versus P and (b) D_τ/D_d. versus P. Source: T. K. Perkins and O. C Johnson, Society of Petroleum Engineers Journal, 3 (1963): 70-84

Impact of p-w velocity on Spreading

- Recall D_m= alpha*v

- When diffusion in minimal:

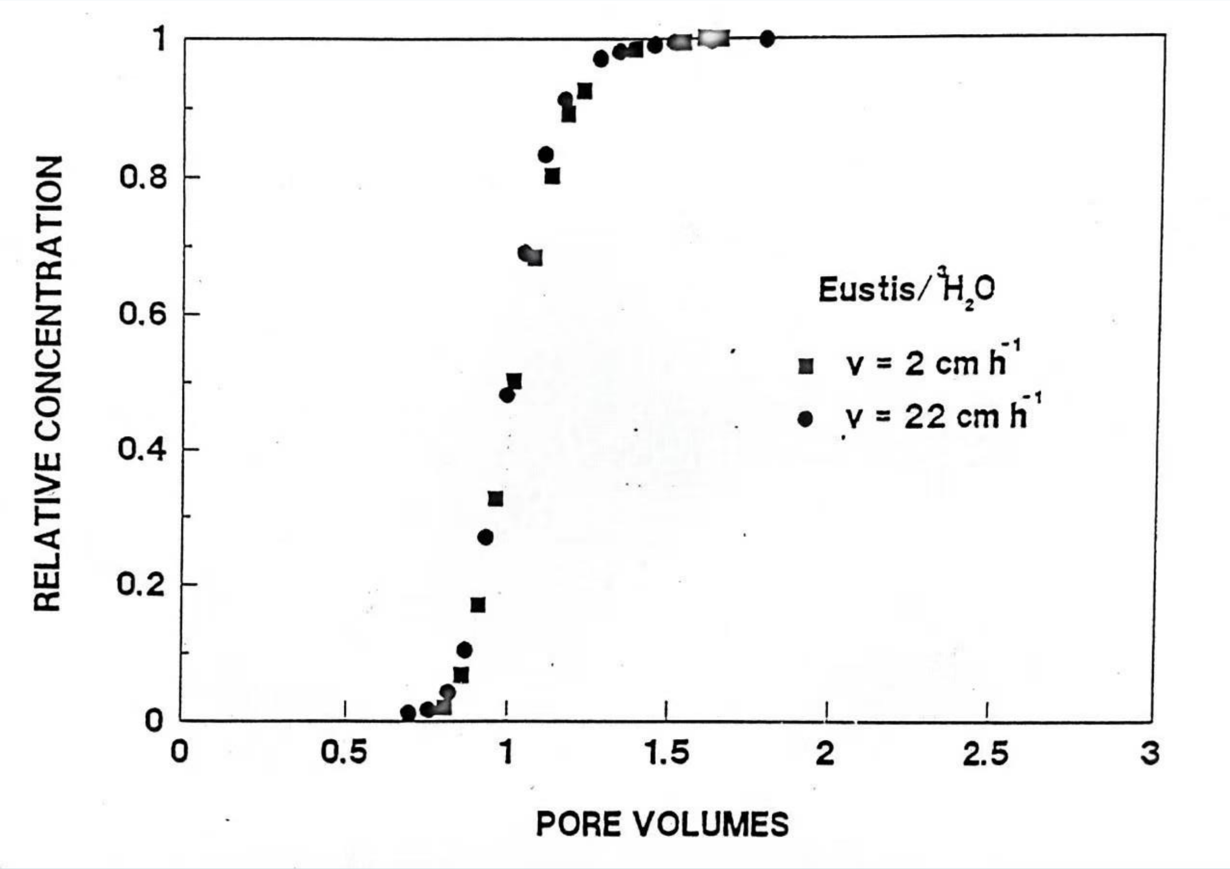
  -No effect (identical BTCs for all velocities)

- When diffusion is important

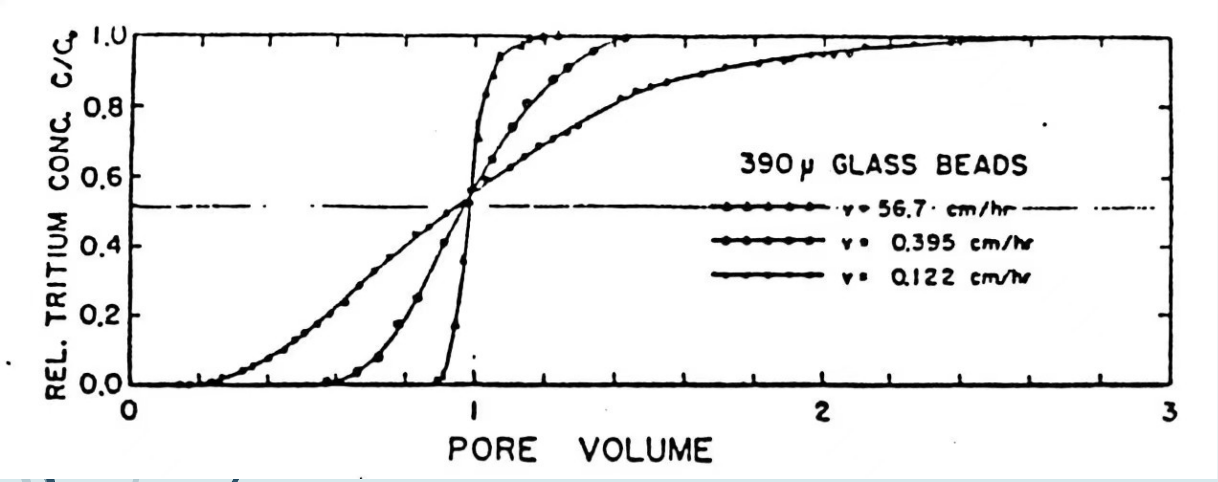
  -Greater spreading at smaller velocities

