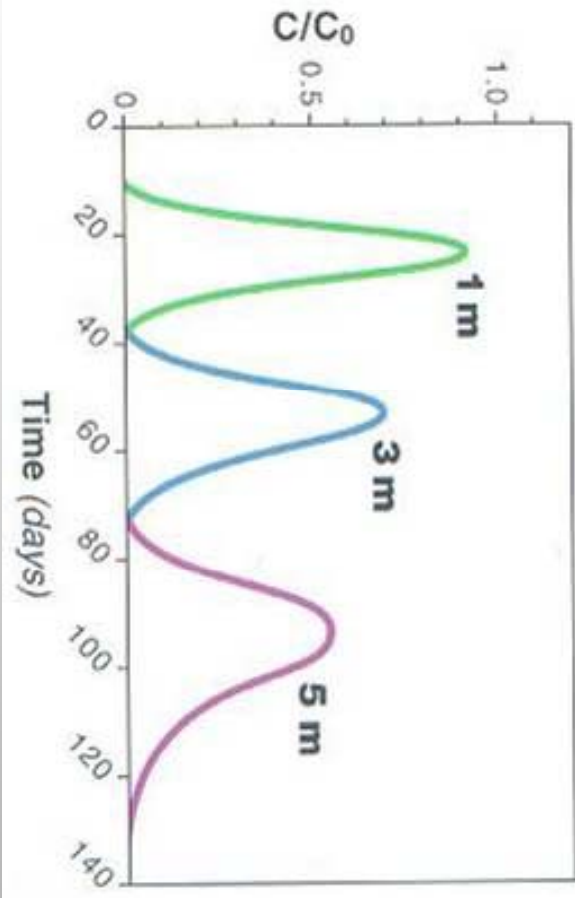


Measuring and modeling of solute transport in soils



- Prediction of the solute transport in soils: fertilizer, salts, pesticides, trace elements
- Influence of different parameter on solute transport
- Determination of solute transport parameter
- Insight into the plant nutrient dynamics in the soil: uptake of nutrients by roots
- Influence of plant uptake on concentrations
- Leaching of plant nutrients from the rooting zone e.g. nitrate
- Development and optimization of the agricultural practice:
 - Minimizing of fertilizer losses
 - prevent the salinization due to irrigation
- Insight into the transport of environmental pollutants: prediction of their behavior in the environment

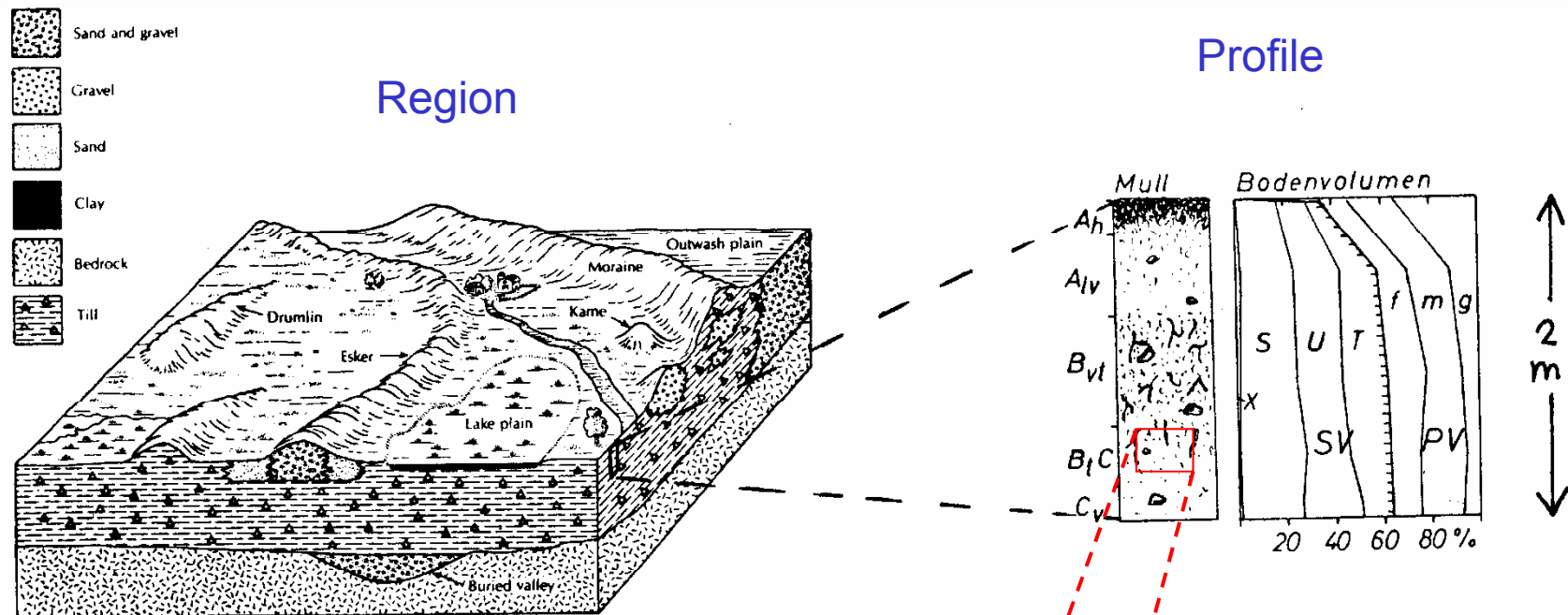
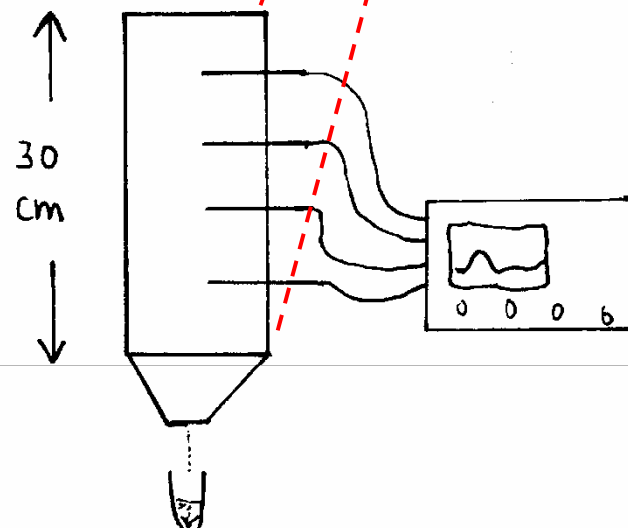


FIGURE 8.1 Distribution of sediments in a glaciated terrane.

