

Tracers in Hydrology

Modeling

Prof. Dr. C. Külls

Content

Transport models

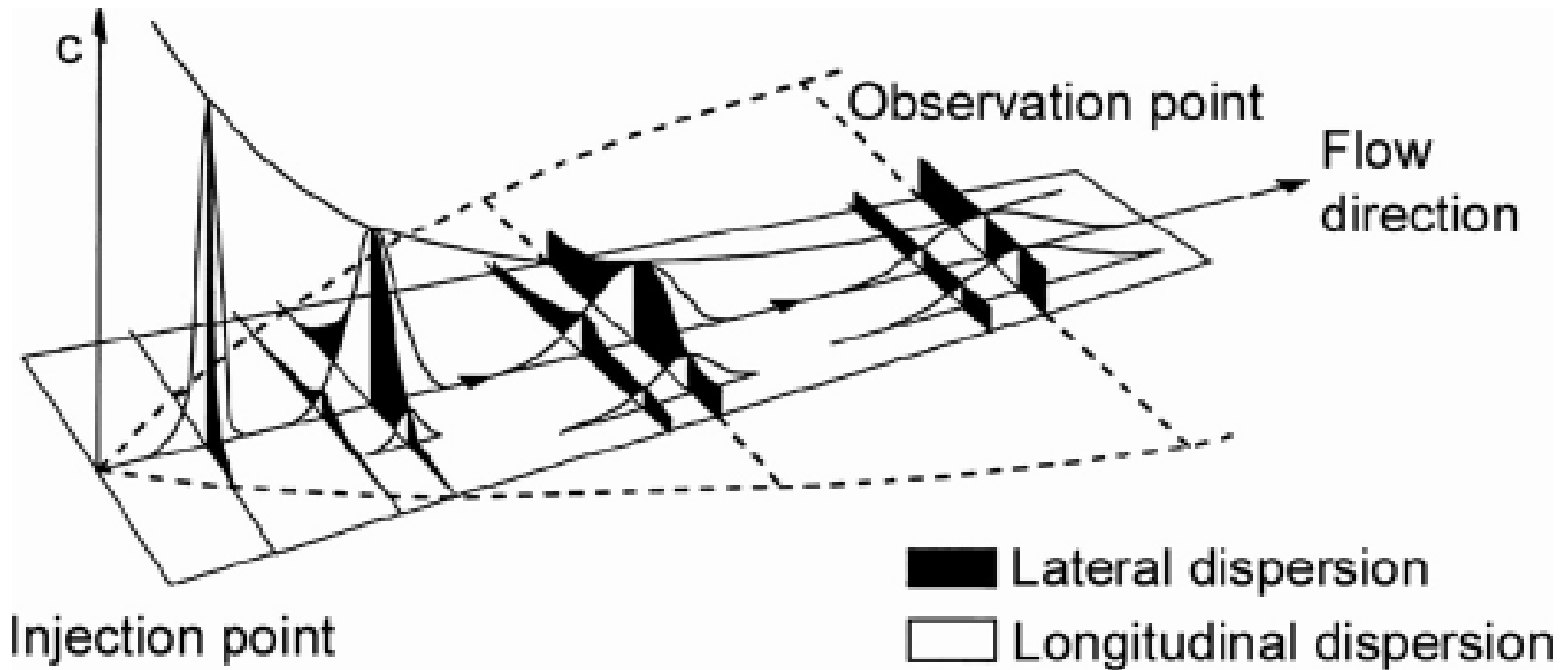
- Conceptual models:
 - Compartment models
 - Application
 - Limits
- Physical models
 - *Transport equation*
 - *Solutions:*
 - *analytical*
 - *numerical*

Rhine Alarm Model



Basics and Theory of Solute Transport

Longitudinal and Transversal Dispersion



- Dispersion transversal and longitudinal
- Gauß-shaped curves

Longitudinal and Transversal Dispersion

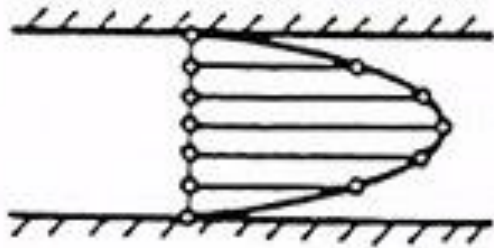
Dispersion of solutes during transport

Concentration decreases and an increasingly large volume of water is contaminated

a) Different velocities

b) Different pore size

c) Different paths



a)

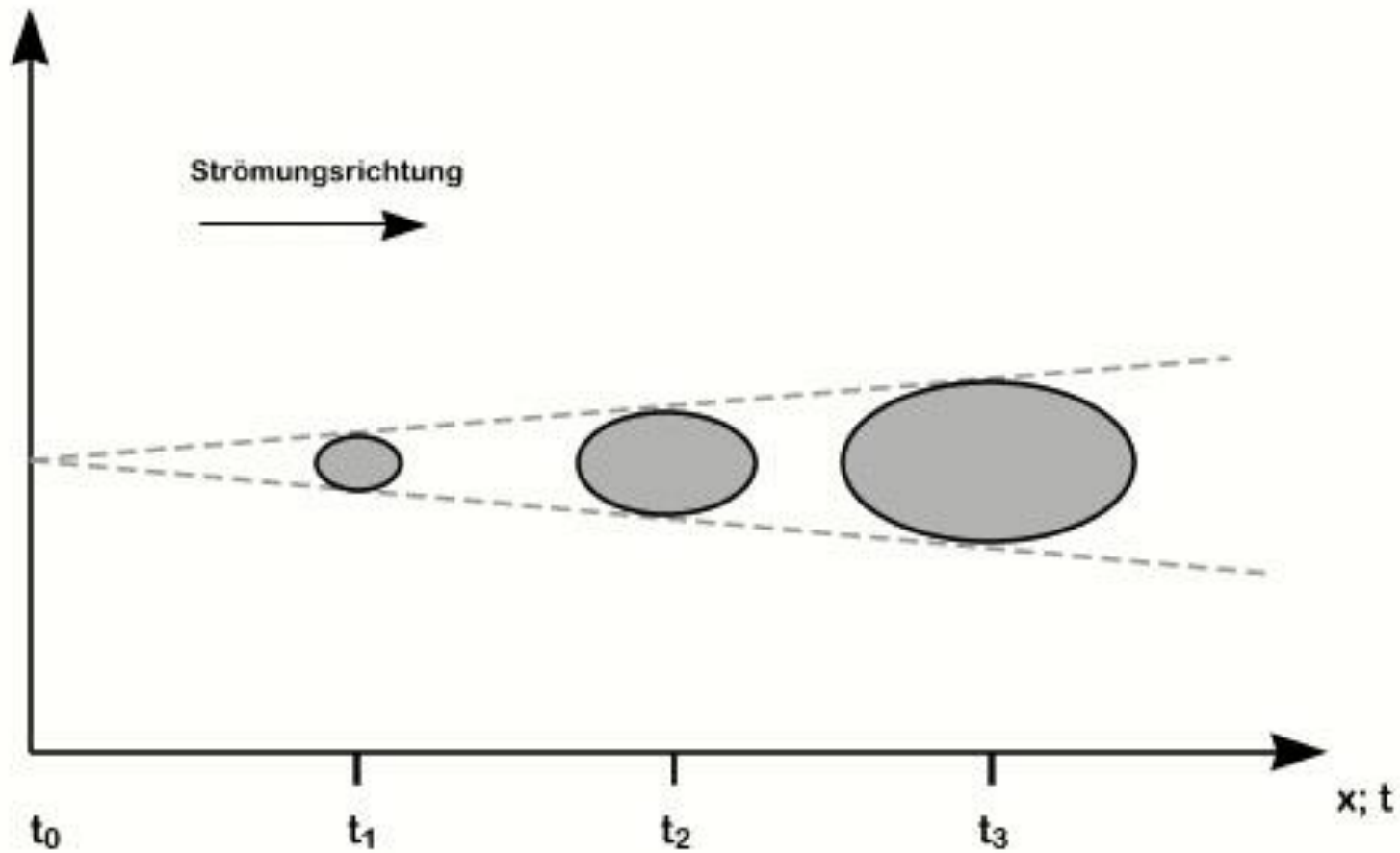


b)

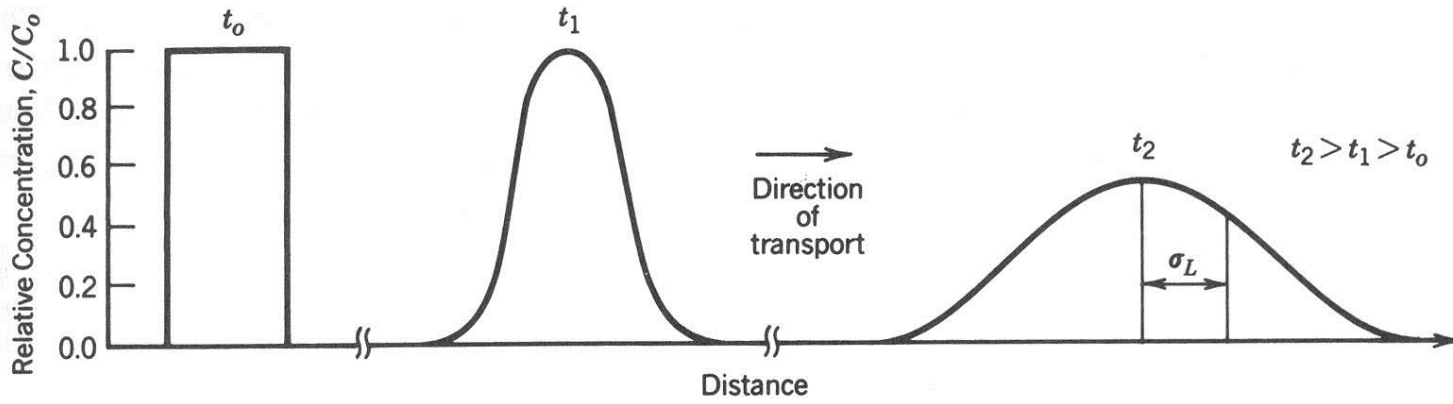


c)

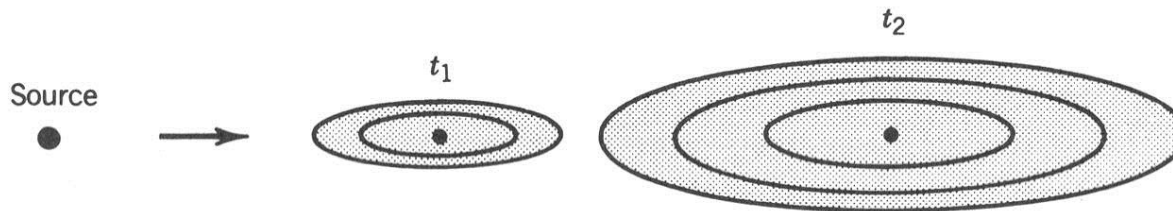
Effect of hydrodynamic dispersion



Quelle: Sächsisches Landesamt für Umwelt und Geologie



(a)



(b)

Figure 10.7

Variation in concentration of a tracer spreading in (a) one or (b) two dimensions in a constant velocity flow system.

Dispersion coefficient

- Dispersion coefficient D (m^2/s)

$$D = \delta * v_a$$

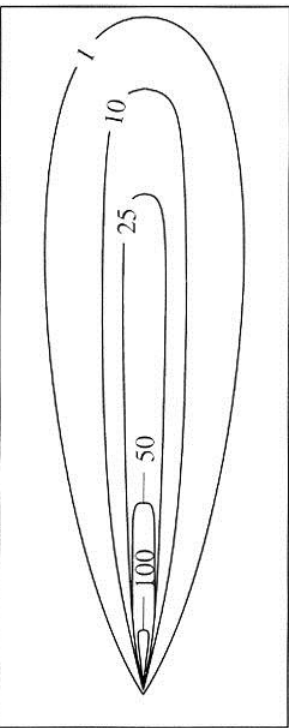
dispersivity δ is scale dependent and describes the heterogeneity

- Laboratory scale
- Field scale
- Regional scale

Transversal / longitudinal Dispersion

- Transversal dispersion 0,1- to 0,2-times longitudinal
- Hydrodynamic dispersion can be determined with column or field experiments

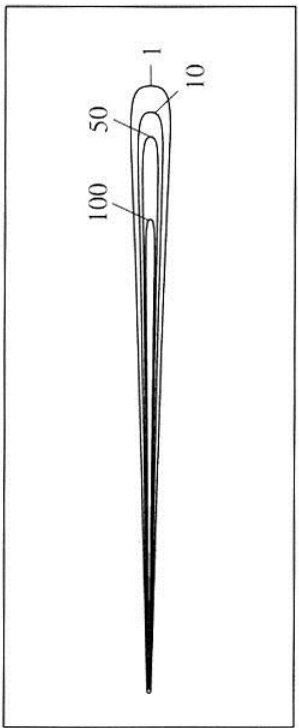
Large and small dispersivity



↑
Flow

$\alpha_L = 3 \text{ m}$ $\alpha_T = 1 \text{ m}$
 $T = 0.0363 \text{ m}^2/\text{sec}$
 $Q = 0.165 \text{ m}^3/\text{sec}$
 $t = 0.01 \text{ yr}$