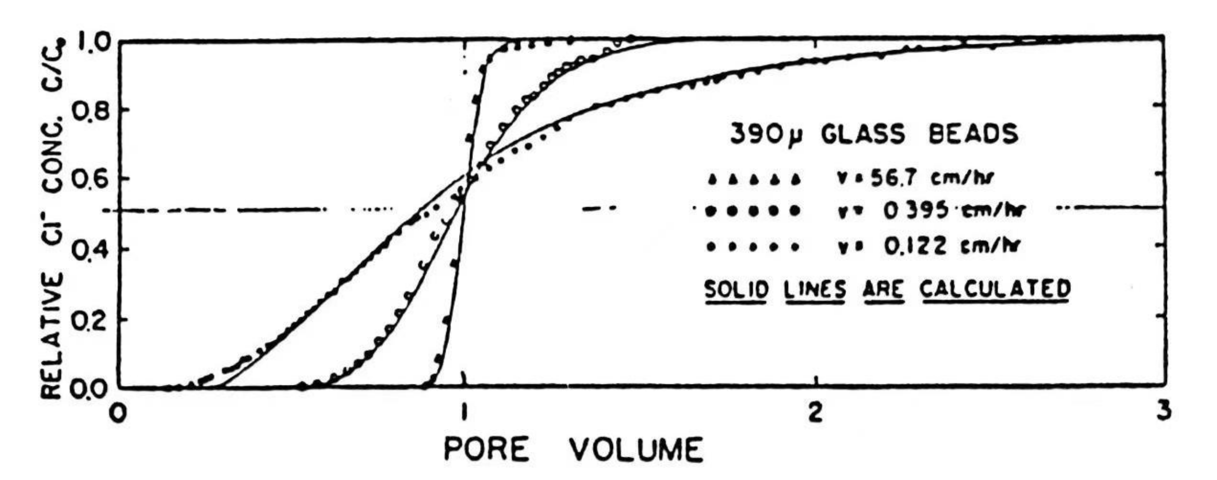
Impact of p-w velocity on Spreading

The effect of pore-water velocity on transport in sandy soil



Impact of p-w velocity on Spreading

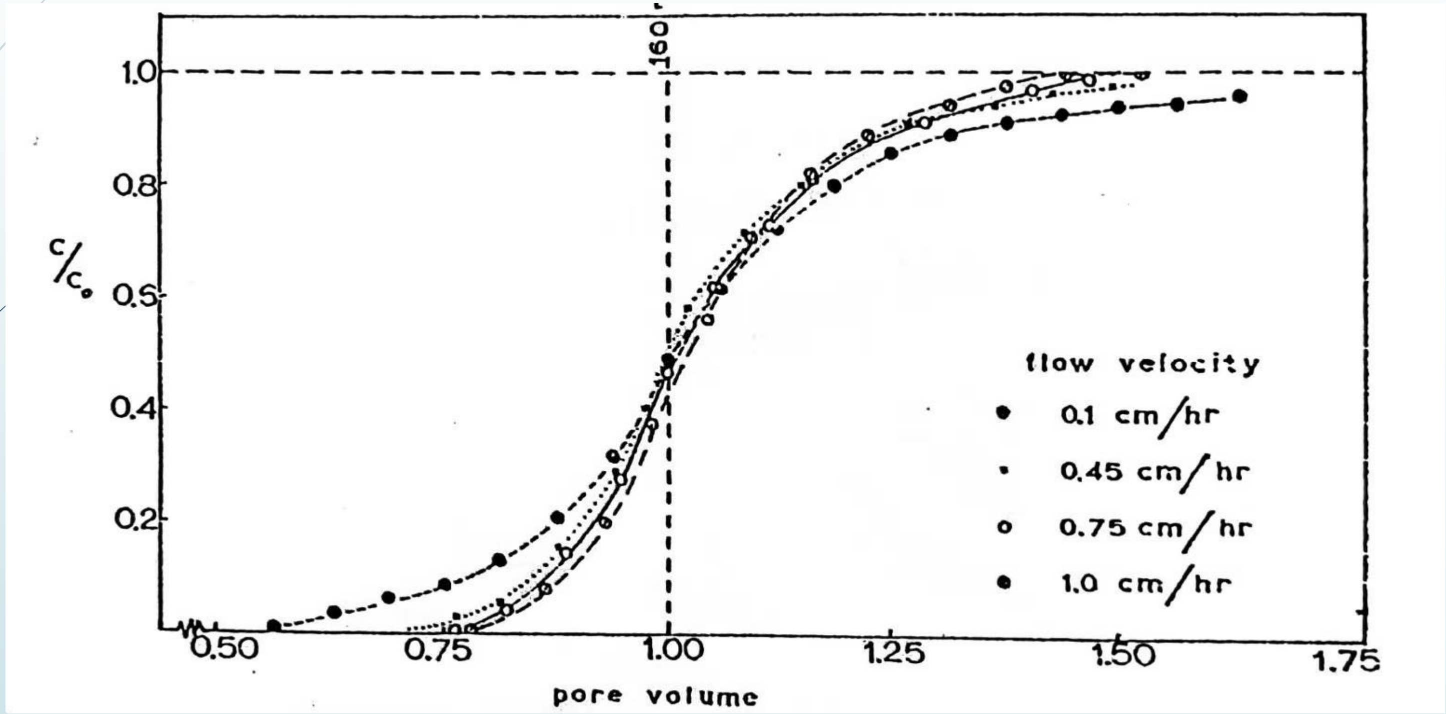




Tritium breakthrough curves from 390μ glass beads for three flow velocities.

Calculated chloride breakthrough curves through measured values from 390μ glass beads.