Soil texture composition

Column



The measurement problem or the difference between a lab column and a field

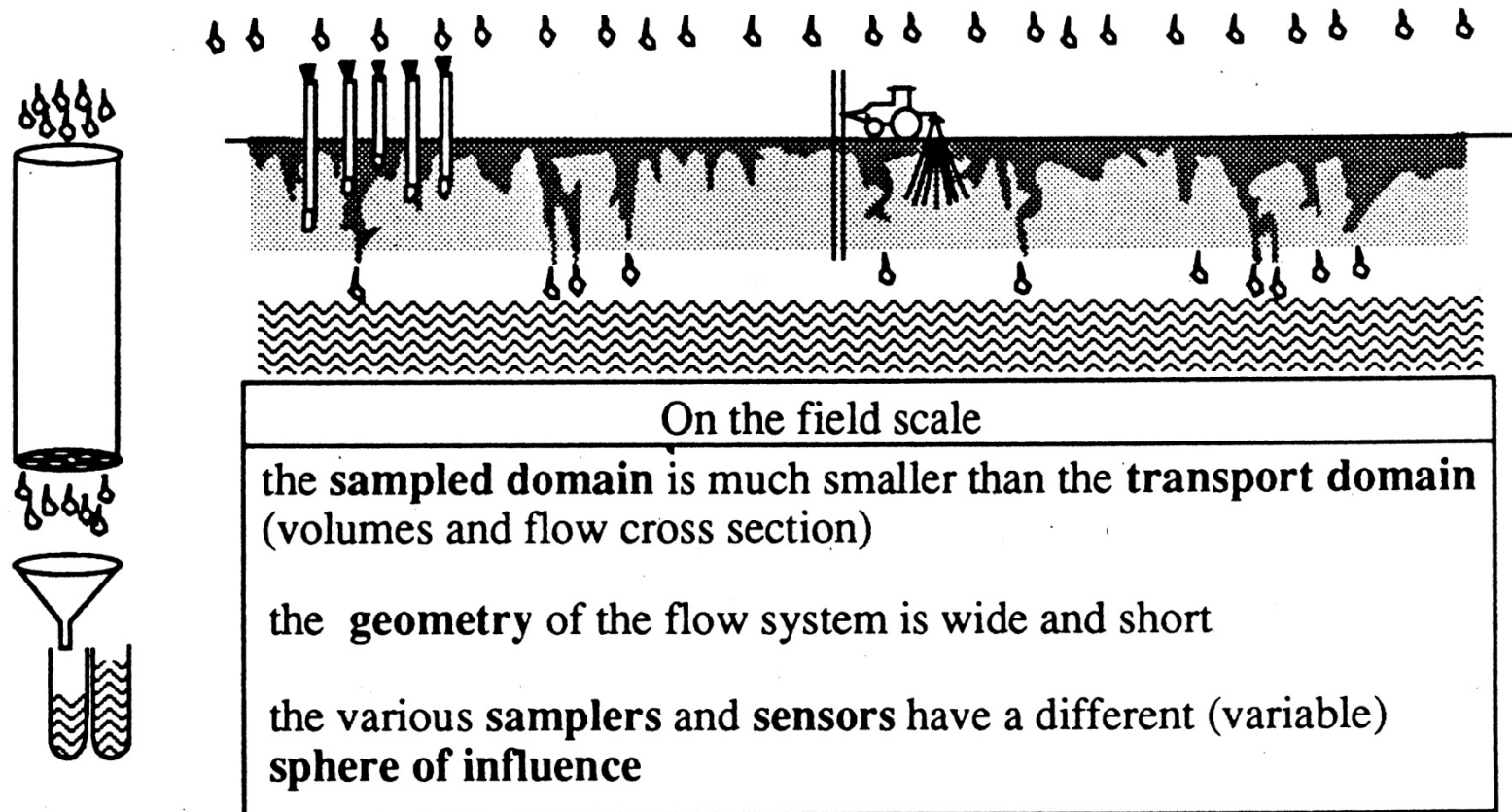


Fig.1 A field (soil) and a laboratory soil column are two very different systems. The scaling-up from lab scale to field scale is a problem which still waits to be resolved.