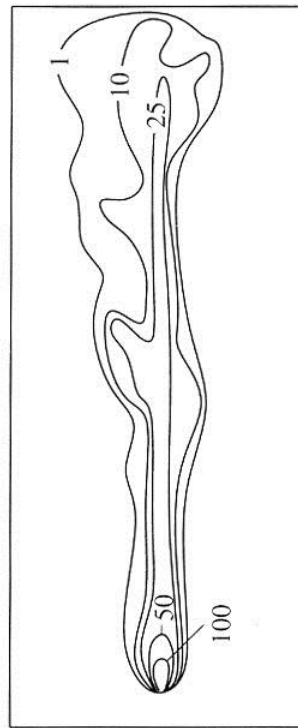
(a)



↑
Flow

$\alpha_L = 0.0003 \text{ m}$ $\alpha_T = 0.00009 \text{ m}$
 $T = 0.0363 \text{ m}^2/\text{sec}$
 $Q = 0.165 \text{ m}^3/\text{sec}$
 $t = 0.01 \text{ yr}$

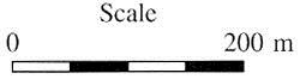
(b)



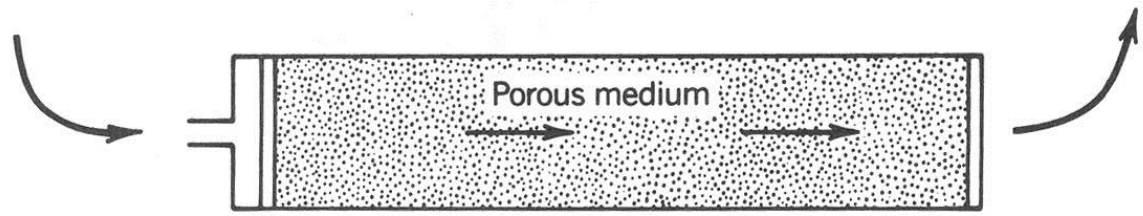
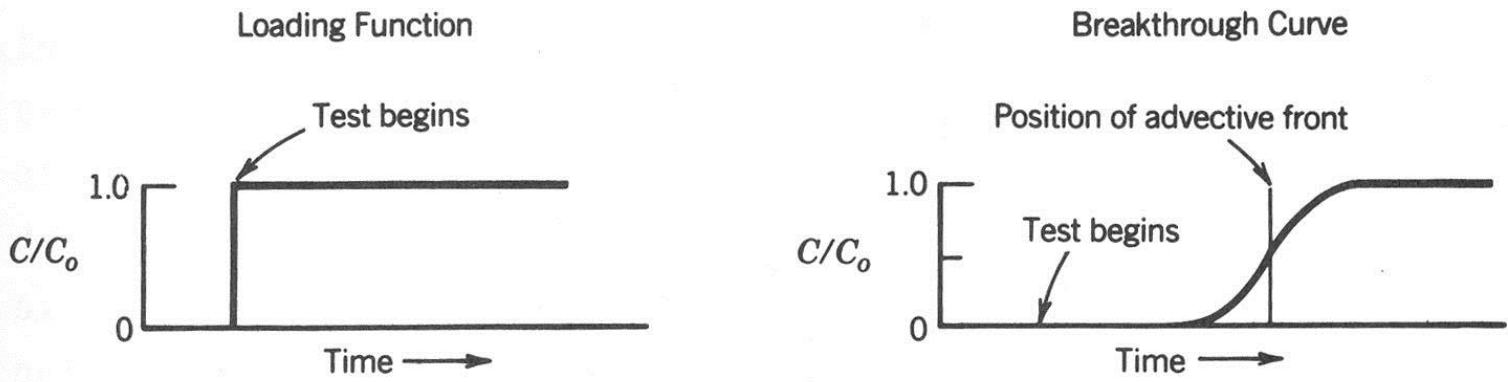
↑
Flow

$\alpha_L = 0.0003 \text{ m}$ $\alpha_T = 0.00009 \text{ m}$
 $T_1 = 0.223 \text{ m}^2/\text{sec}$ $T_2 = 0.0223 \text{ m}^2/\text{sec}$
 $Q = 0.165 \text{ m}^3/\text{sec}$
 $t = 0.01 \text{ yr}$

(c)



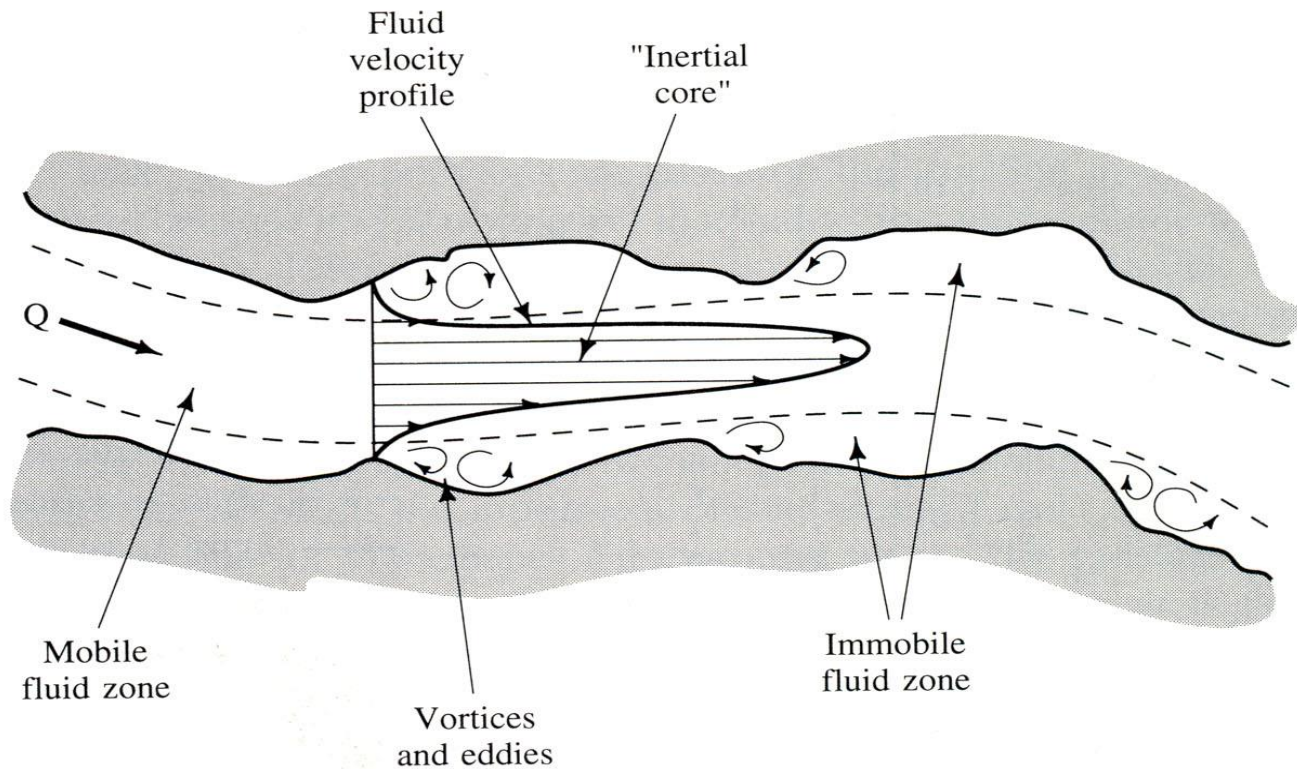
Dispersion in column experiment



(a)

Experimental apparatus to illustrate dispersion in a column. The test begins with a continuous input of tracer $C/C_0 = 1$ at the inflow end. The relative concentration versus time function at the outflow characterizes dispersion in the column.

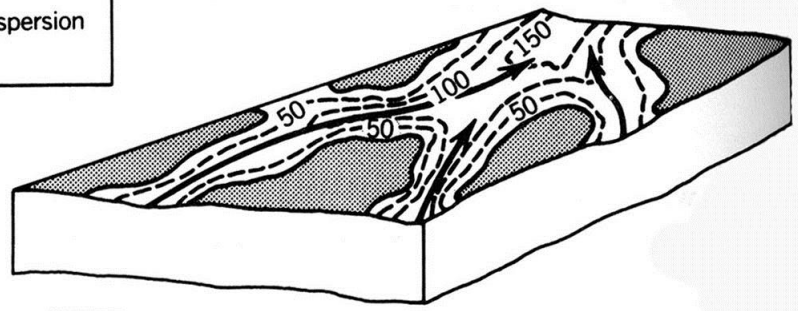
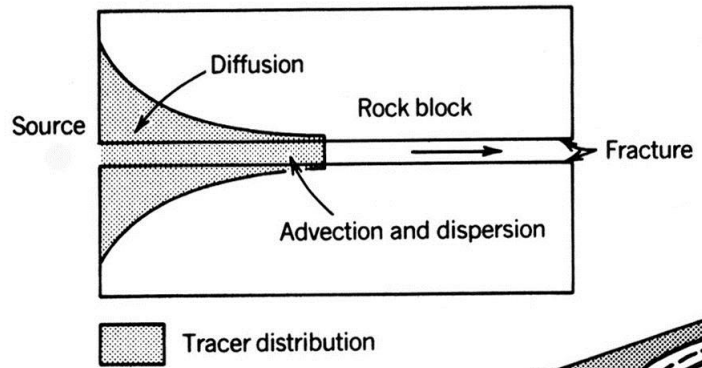
Immobile zones and dispersion



Zones of mobile and immobile water in a fracture. Source: K. G. Raven, K. S. Novakowski, and P. A. Lapcevic, *Water Resources Research* 24, no. 12 (1988):2019–32. Published by the American Geophysical Union.

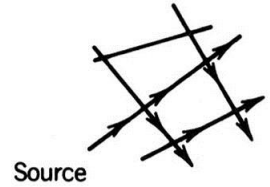
Scales of dispersion

(a) Diffusion into the Matrix

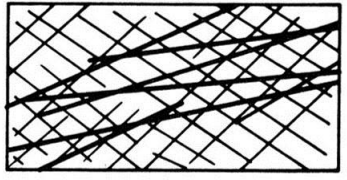


■ Closed fracture
--- Fracture aperture (μm)

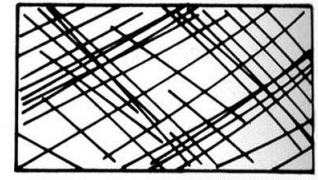
(b) Variability in Velocity due to Fracture Roughness