Impact of p-w velocity on Spreading



Chloride breakthrough curves for flow velocities of 1.0 cm/hr, 0.75cm/hr, 0.45 cm/hr, and 0.1 cm/hr in saturated columns containing sand plus 5 percent powdered Clackline clay.

Impact of Solute Size on Spreading

- Recall Do correlates to 1/MW

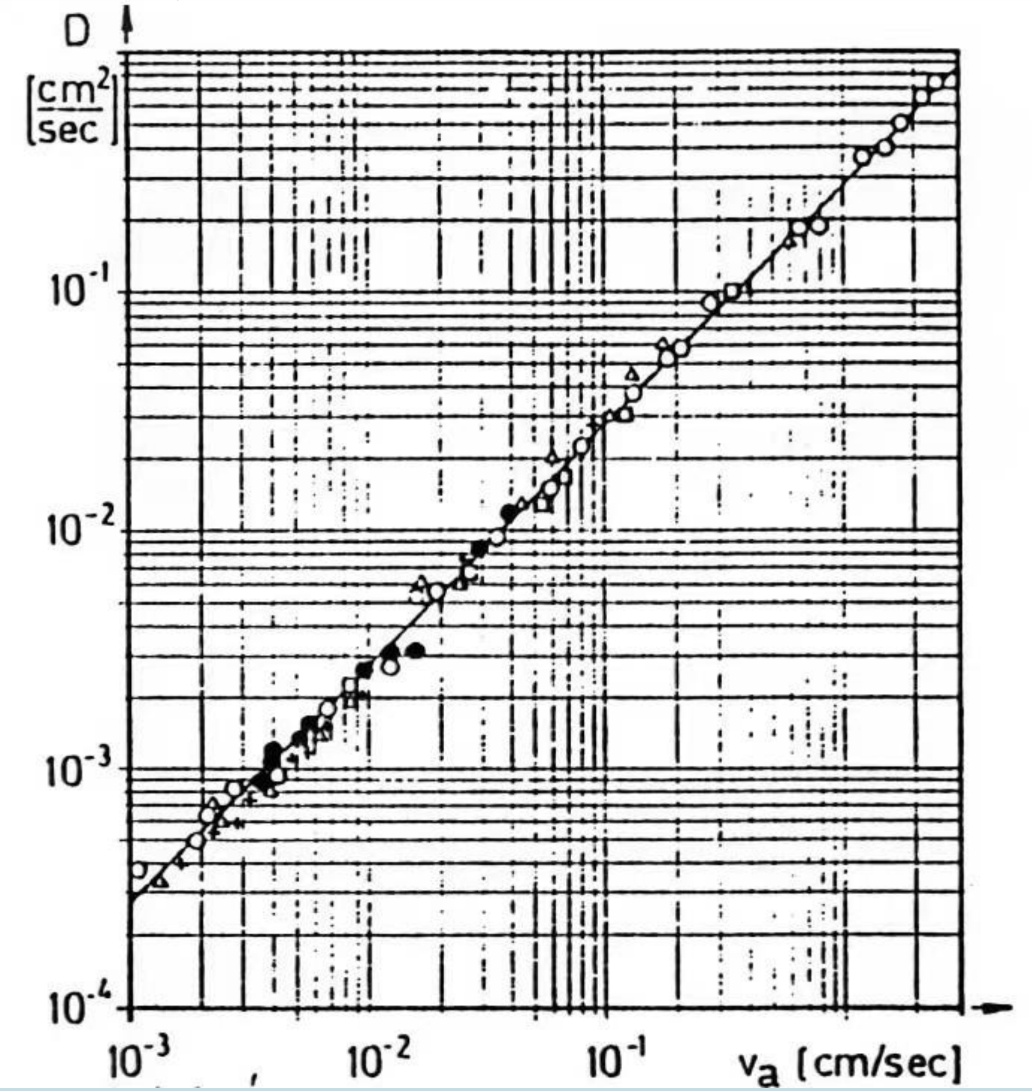
- When diffusion in minimal:

  - No effect(identical BTCs for all solutes)