Macropores

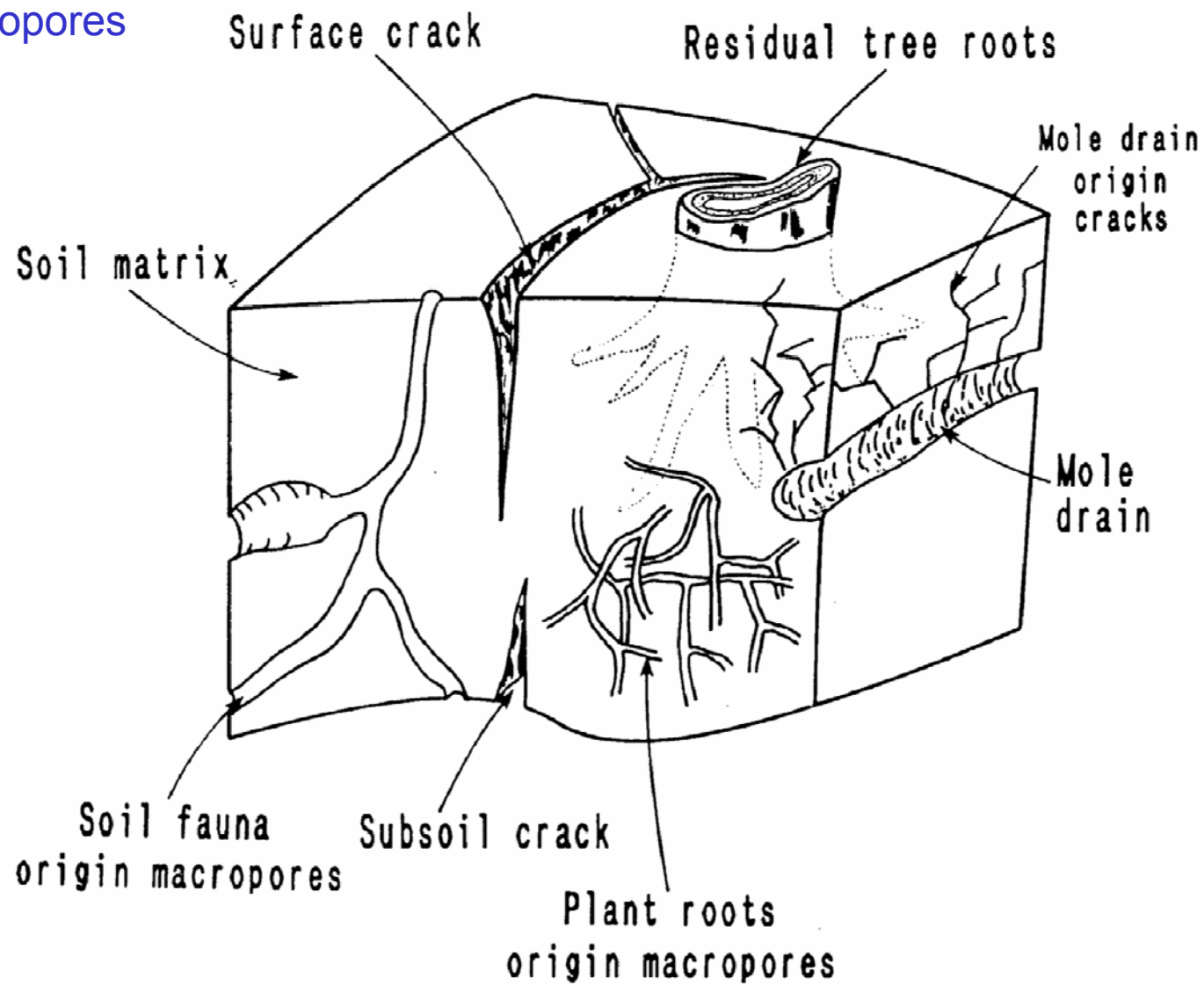
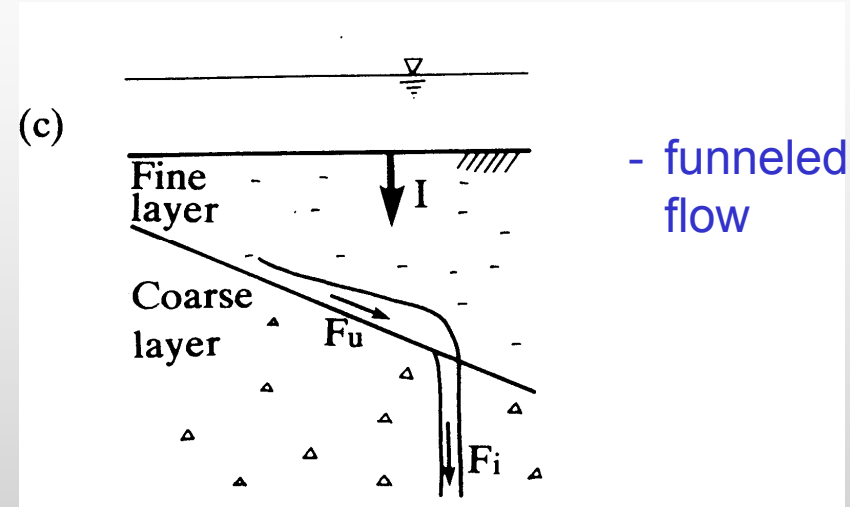