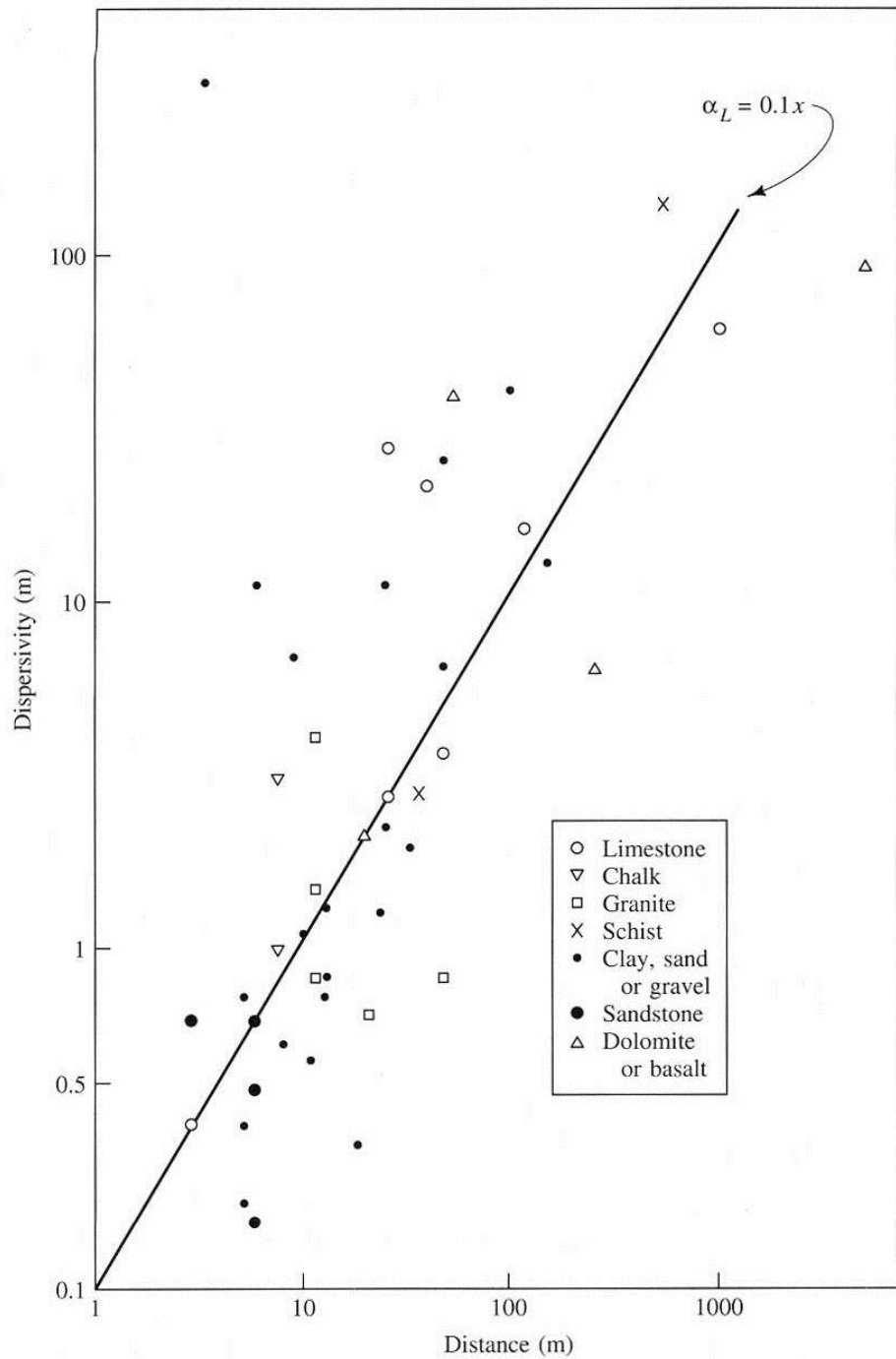
(c) Mixing at Fracture Intersections



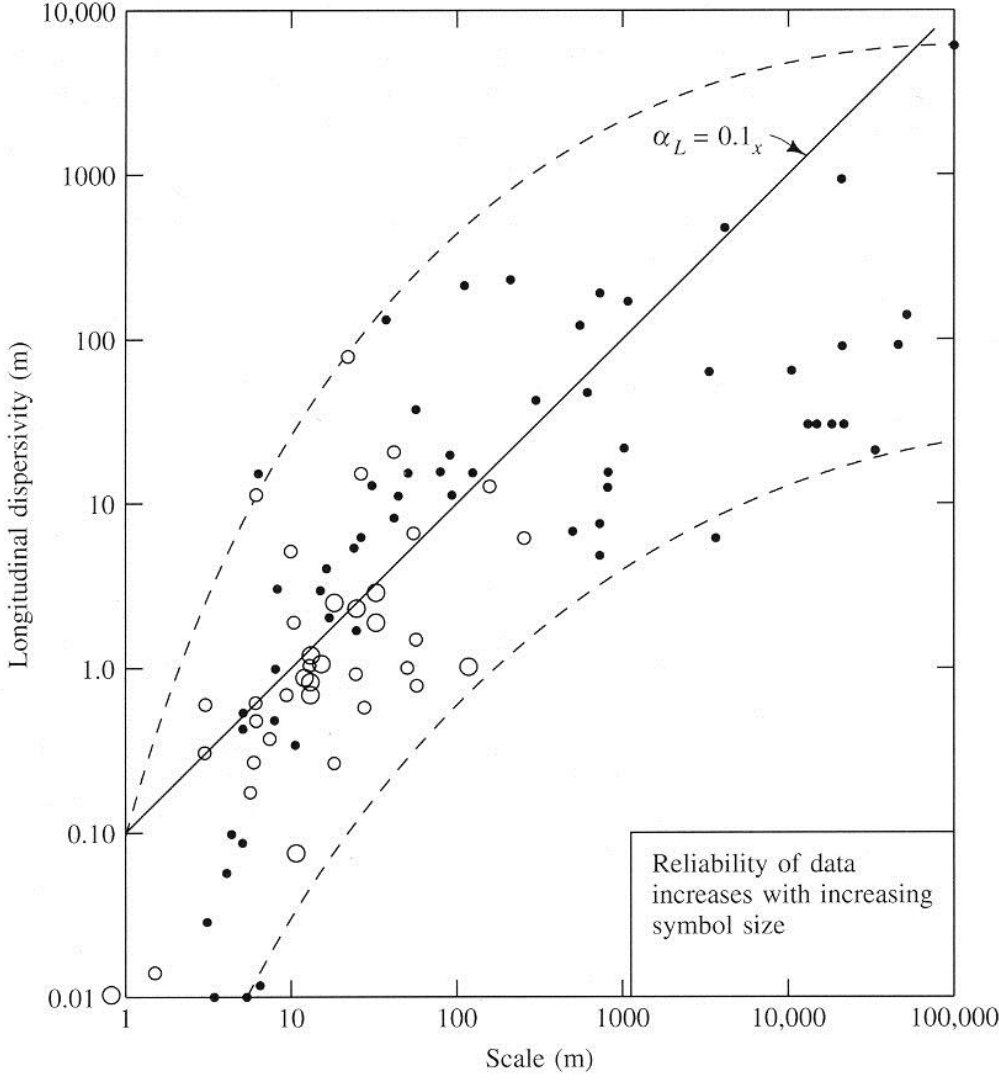
(d) Variability in Velocity due to Differing Scales of Fracturing



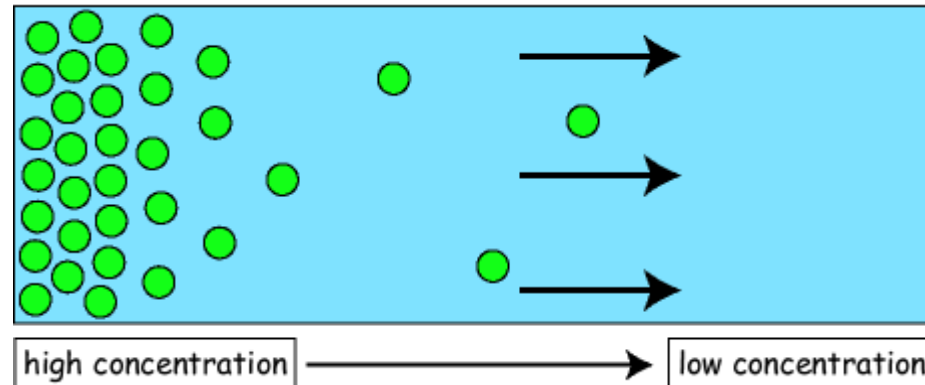
(e) Variability in Velocity due to Variable Fracture Density



Scale effects



Diffusion



$$f_{diff}^* = -d_o \cdot i_c \quad \text{mit} \quad i_c = \frac{\partial c}{\partial x}$$

f_{diff}^* Diffusiver Massenfluß im freien Wasservolumen [kg/(m²s)]

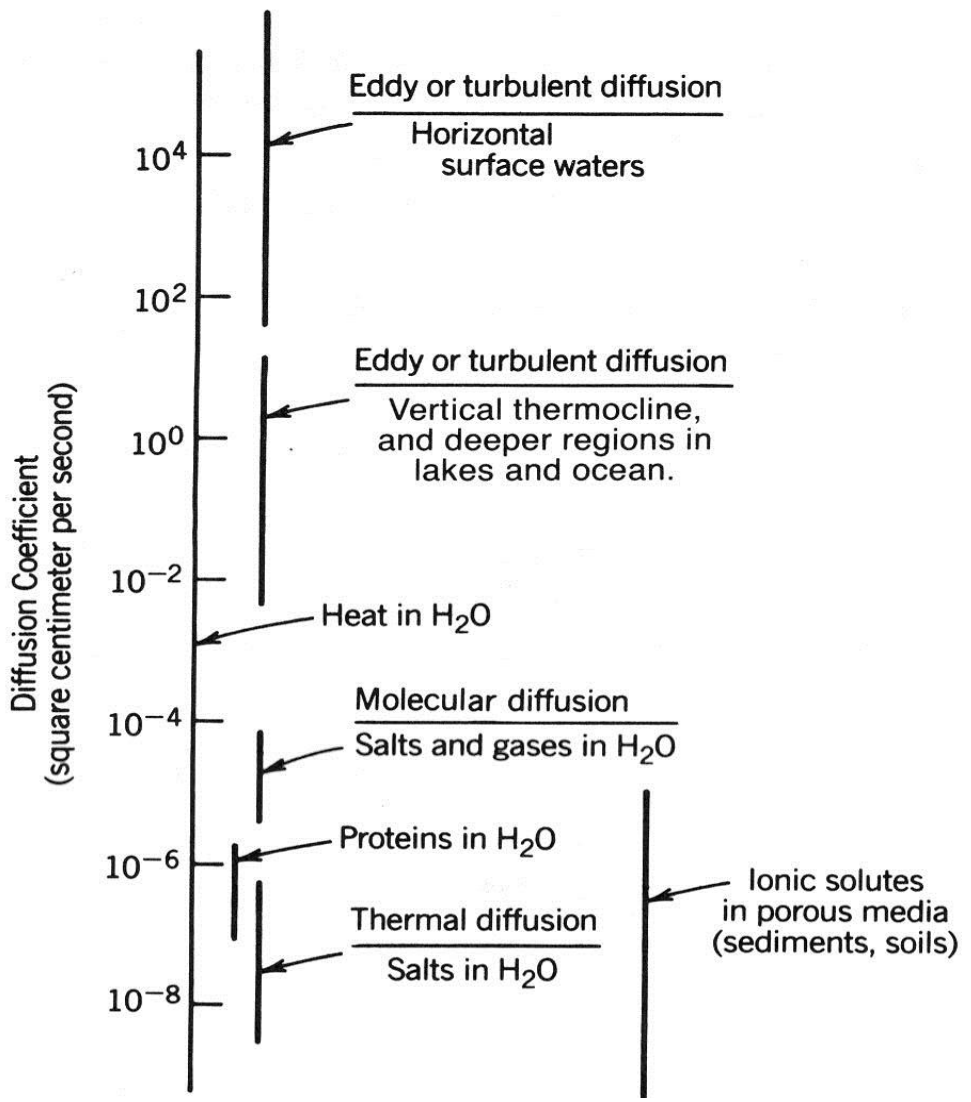
d_o Diffusionskoeffizient im freien Wasservolumen [m²/s]

i_c Konzentrationsgradient [kg/m⁴]

c Konzentration des wassergelösten Inhaltsstoffes [kg/m³]

x Abstand zwischen 2 Konzentrationsmeßpunkten [m]

Diffusion coefficient

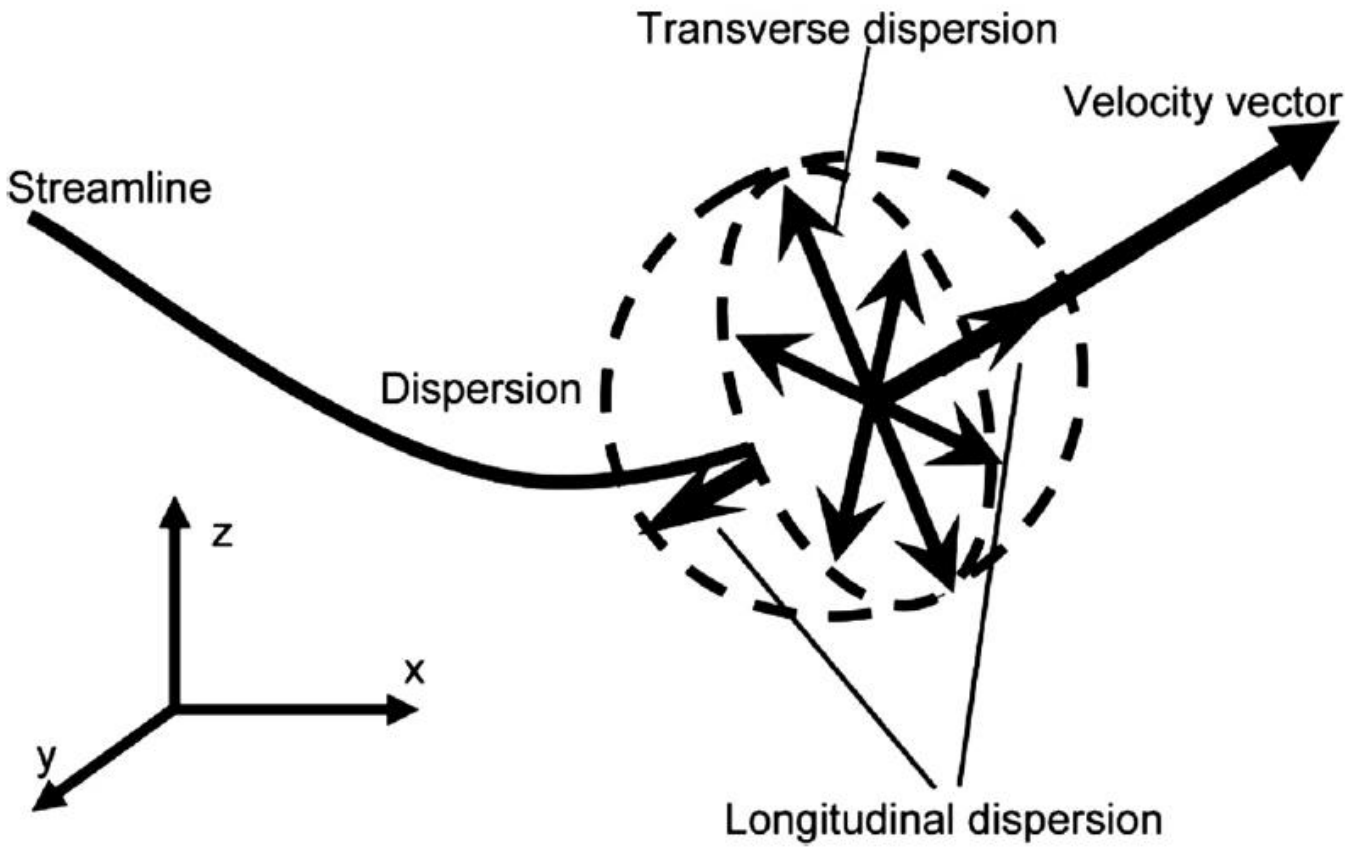


Transport equation

$$\begin{aligned} & \frac{\partial}{\partial x} \left(D_{xx} \frac{\partial C}{\partial x} + D_{xy} \frac{\partial C}{\partial y} + D_{xz} \frac{\partial C}{\partial z} - v_x C \right) \\ & + \frac{\partial}{\partial y} \left(D_{yx} \frac{\partial C}{\partial x} + D_{yy} \frac{\partial C}{\partial y} + D_{yz} \frac{\partial C}{\partial z} - v_y C \right) \\ & + \frac{\partial}{\partial z} \left(D_{zx} \frac{\partial C}{\partial x} + D_{zy} \frac{\partial C}{\partial y} + D_{zz} \frac{\partial C}{\partial z} - v_z C \right) = \frac{\partial C}{\partial t} \end{aligned}$$