- When diffusion is important

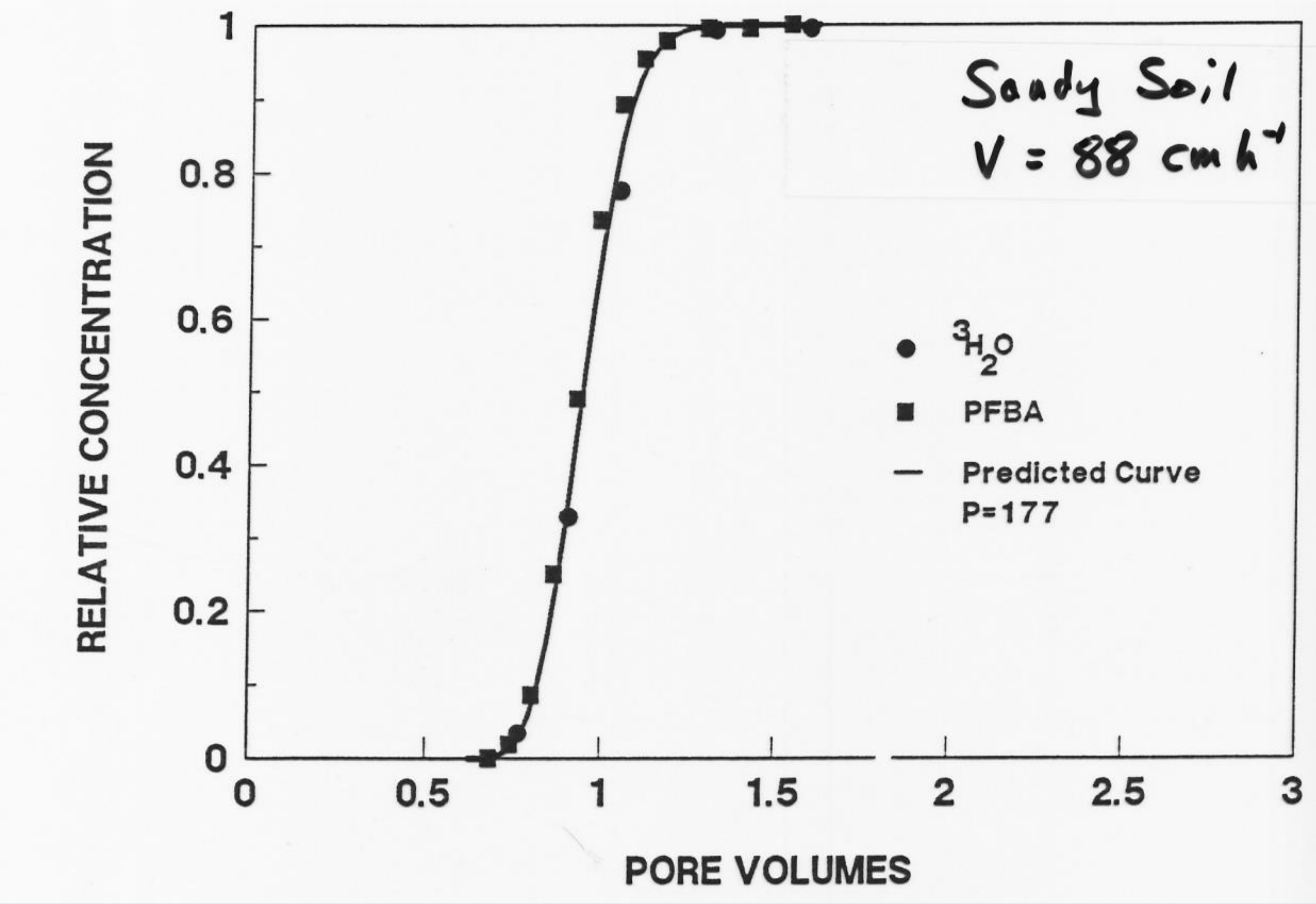
  - Greater spreading for smaller solute

Impact of Solute Size on Spreading

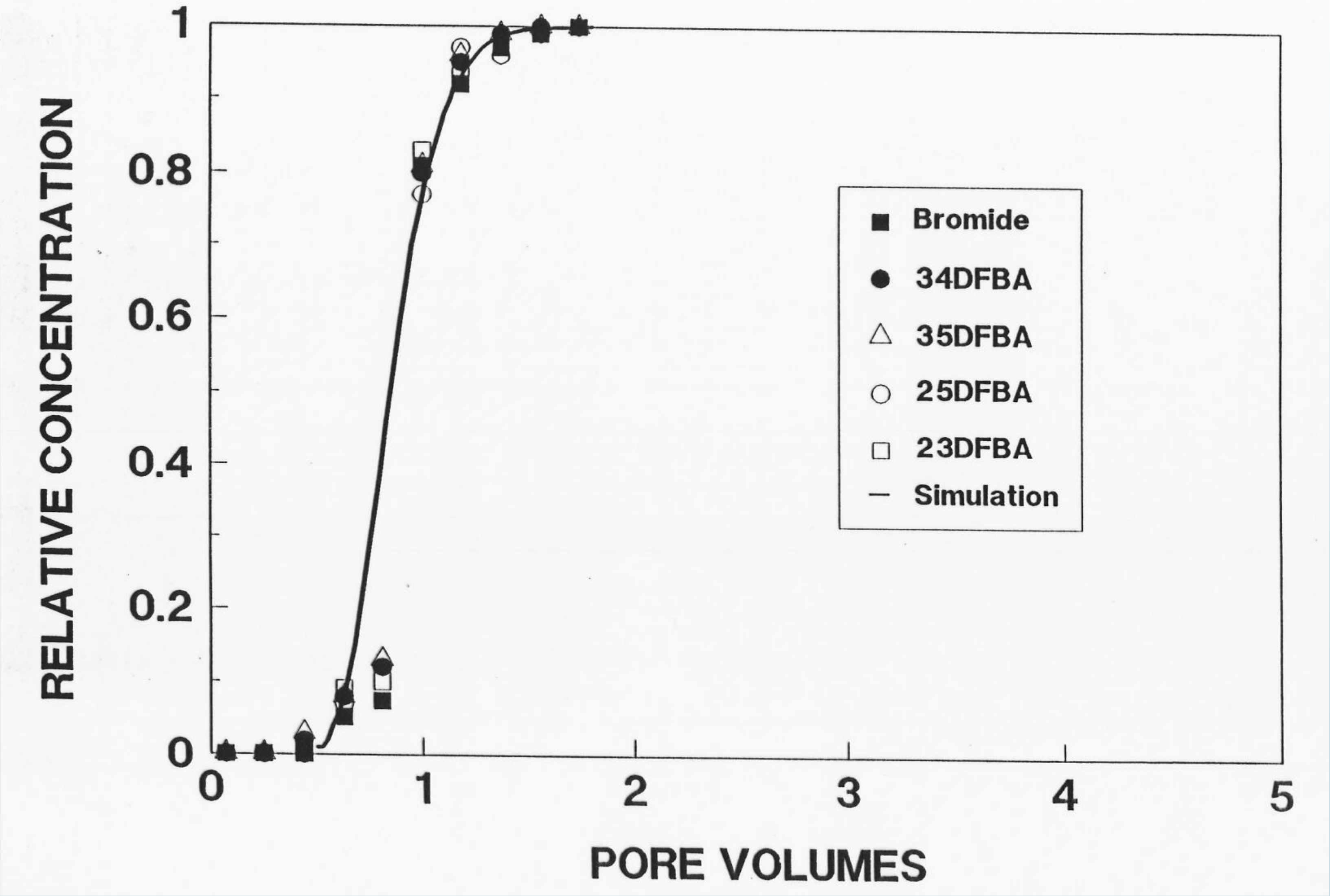


Longitudinal dispersion coefficient D in relation to distance velocity v_a using different tracer solutions: C NH_4 ^{82}Br, Na^{131}. ΔNaCl, □Uranin A. + ^{51}Cr-EDTA. Porous medium (total porosity n =0.38).