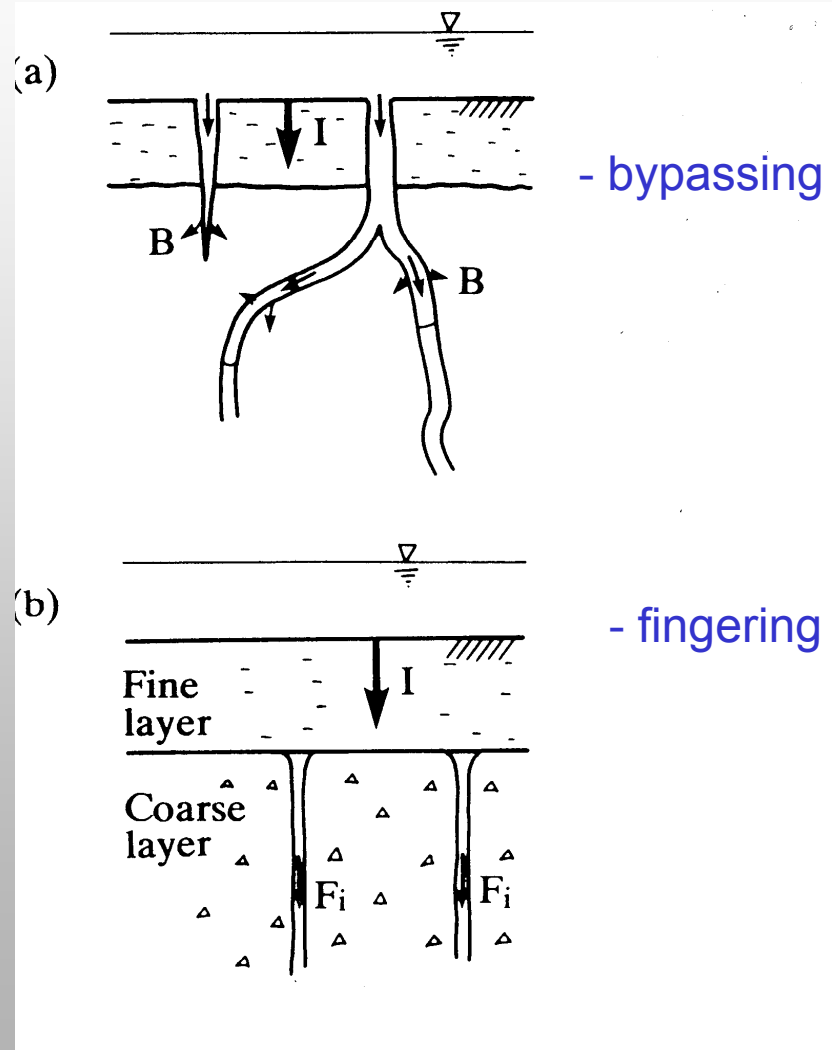
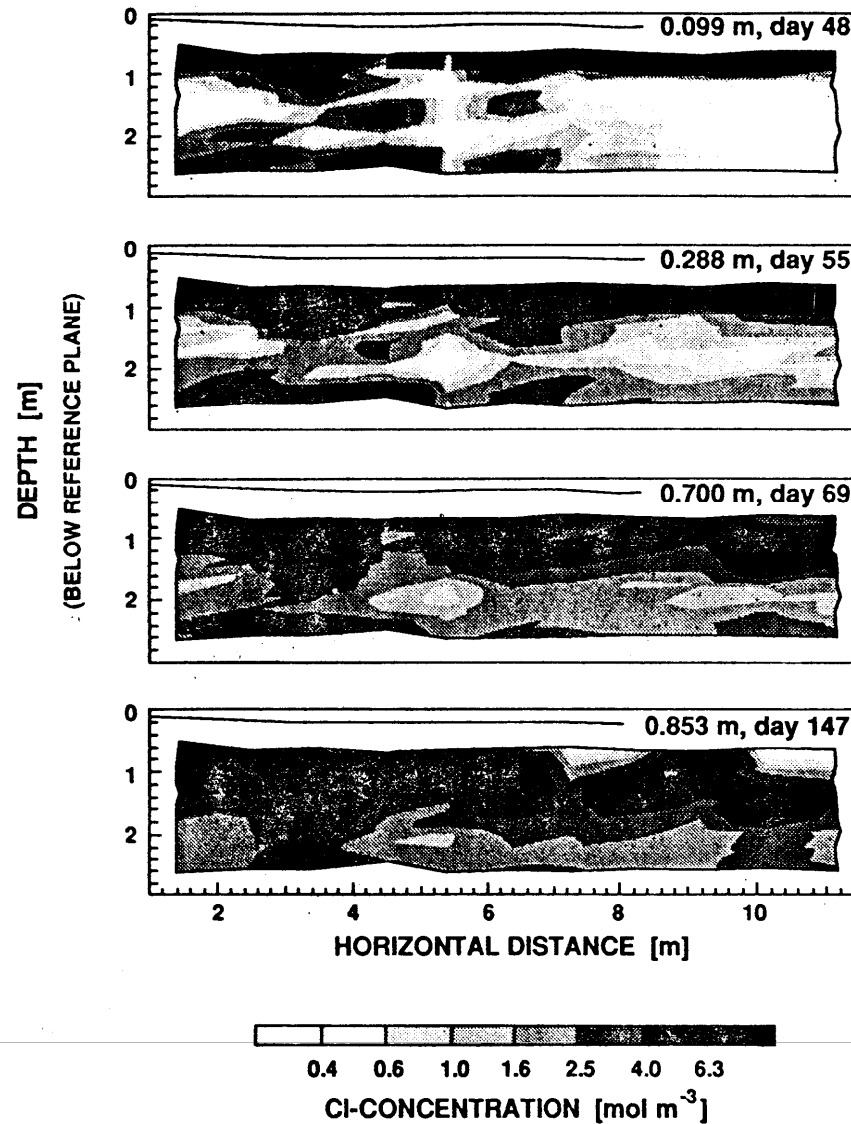