- D_{ij} dispersion coefficient x, y, z direction
- C concentration t time
- v_i flow velocity

Dispersion effects



Dispersivity and dispersion coefficient

$$D_L = \alpha_L v$$

$$D_T = \alpha_T v$$

$$v = \sqrt{v_x^2 + v_y^2 + v_z^2}$$

- D dispersion coefficient
- α dispersivity
- v flow velocity

Definition for Dispersivity and Tortuosity

$$D_{xx} = D_L \left(\frac{v_x^2}{v^2} \right) + D_T \left(\frac{v_y^2}{v^2} \right) + D_T \left(\frac{v_z^2}{v^2} \right) + \frac{D_m}{\tau}$$

$$D_{yy} = D_T \left(\frac{v_x^2}{v^2} \right) + D_L \left(\frac{v_y^2}{v^2} \right) + D_T \left(\frac{v_z^2}{v^2} \right) + \frac{D_m}{\tau}$$

$$D_{zz} = D_T \left(\frac{v_x^2}{v^2} \right) + D_T \left(\frac{v_y^2}{v^2} \right) + D_L \left(\frac{v_z^2}{v^2} \right) + \frac{D_m}{\tau}$$

$$D_{xy} = D_{yx} = (D_L - D_T) \left(\frac{v_x v_y}{v^2} \right)$$

$$D_{xz} = D_{zx} = (D_L - D_T) \left(\frac{v_x v_z}{v^2} \right)$$

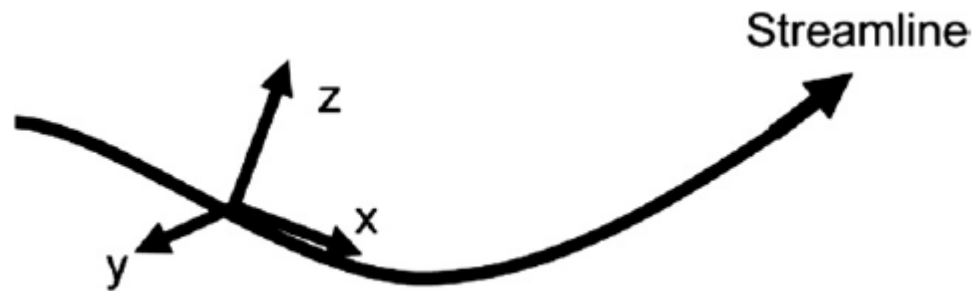
$$D_{zy} = D_{yz} = (D_L - D_T) \left(\frac{v_z v_y}{v^2} \right)$$

- T Tortuosity
- D_ Dispersion coefficienten
- L, T for lateral and transversal

3D

3D equation

$$D_{xx} \frac{\partial^2 C}{\partial x^2} + D_{yy} \frac{\partial^2 C}{\partial y^2} + D_{zz} \frac{\partial^2 C}{\partial z^2} - v \frac{\partial C}{\partial x} = \frac{\partial C}{\partial t}$$



- 3D Transport
- Translation and dispersion

3D

$$D_{xx} = D_L + \frac{D_m}{\tau}$$

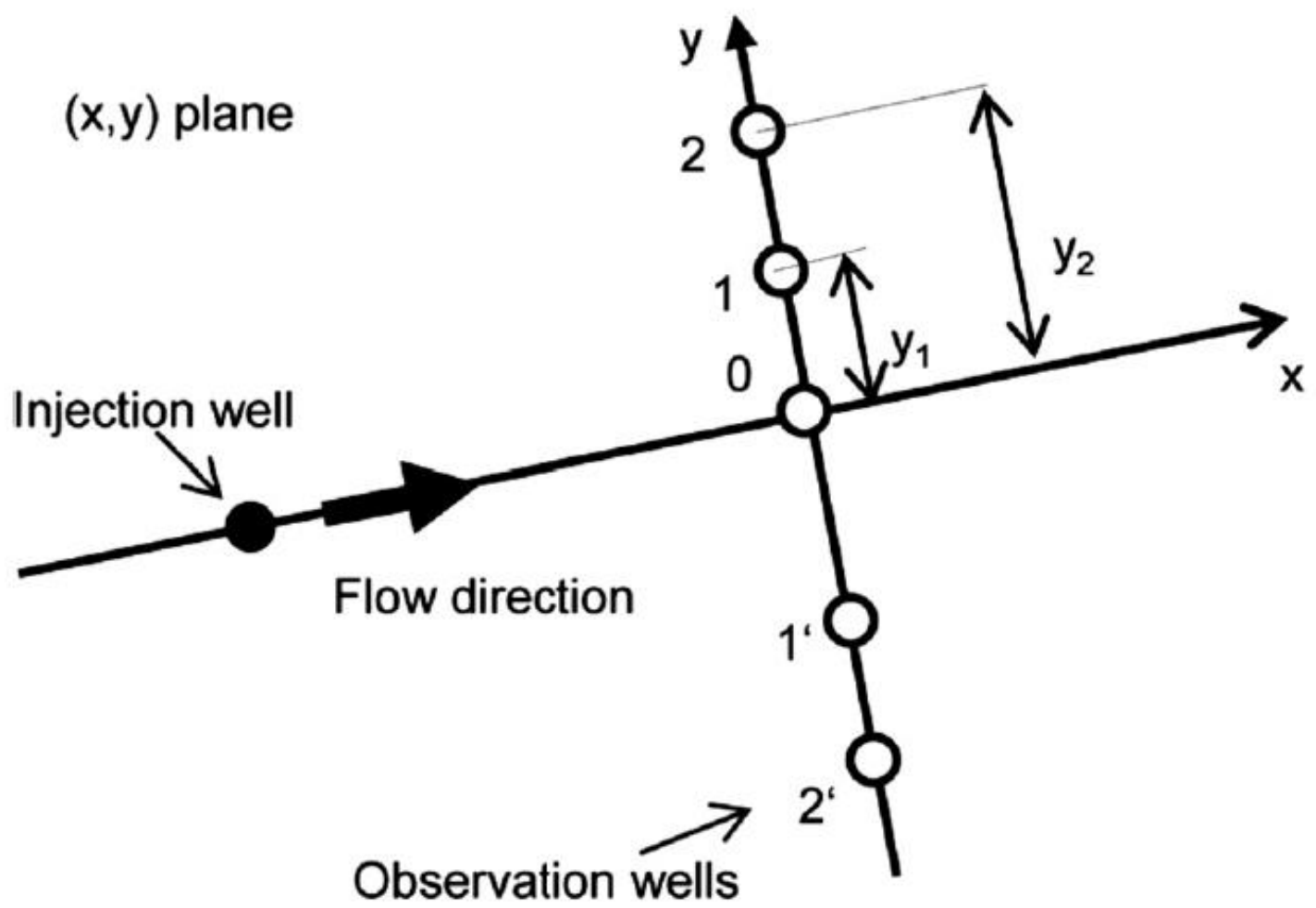
$$D_{yy} = D_T + \frac{D_m}{\tau}$$

$$D_{zz} = D_T + \frac{D_m}{\tau}$$

- $v < 0.1$ m/Tag :
 - $D_L = D_{xx}$
 - $D_T = D_{yy} = D_{zz}$

2D

Boundary conditions



2D

if

$$\frac{\partial C}{\partial z} = 0$$

then

$$D_L \frac{\partial^2 C}{\partial x^2} + D_T \frac{\partial^2 C}{\partial y^2} - v \frac{\partial C}{\partial x} = \frac{\partial C}{\partial t}$$

Boundary conditions

$$C(x = 0, y = 0, t) = \frac{M}{nH} \delta(t) \delta(x) \delta(y)$$

$$C(x, y, t = 0) = 0$$

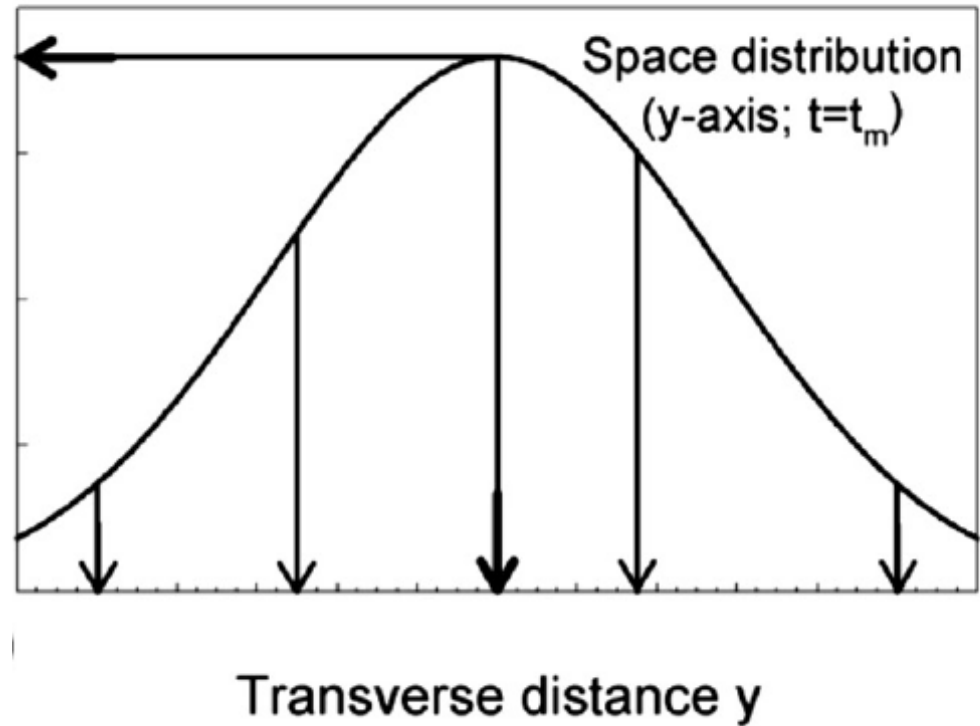
$$\lim_{(x, y) \rightarrow \infty} C(x, y, t) = 0$$

- M mass (g)
- n porosity
- H is thickness

Analytical solution 2D

$$C(x, y, t) = \frac{M}{nH} \frac{x}{4\pi vt^2 \sqrt{D_L D_T}} \exp \left[-\frac{(x - vt)^2}{4D_L t} - \frac{y^2}{4D_T t} \right]$$

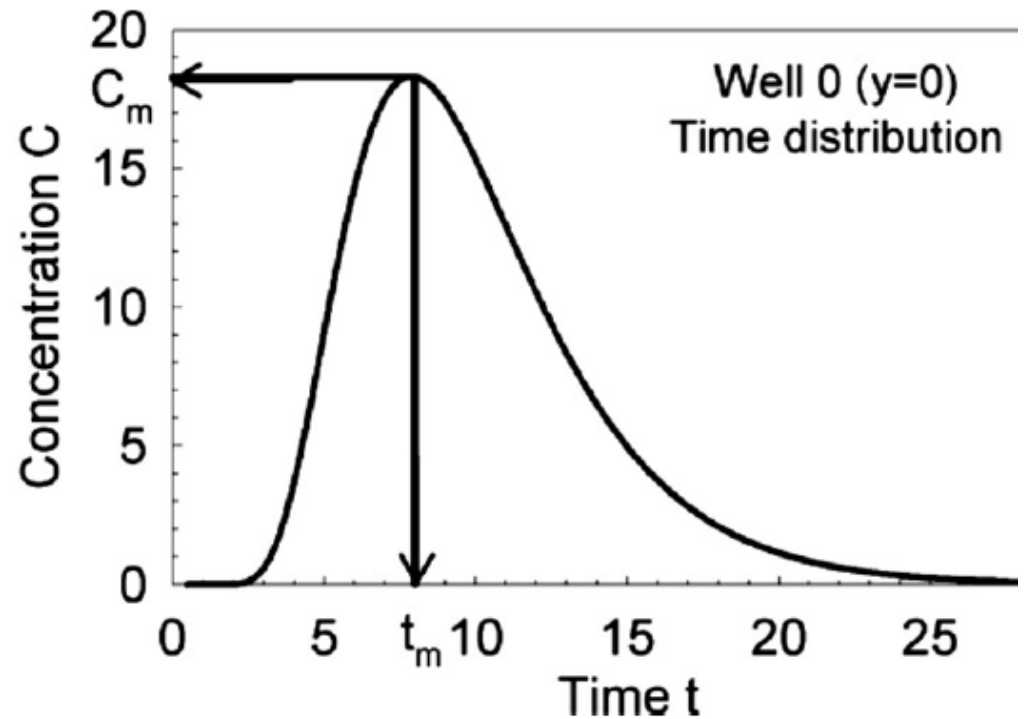
- M is mass (g)
- n is porosity
- H is thickness
- D_L is longitudinal
 D_T is transversal
Dispersion



Time equation 2D

$$C(t) = C_m \left(\frac{t_m}{t} \right)^2 \exp \left[-\frac{(x - vt)^2}{4D_L t} + \frac{(x - vt_m)^2}{4D_L t_m} \right]$$

- t_m is residence time*



Transverse dispersion

$$C(y) = C_m \exp \left[-\frac{y^2}{4D_T t_m} \right]$$

- y is transverse distance
- D_T is transversal dispersion coefficient
- t_m is residence time

Finally ...