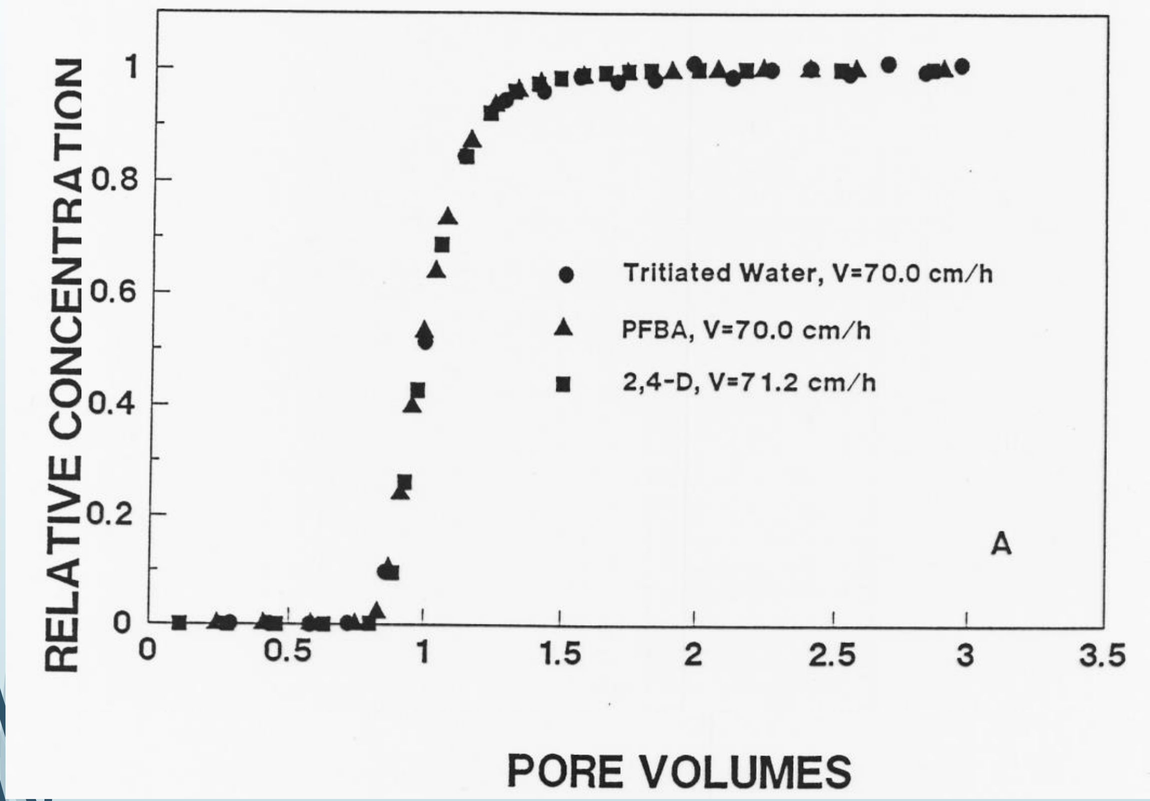
Impact of Solute Size on Spreading

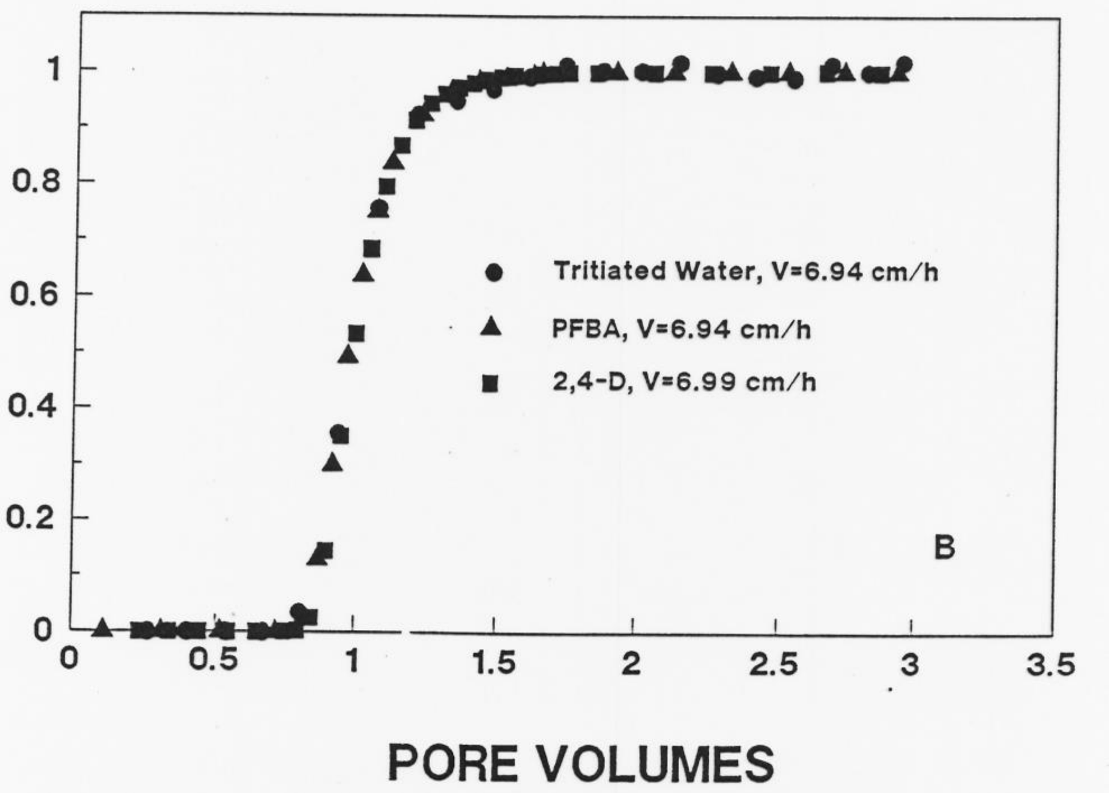


Impact of Solute Size on Spreading