Figure 9.22 Exaggerated macropores in soils.

Preferential flow



ROTH ET AL.: CHLORIDE TRANSPORT THROUGH AN UNSATURATED FIELD SOIL



6. Spatial distribution of the tracer after a cumulative infiltration of 0.099 m (beginning of irrigation), 0.288 m (one third of the irrigation), 0.700 m (end of irrigation) and 0.853 m (end of the experiment).

Preferential flow





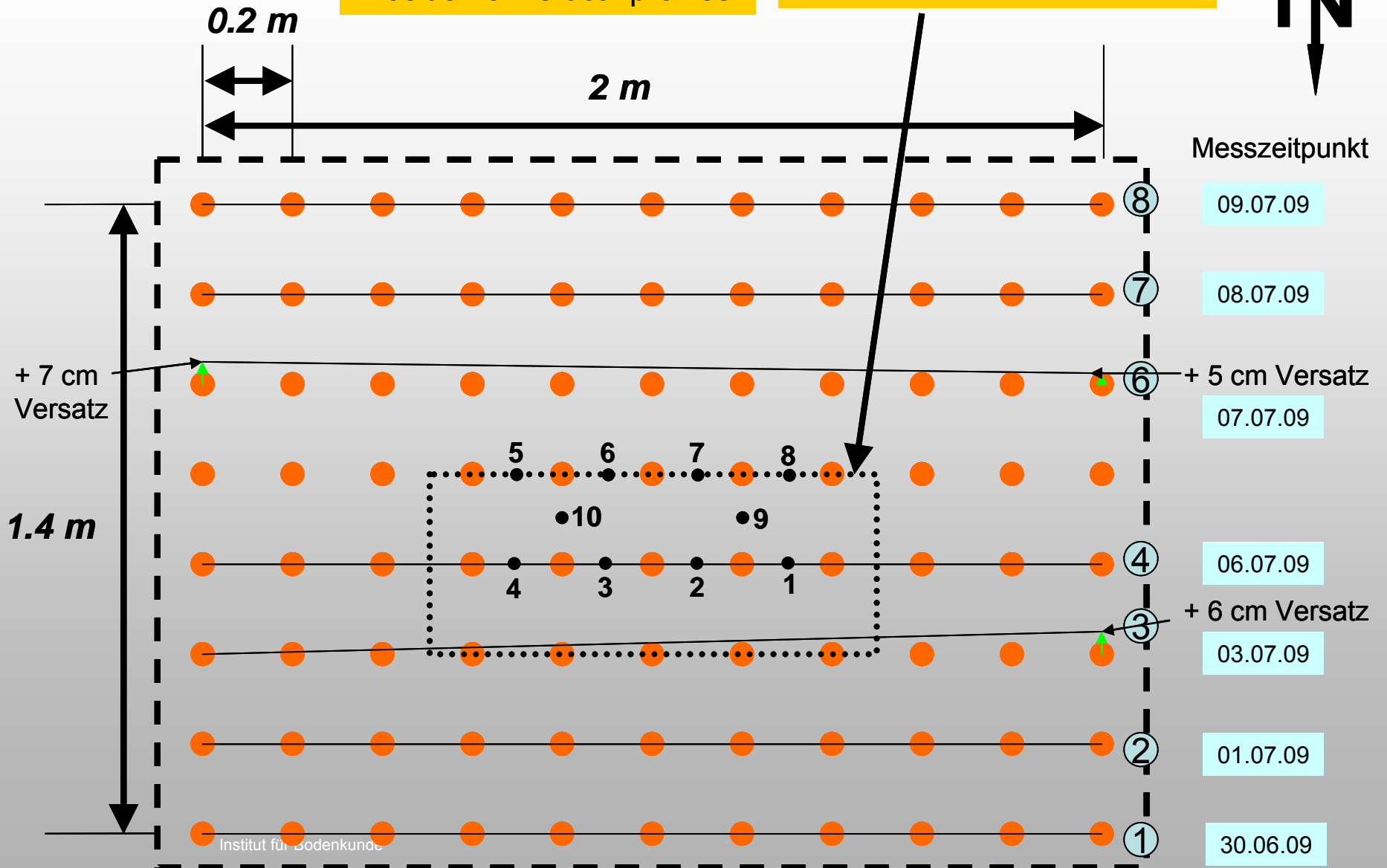
Infiltration experiment with:
- ERT-measurements
- soil physical measurements

Solute transport

● ERT-Elektroden ● Tensiometer

Position of vertical profiles

Water application area 0.4 x 1.0 m²



Institut für Bodenkunde

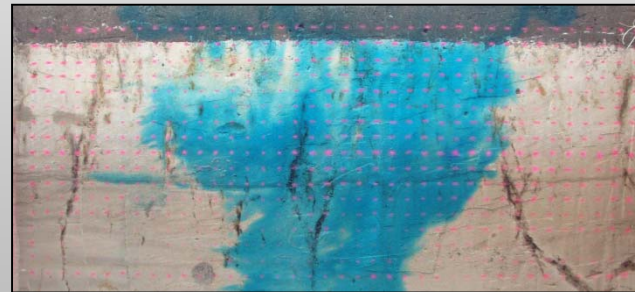
Ganz et al., 2010)

Tracer experiment 2009: - water application area 0.40 * 1.00 m
- Brilliant Blue
- water application amount 200 mm in 8 h.

Vertical profile 2
(40 cm from center)



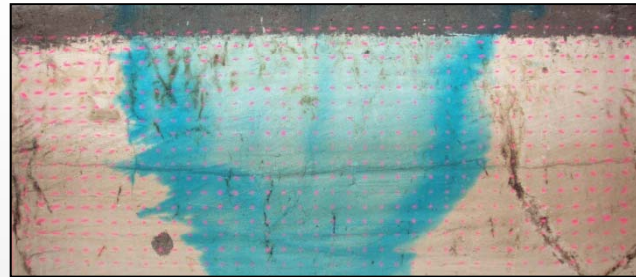
Vertical profile 3
(20 cm from center)



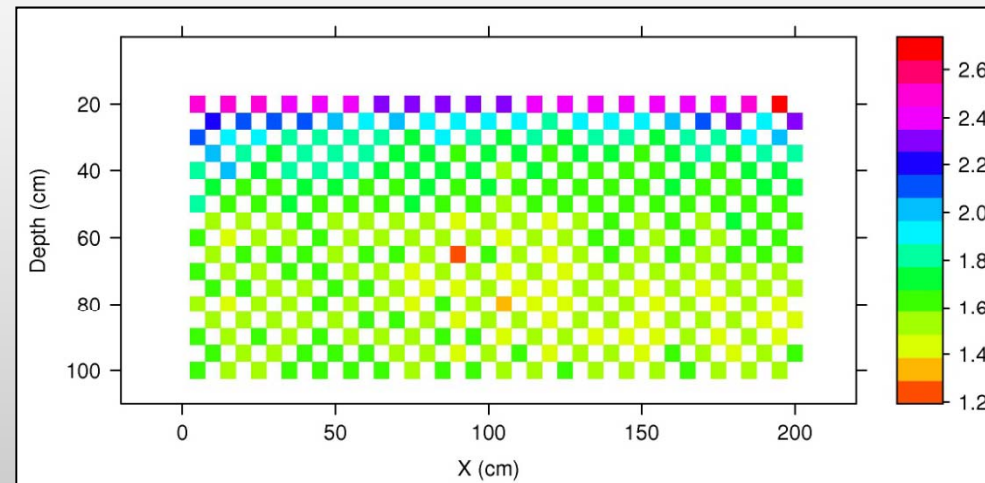
Vertical profile 4
(center)