1D

Momentaneous injection



- Dirac-Stoß

1D

if

$$\frac{\partial C}{\partial y} = \frac{\partial C}{\partial z} = 0$$

then:

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

- 1D no change in y and z
- Rivers and columns

Boundary conditions 1D

$$C(x = 0, t) = \frac{M}{Q} \delta(t)$$

$$C(x, t = 0) = 0$$

$$\lim_{x \rightarrow \infty} C(x, t) = 0$$

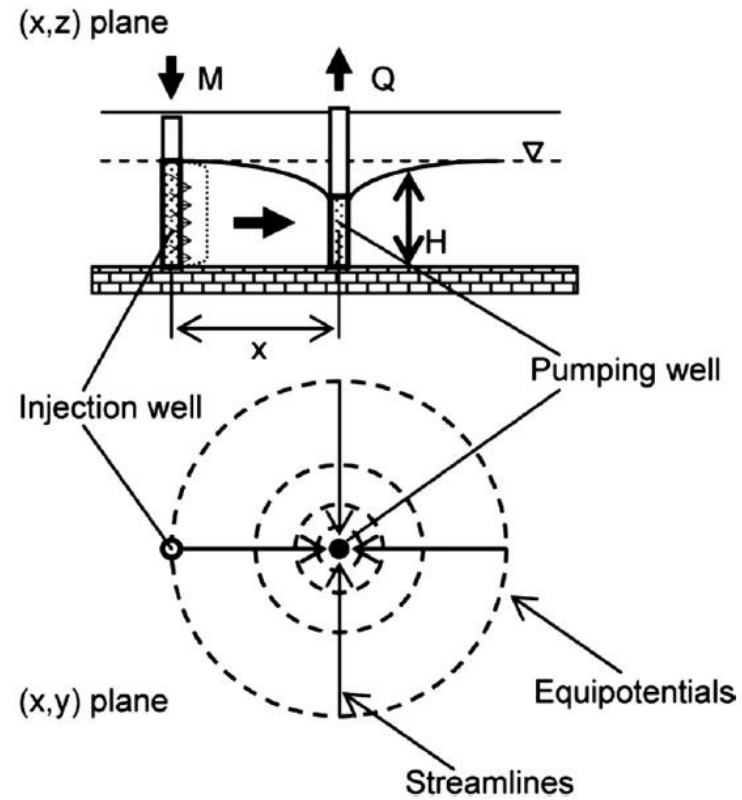
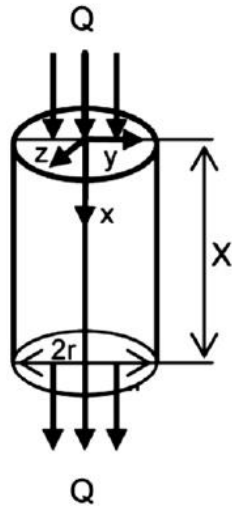
$$x \rightarrow \infty$$

Solution 1D

$$C(x, t) = \frac{M}{Q} \frac{x}{\sqrt{4\pi D_L t^3}} \exp \left[-\frac{(x - vt)^2}{4D_L t} \right]$$

- Main equation 1D
- C depends on M and 1/Q and $D_L^{-1/2}$ and $1/t^{3/2}$ and decreases exponentially with x^2

Radial 1D



- Applicable to wells

Residence time

$$t_0 = \frac{x}{v}$$

$$t_0 = \frac{V}{Q}$$

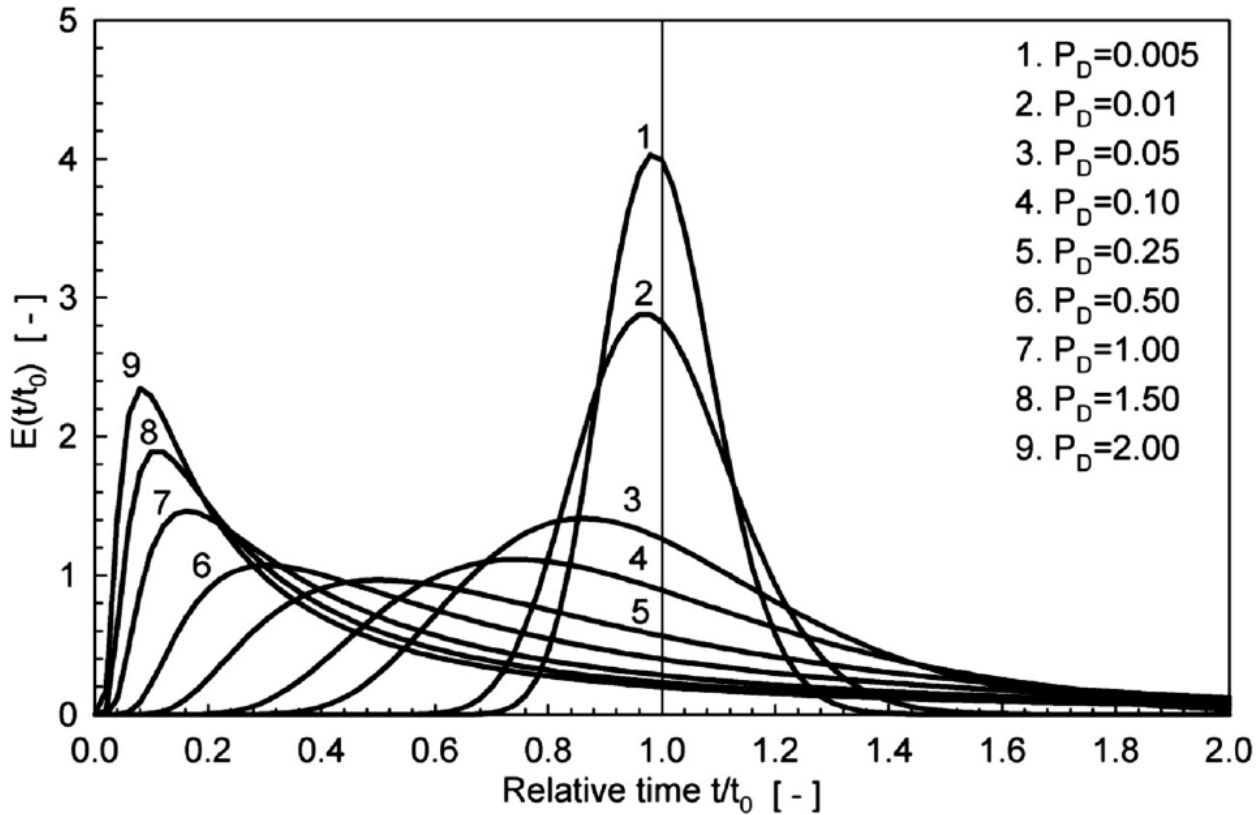
- In proportion to Volume and
- In inverse proportion to discharge

Dispersion parameter (Definition)

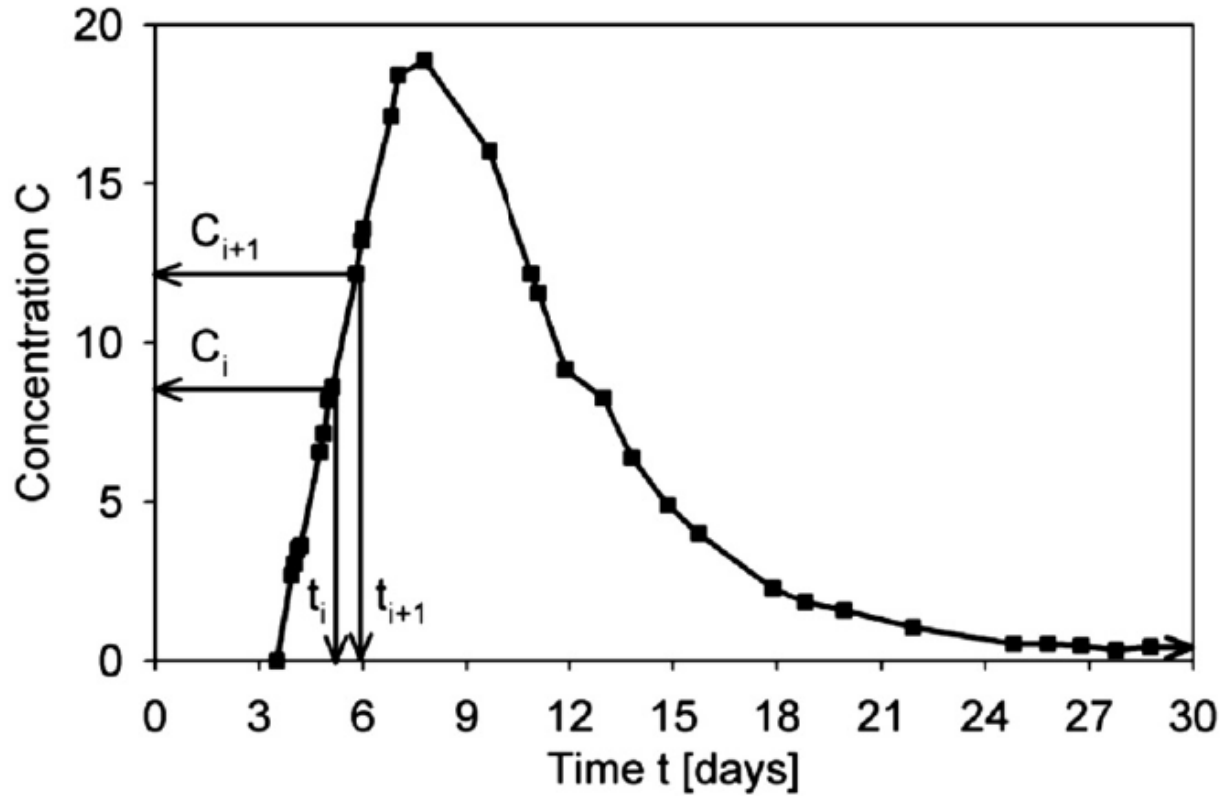
$$P_D = \frac{D_L}{vx} = \frac{\alpha_L}{x}$$

- Dispersion coefficient per velocity
- Dispersivity per length x
- Dispersion parameter corresponds to α/x