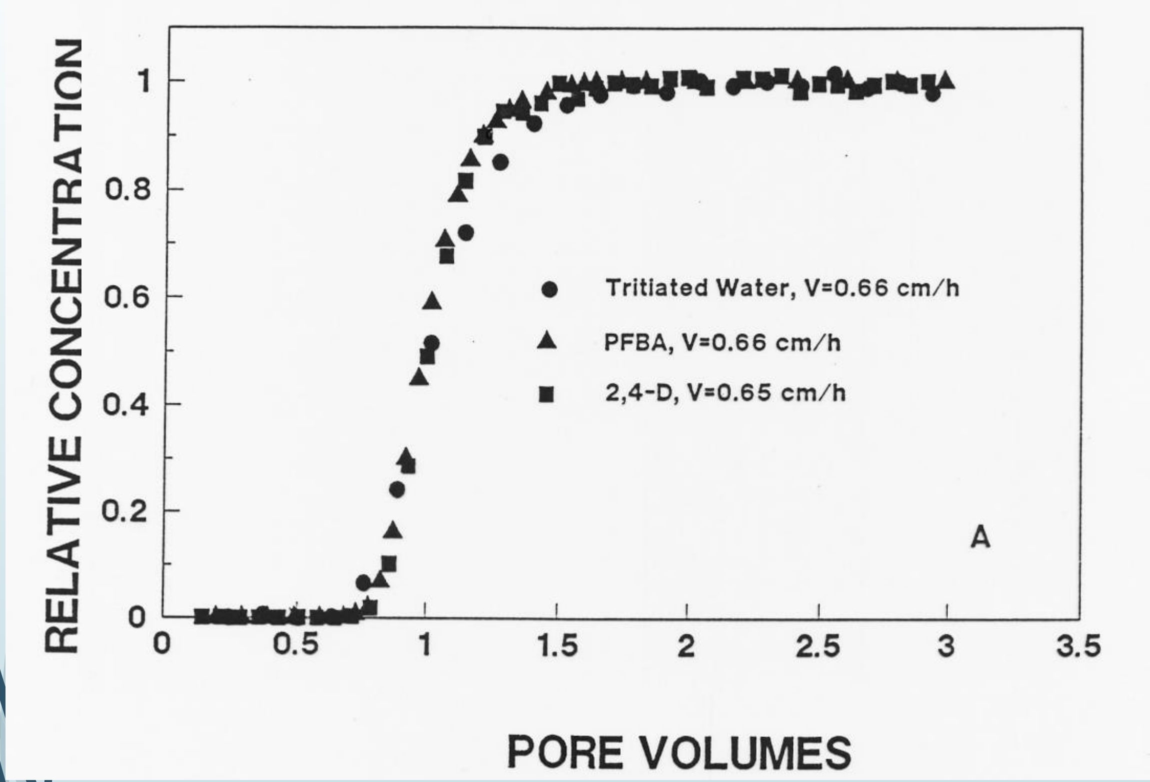


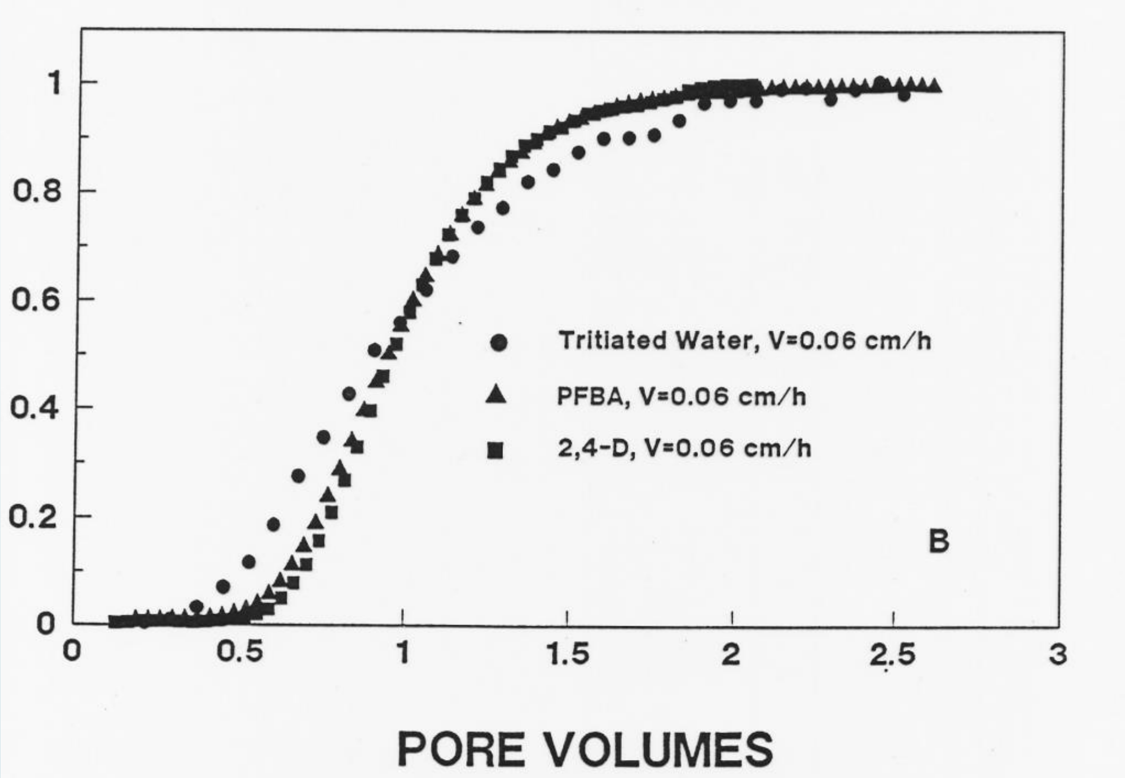
Impact of Solute Size on Spreading



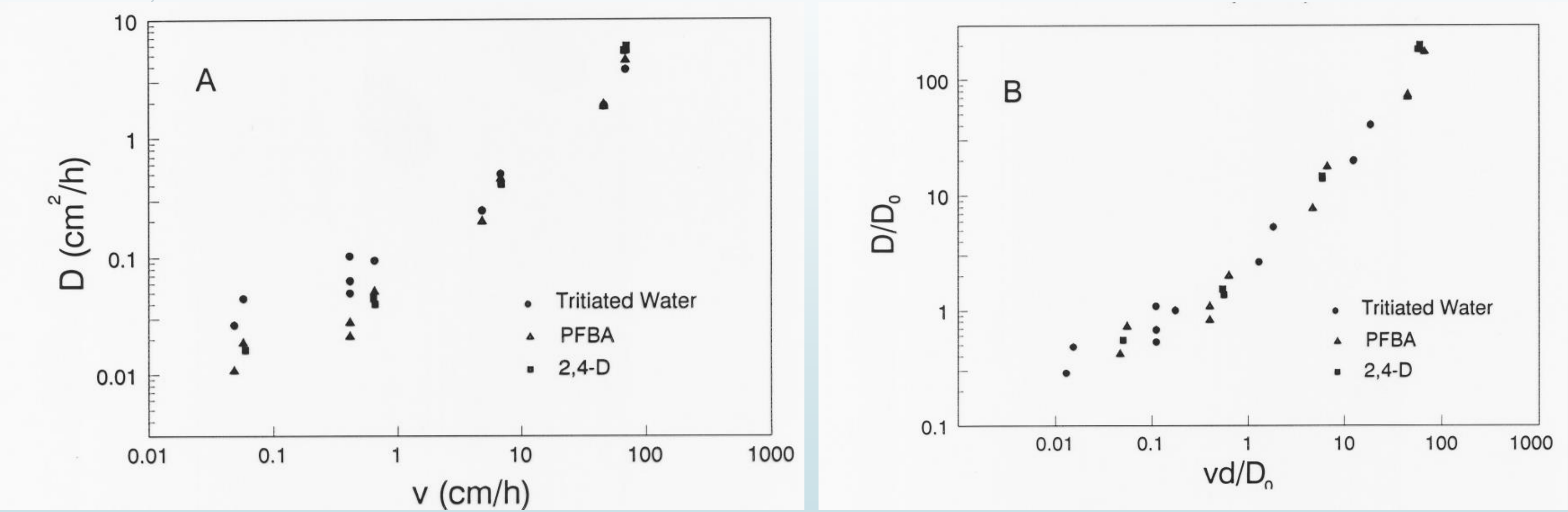