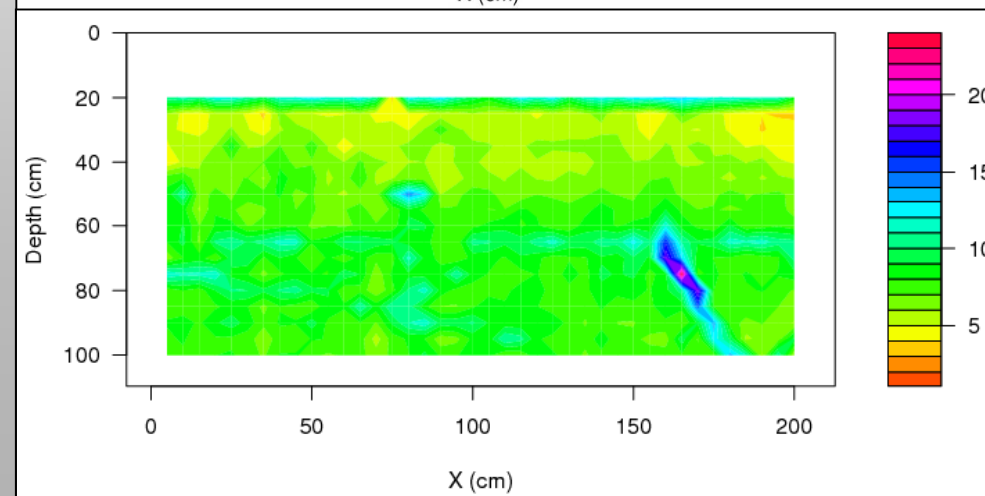
Vertical profile 4 (center)



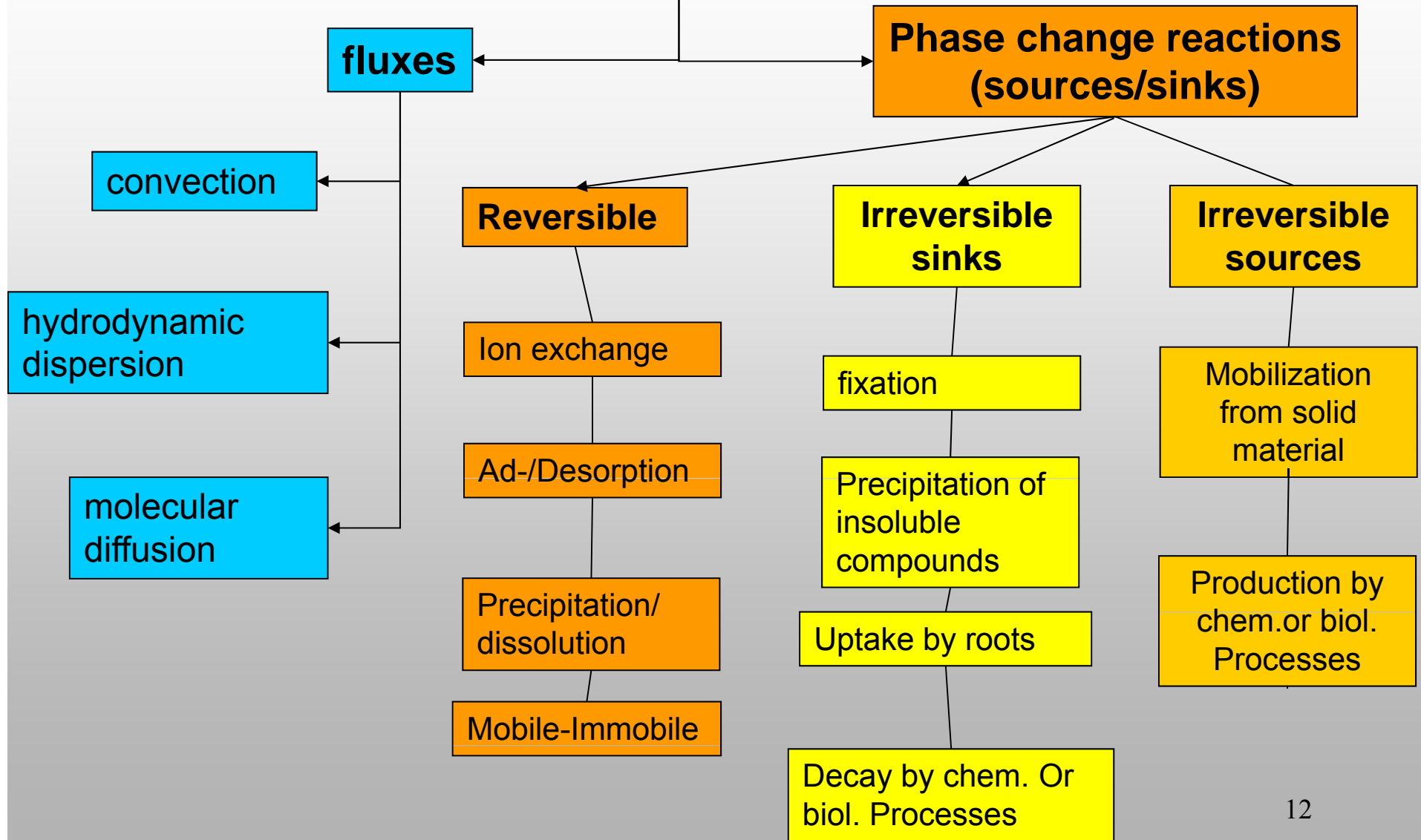
matric potential (pF)



Water content (%-vol.)