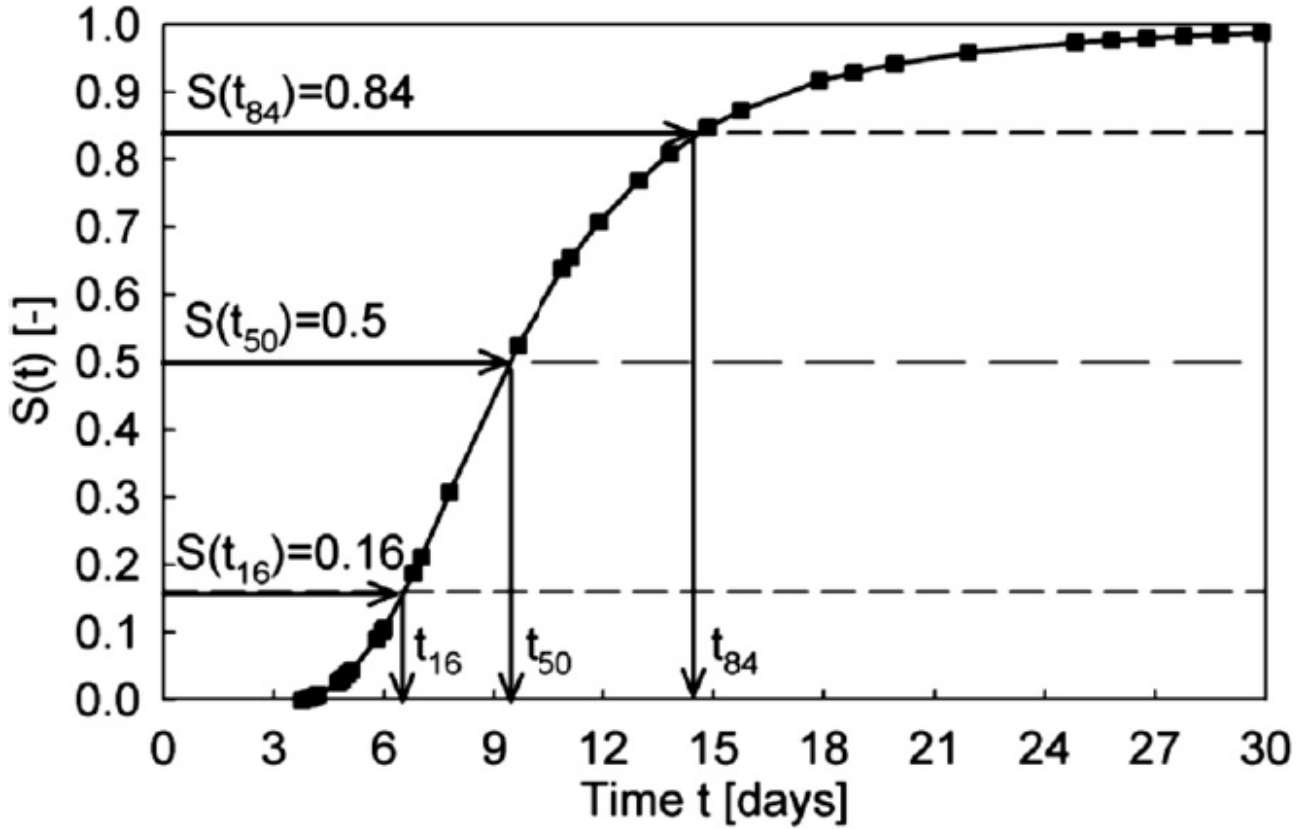
Normalized curves



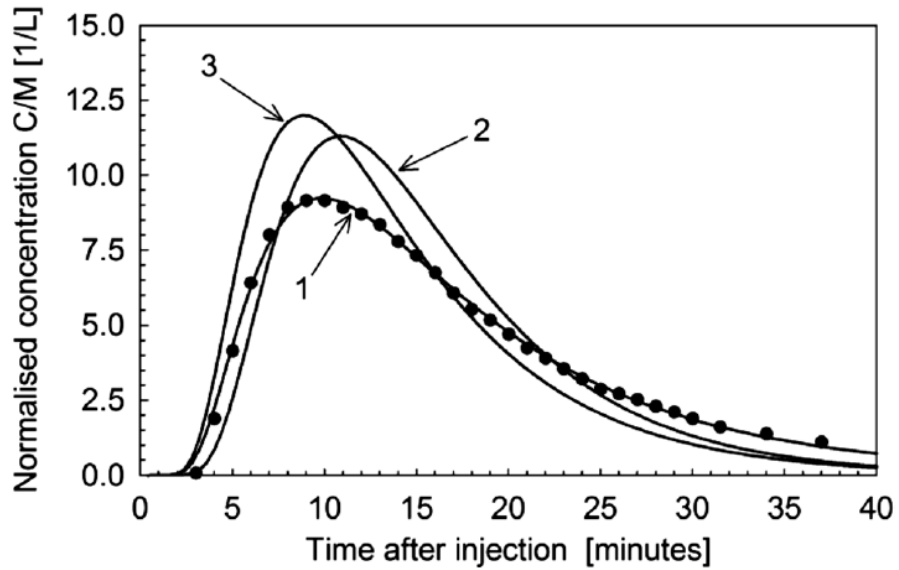
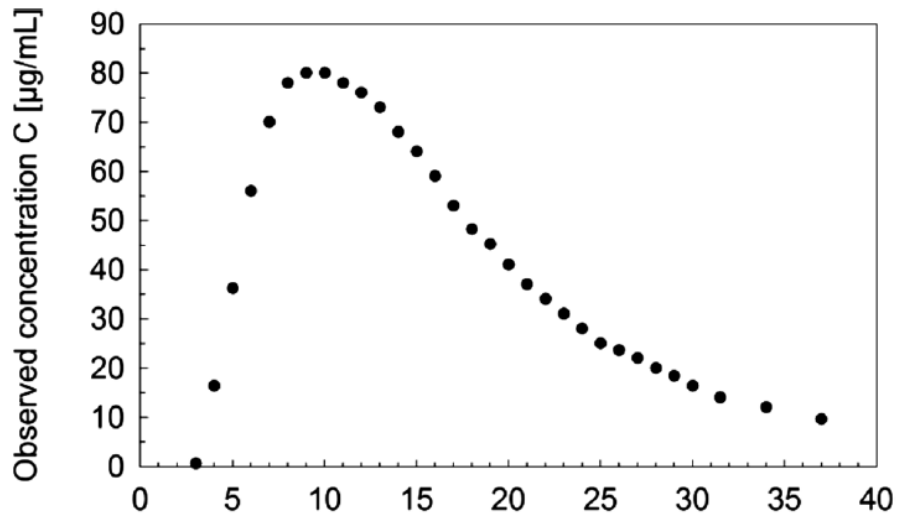
Measurements



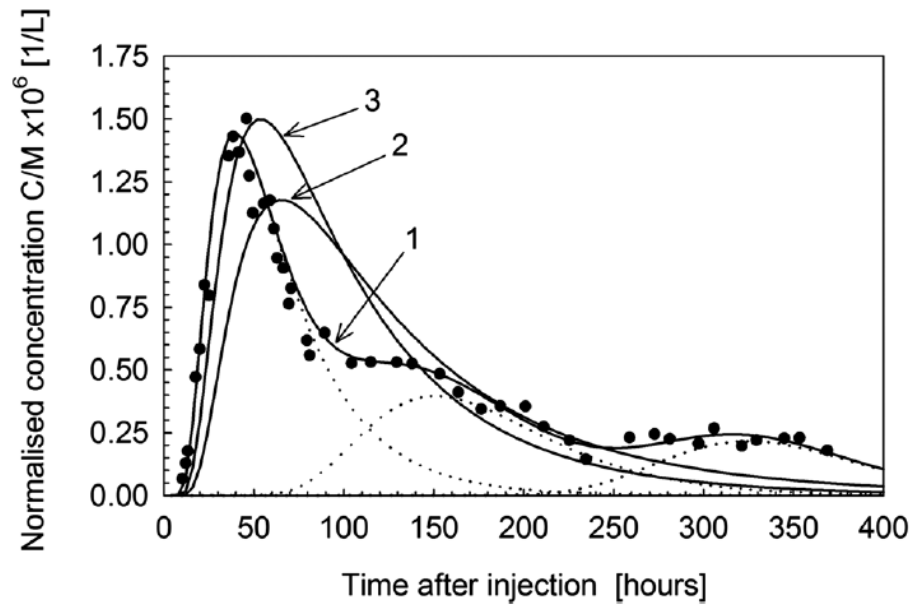
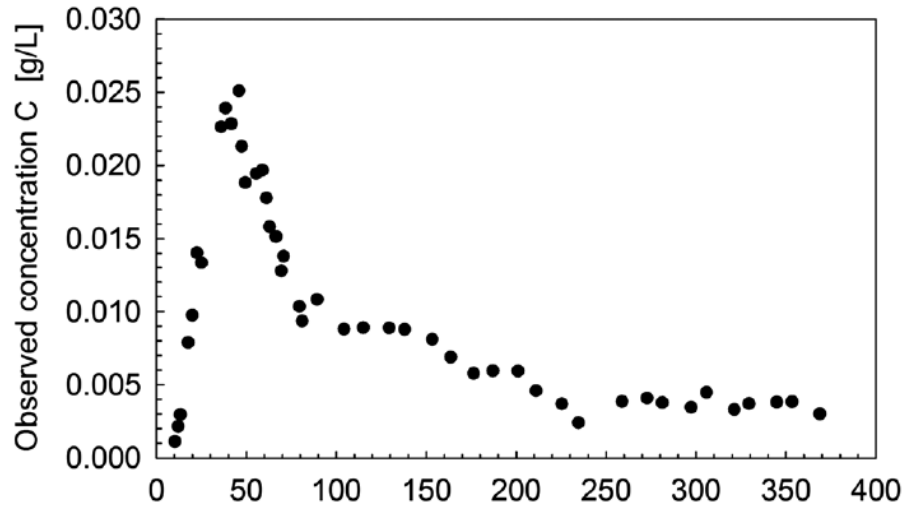
Mass curve