Impact of Solute Size on Spreading





Impact of Solute Size on Spreading

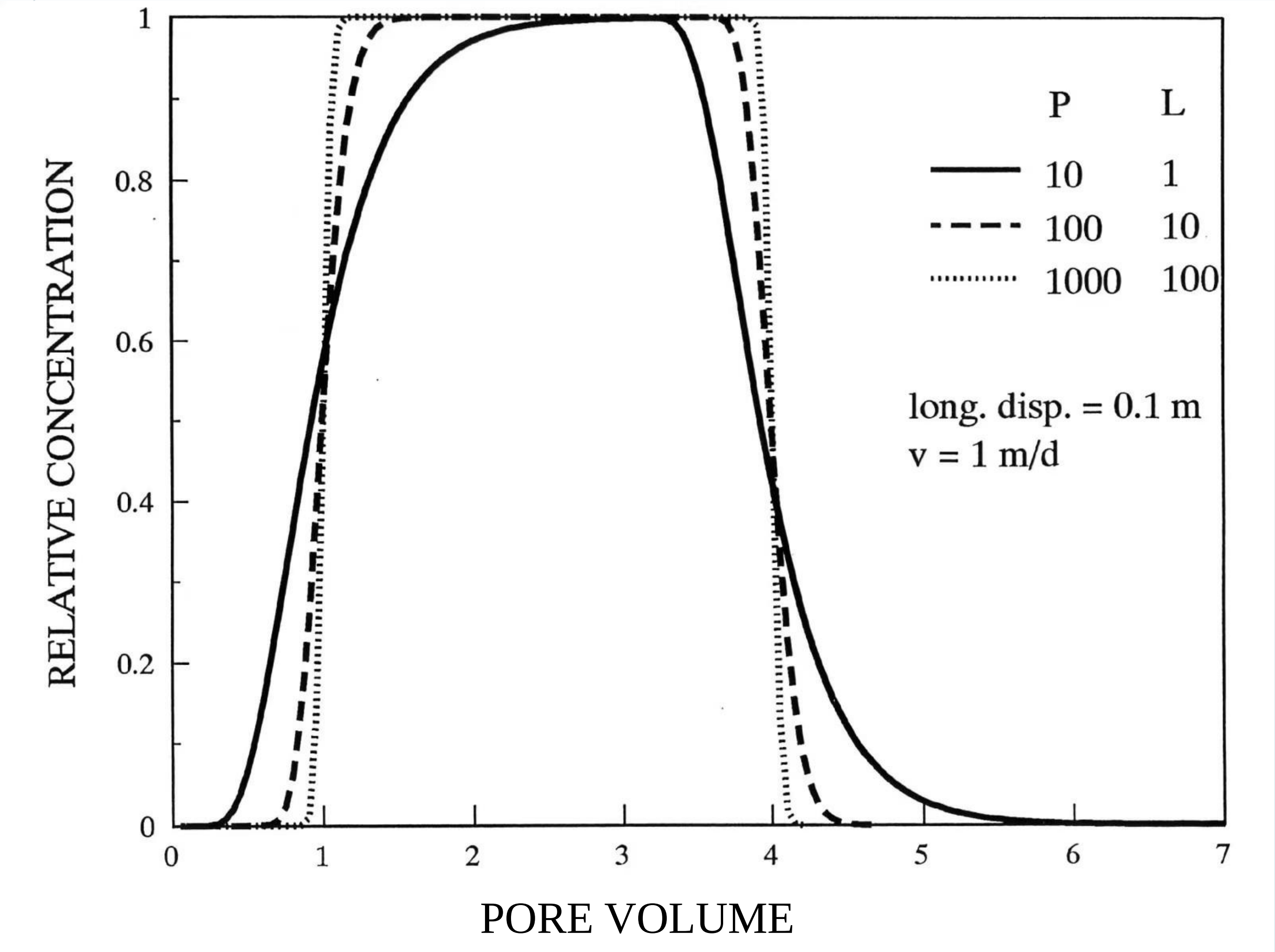


Spreading and Travel Distance