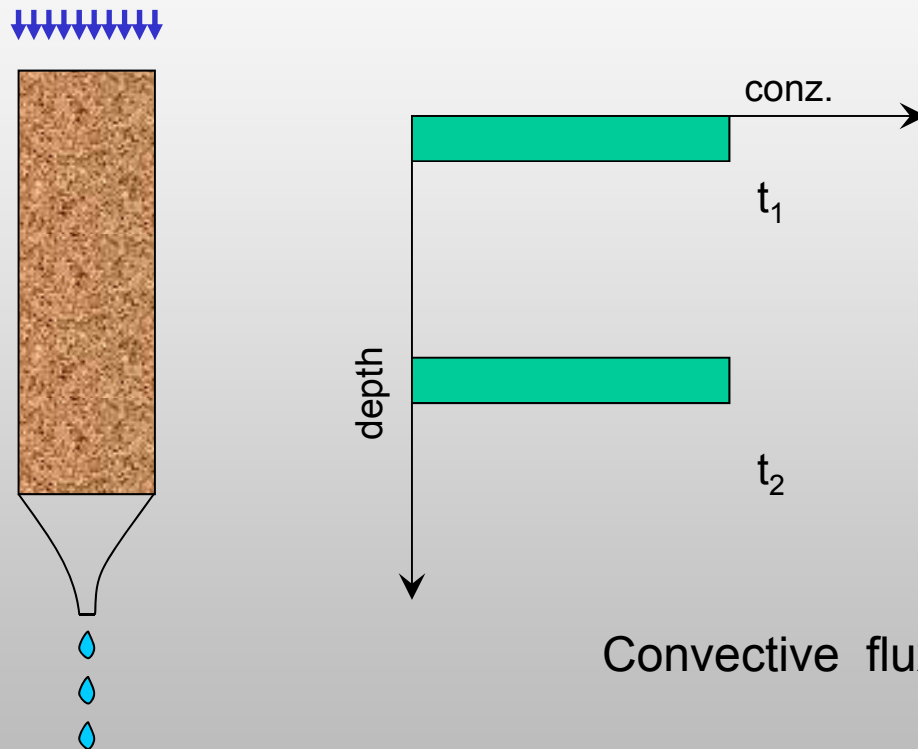


Transport mechanism and processes in soils



Mass flow or transport by convection

In water dissolved solutes are transported with the water



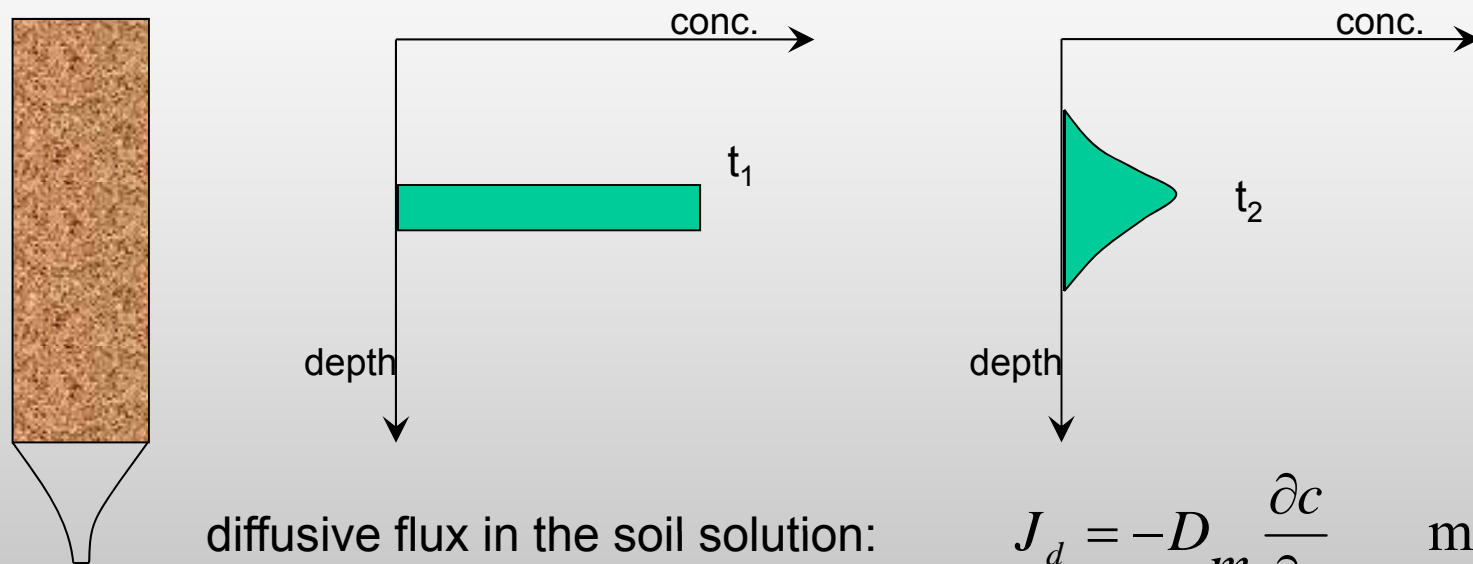
„Piston flow“

Convective flux: $J_c = q \cdot c$ mg.cm⁻².d⁻¹

q = Darcy- flux in the soil [cm³.cm⁻².d⁻¹]

c = concentration in the soil solution [mg.cm⁻³]