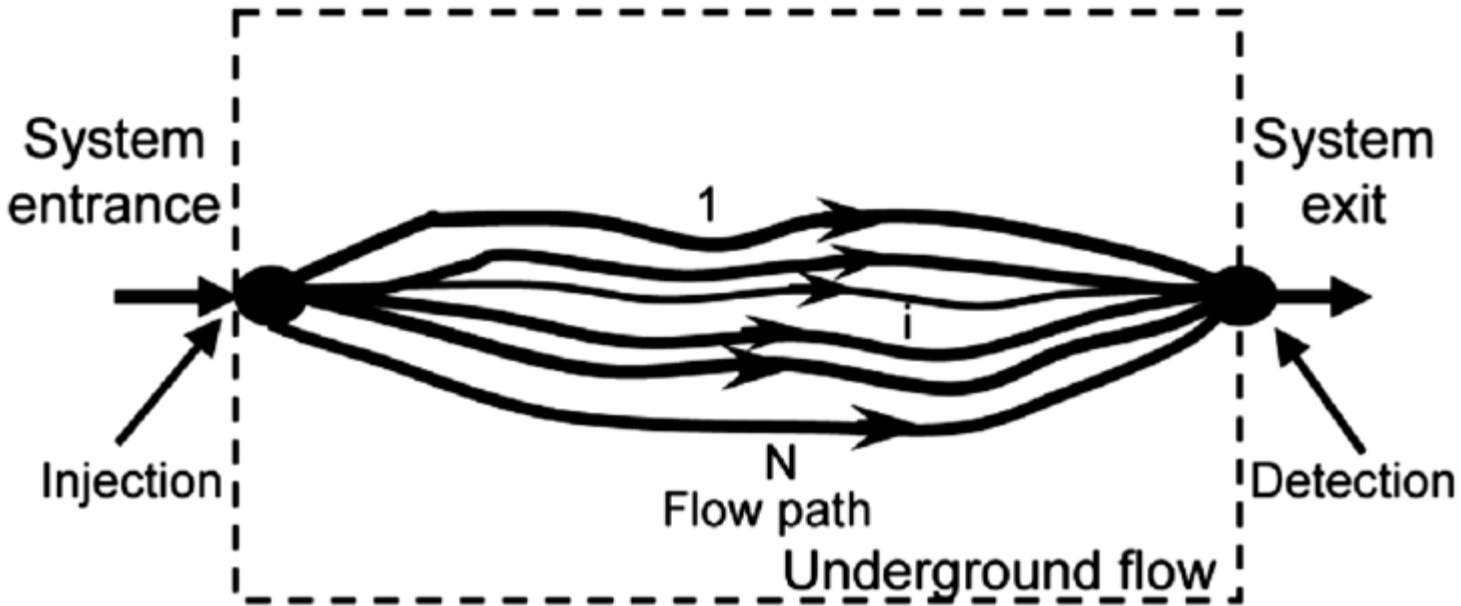
Fitting



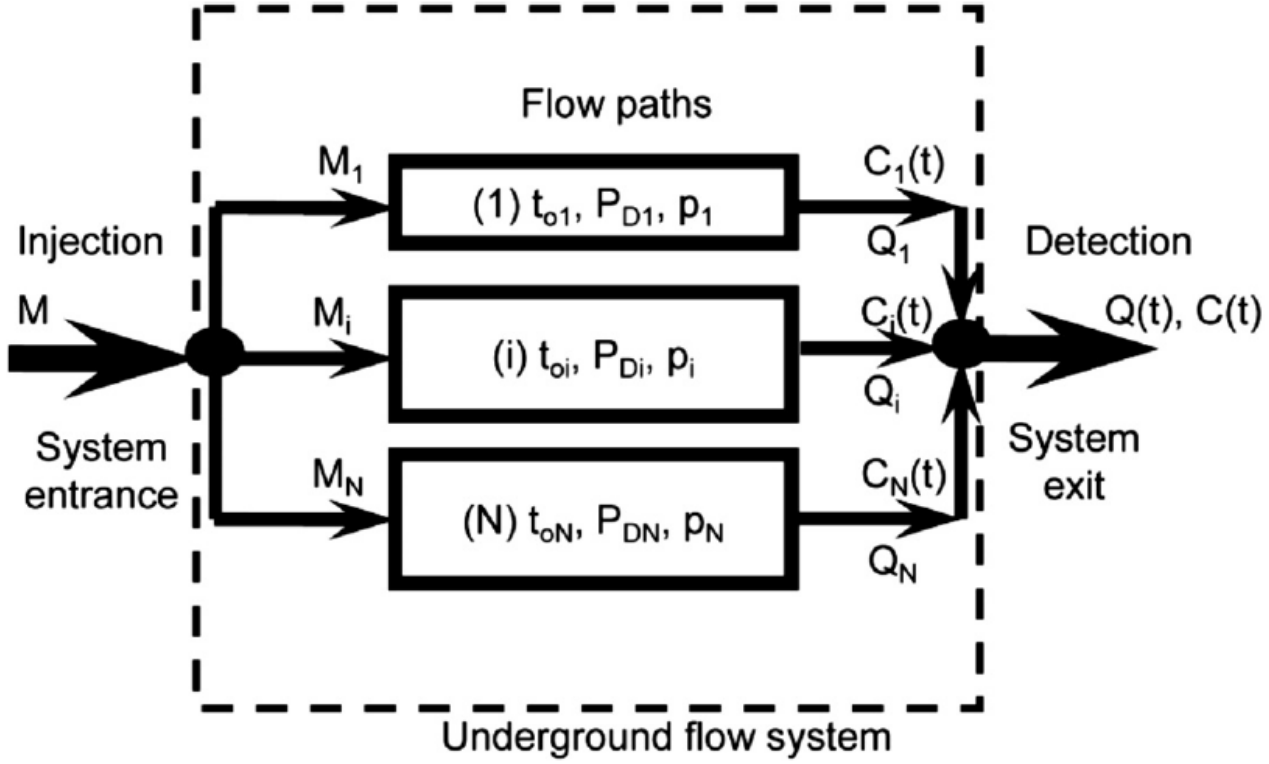
Multifinalität



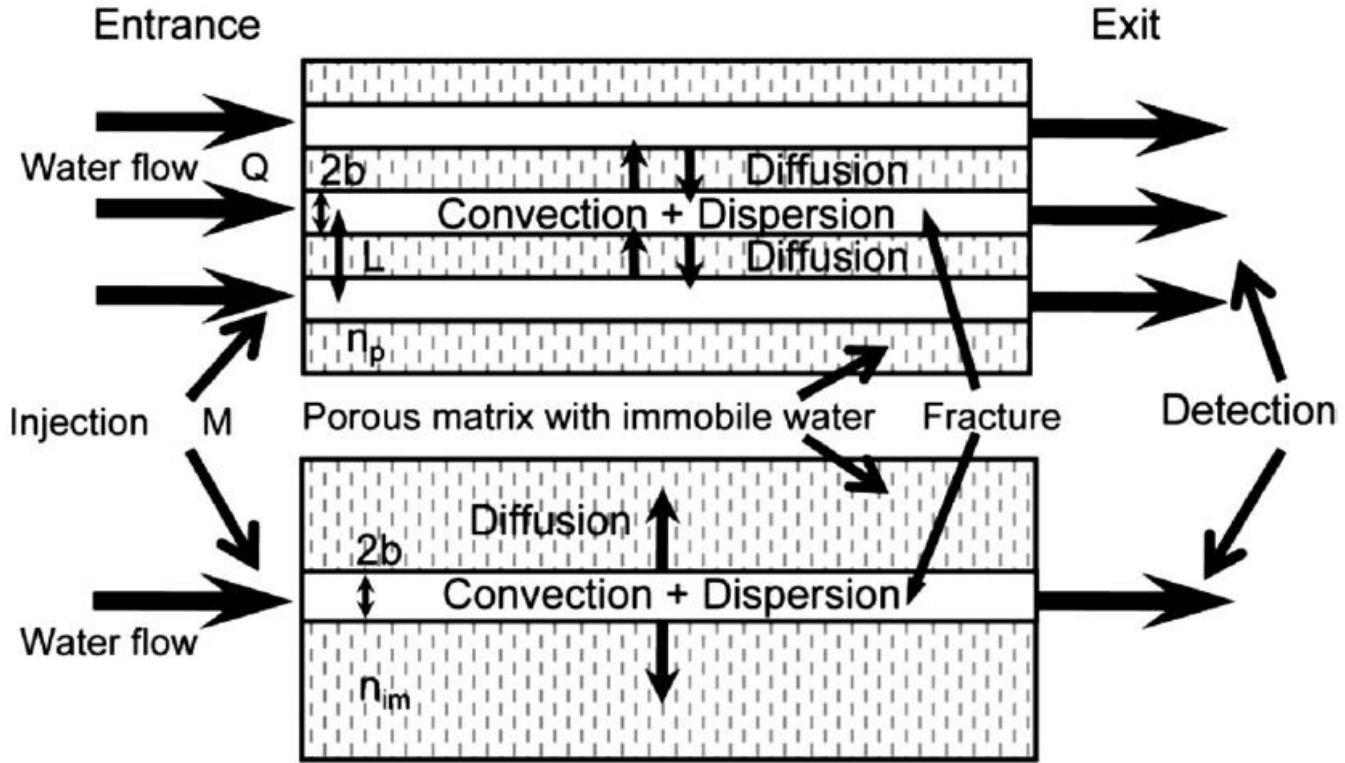
Conceptual model



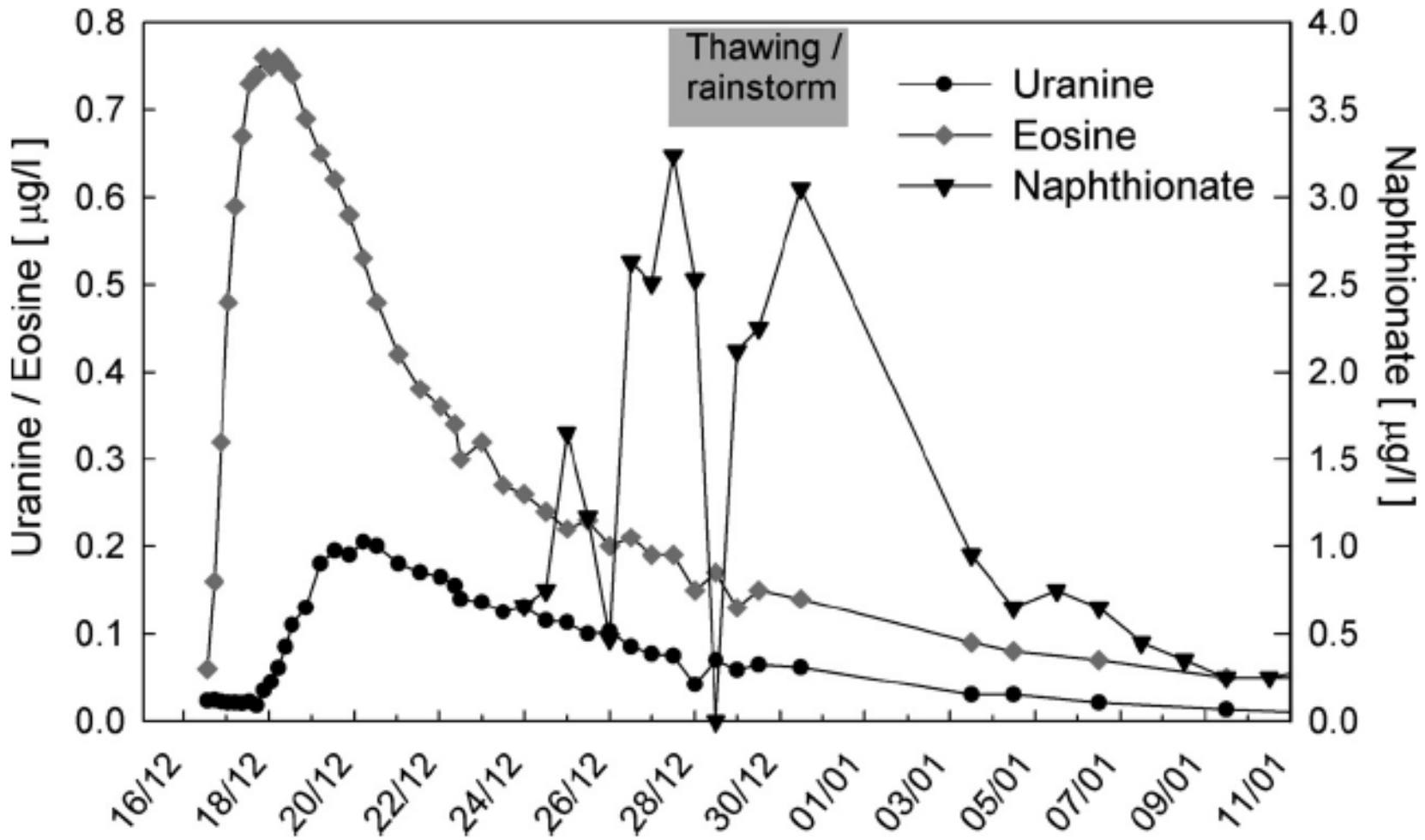
Parallel ADV Models



Dispersion and Diffusion



Example



Rhein

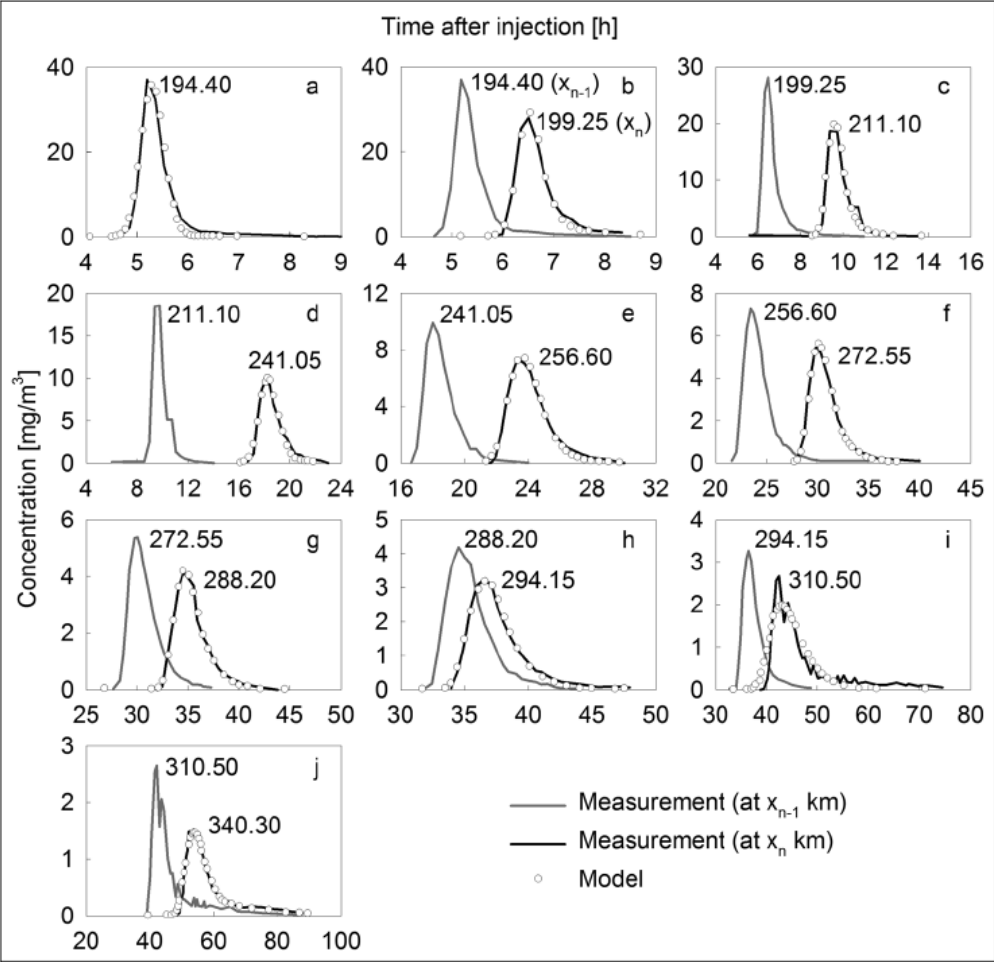


Figure 7.24 Experiment 04/89. Measured tracer breakthroughs at the following river sections (x_n): Ottmarsheim (km 194.4), Neuenburg (km 199.25), Fessenheim (km 211.1), Marckolsheim (km 241), Rheinau (km 256.6), Gerstheim (km 272.5), Strasbourg (km 288.2), Kehl (km 294.1), Gambsheim (km 310.5), Plittersdorf (km 350.3).