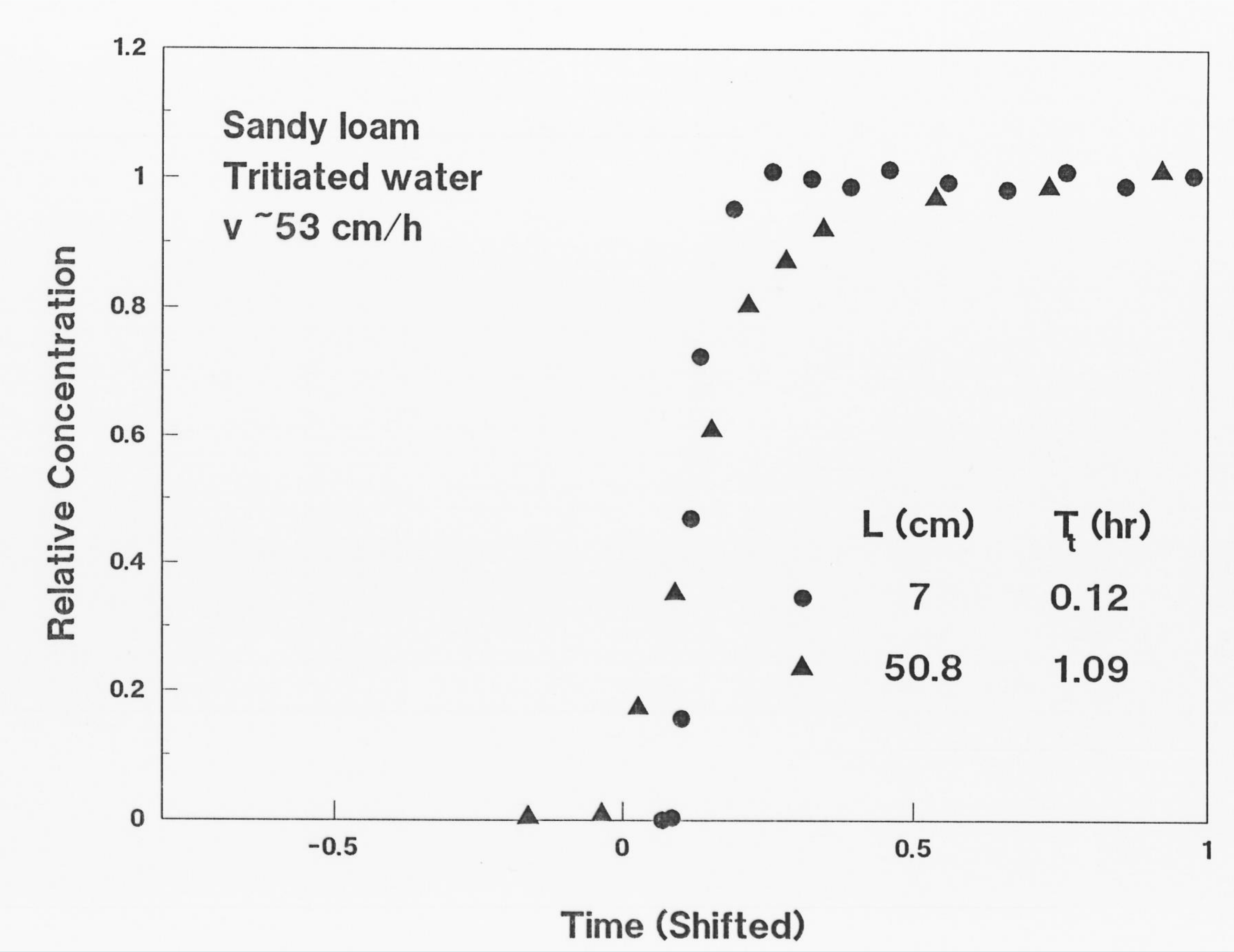
- P= L/alpha

  -Assume diffusion is minimal

Spreading and Travel Distance



Spreading and Travel Distance



Spreading and Travel Distance