Fitting of models

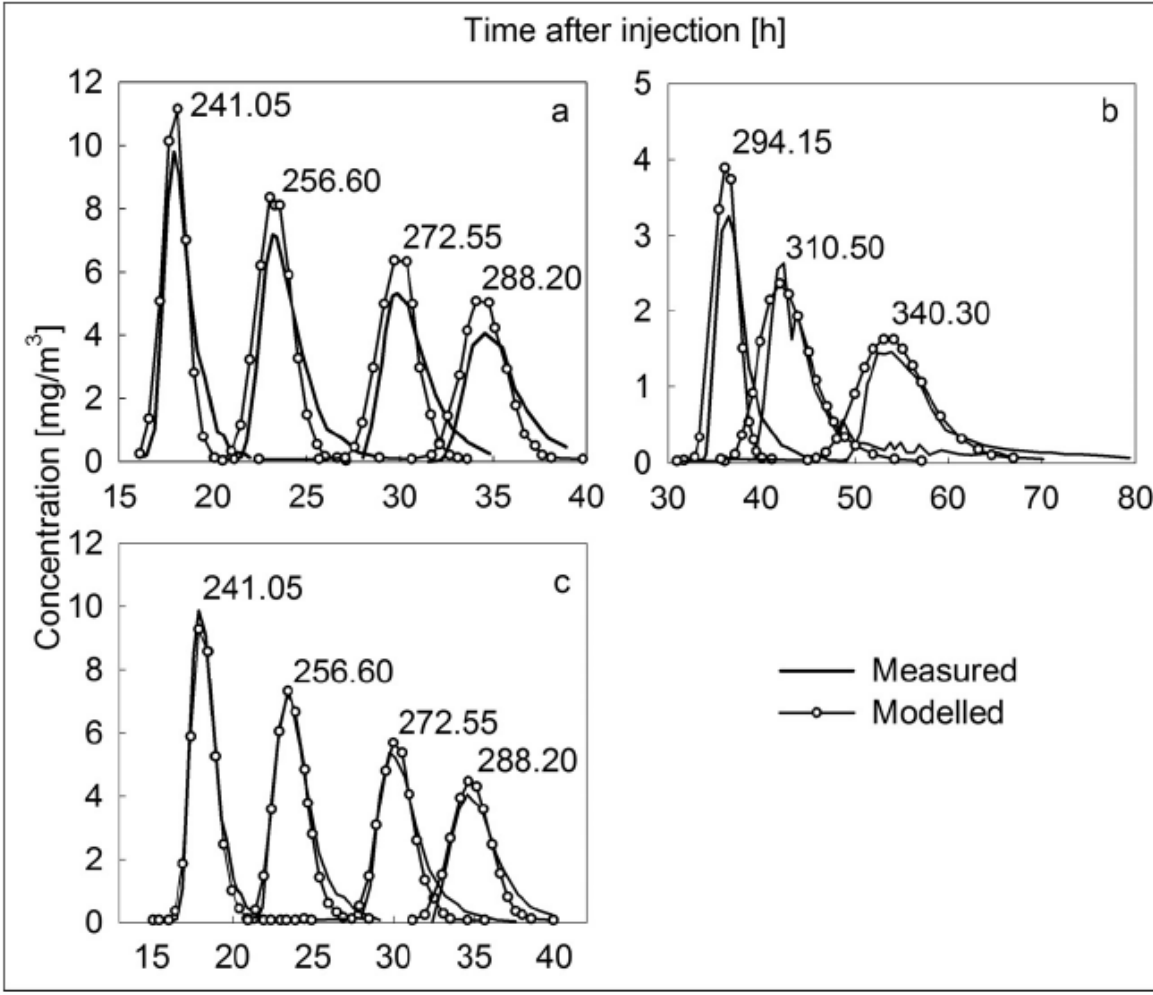
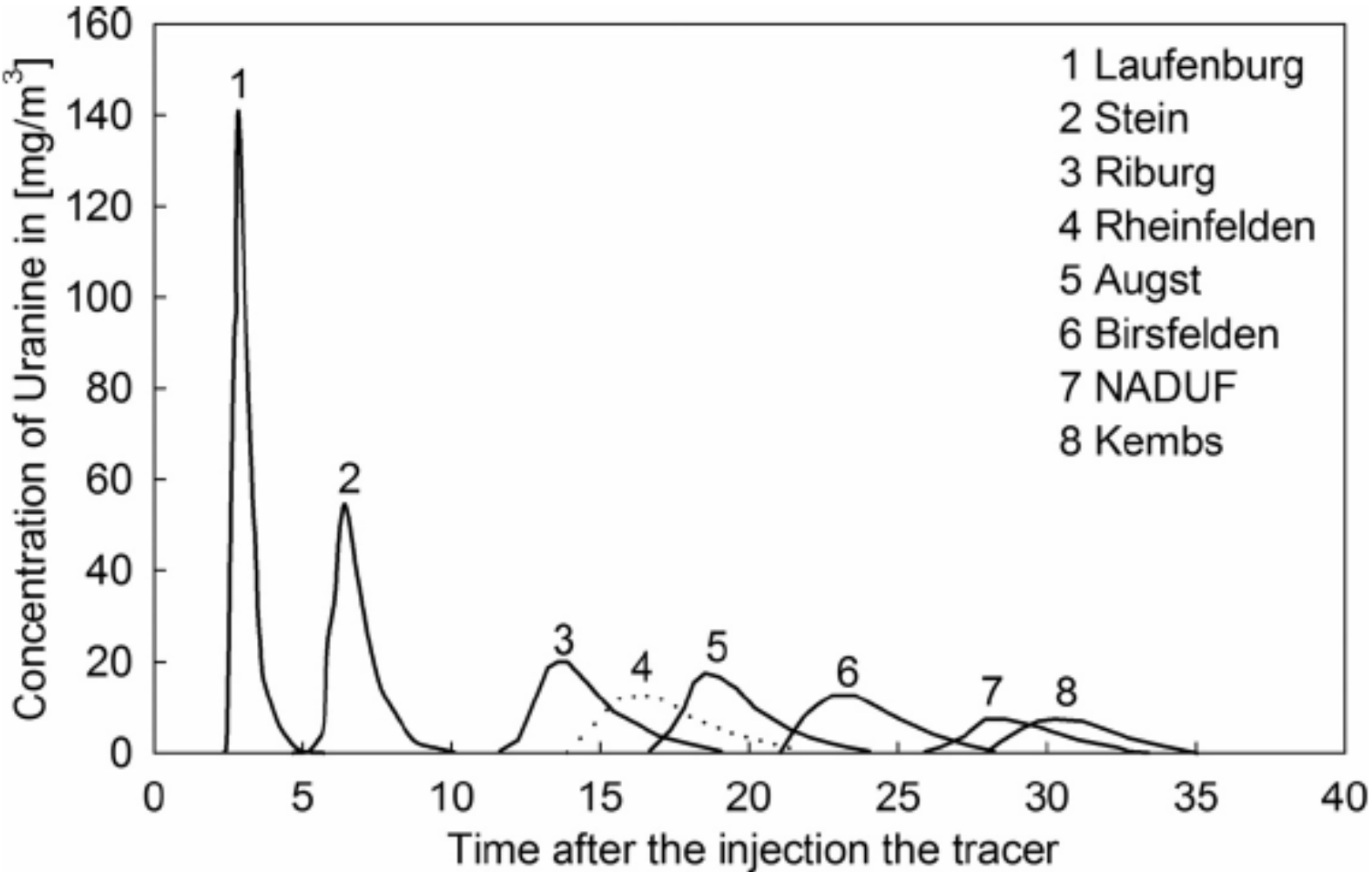


Figure 7.25 Validation of the Upper Rhine river sections: a) postmodelling, Rhine km 241.05–288; b) postmodelling, Rhine km 294.15–340.3; c) forecast improvement, Rhine km 241.05–288.2.

Warning model

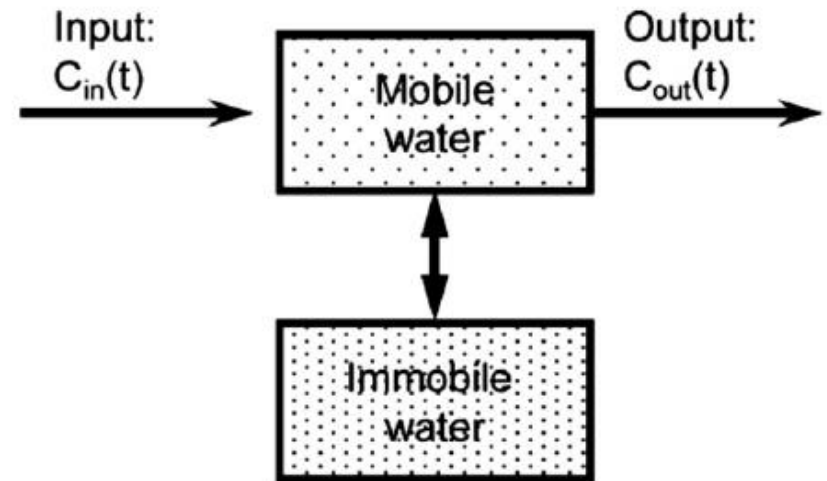


Combining advection dispersion and diffusion into dead zones

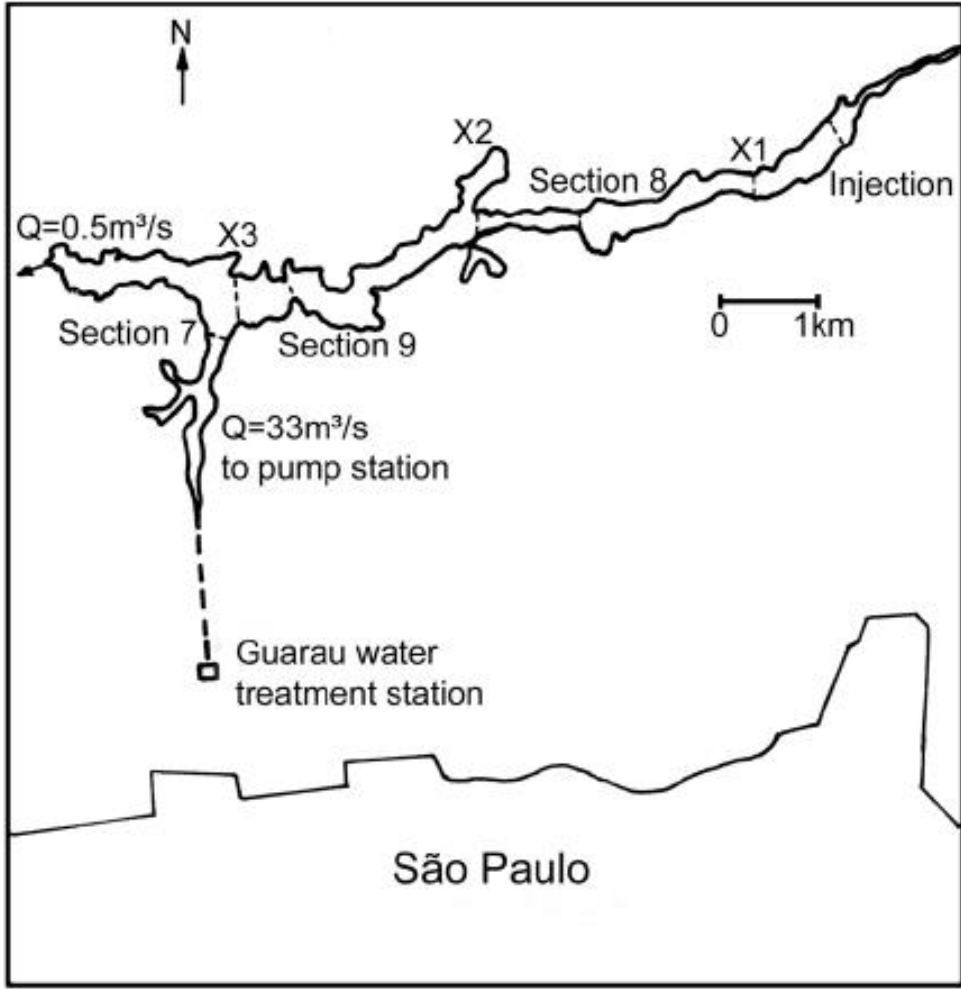
Single-porosity medium



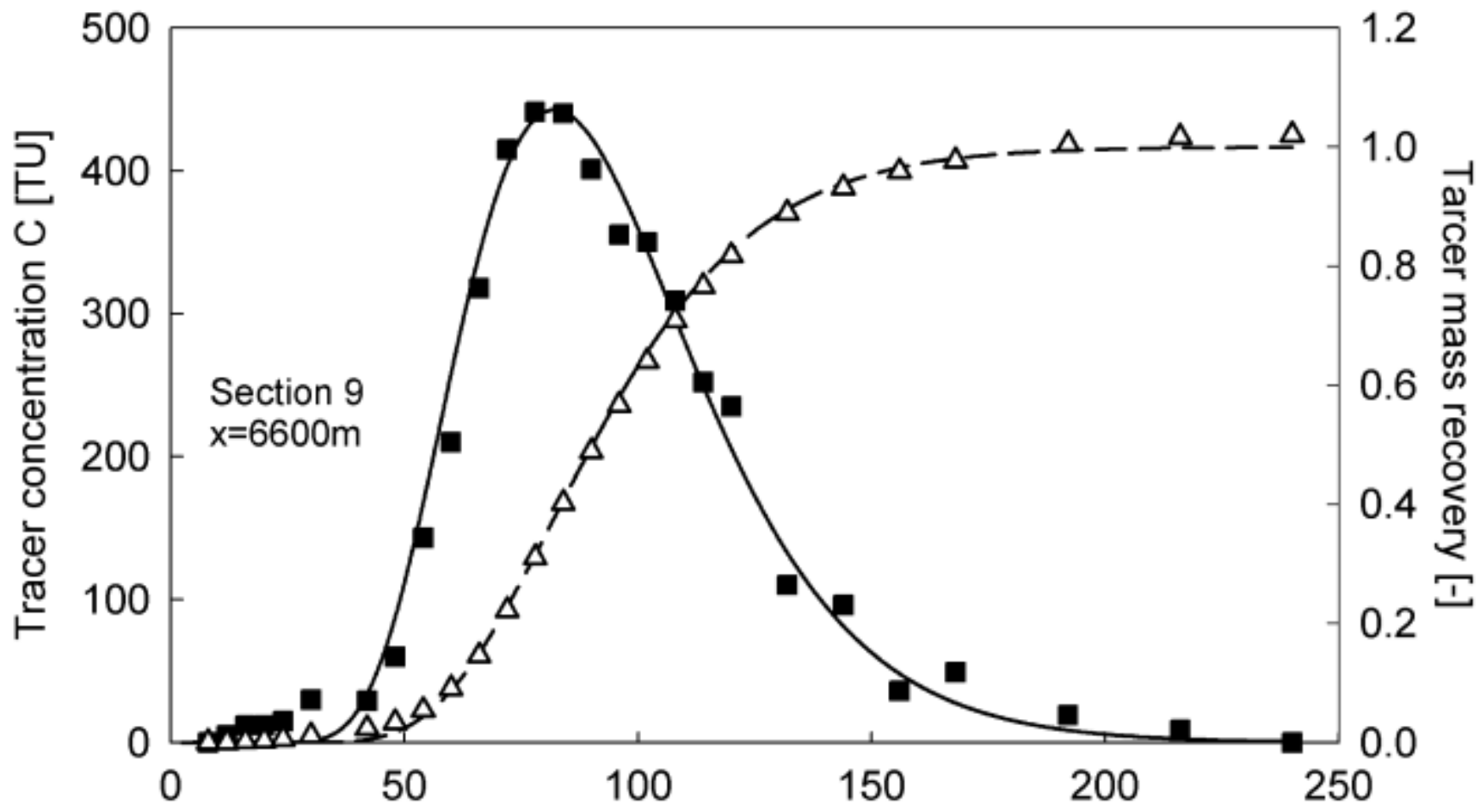
Double-porosity medium



Brasil



Determining the residence time of water in a surface reservoir in Brasil near Sao Paulo



Summary

- ADV has analytical solutions for 1D, 2D
- Can be used to predict breakthrough
- Can be used to calculate mass M
- Fundamental equations for predicting mass transport