Diffusion: thermal movement of molecules of in water solved solutes
(Brownian motion)



diffusive flux in the soil solution:

$$J_d = -D_m \frac{\partial c}{\partial z} \quad \text{mg.cm}^{-2} \cdot \text{d}^{-1}$$

D_m = molecular diffusion coefficient
in the oil solution $[\text{cm}^2 \cdot \text{d}^{-1}]$

$\frac{\partial c}{\partial z}$ = concentration gradient $[\text{mg} \cdot \text{cm}^{-4}]$

The molecular diffusion coefficient is less as in free water :

- Tortuosity - water content - Pore diameter - elektrochemical effects

$$\tau = \frac{\theta^{10/3}}{n^2} \quad \text{--- Millington und Quirk (1961)}$$

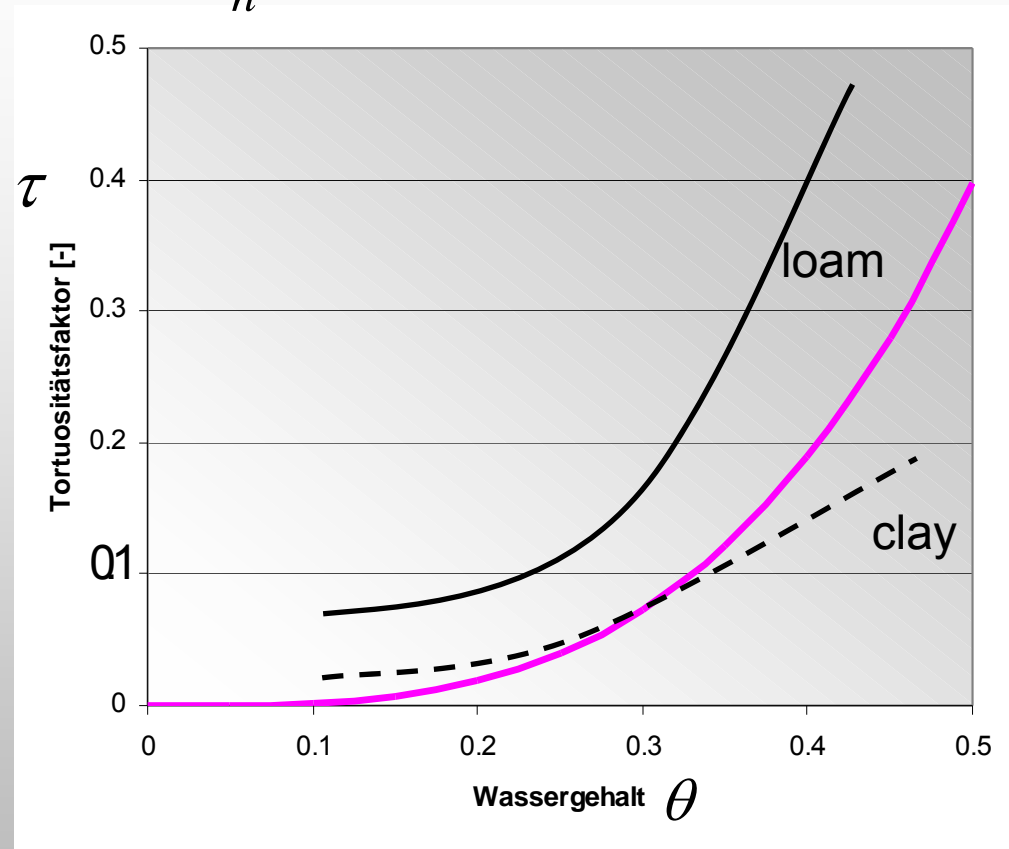
tortuosity faktor τ

$$\tau = f(\theta)$$

$$D_m = \tau \cdot D_o$$

D_o = molecular diffusion coefficient
in free water

For Cl, NO₃: $D_o = 1.6 \text{ cm}^2 \cdot \text{d}^{-1}$



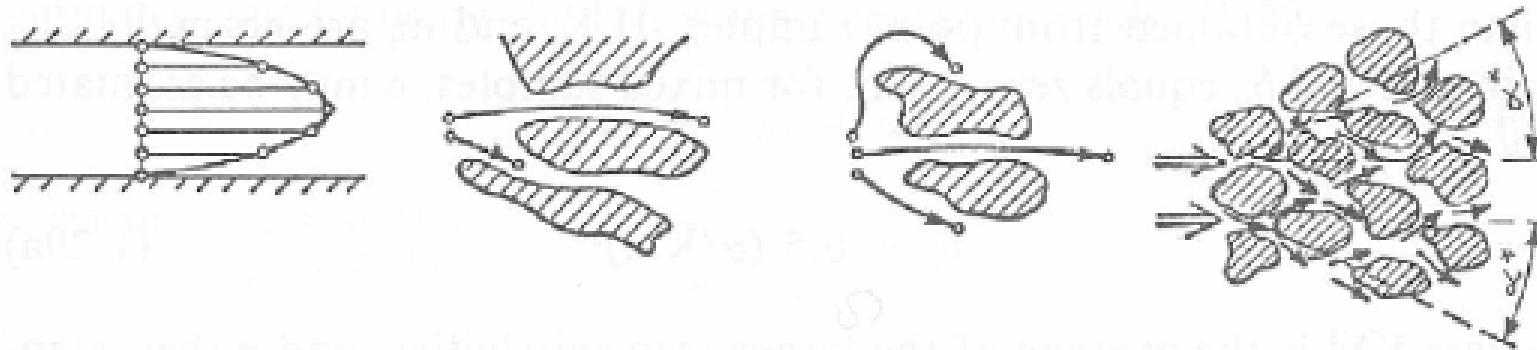
Olsen and Kemper (1968): $\tau = a \cdot e^{b \cdot \theta}$

with $b = 10$ and
 clay: $a = 0.001$ ¹⁵
 loam: $a = 0.005$

Hydrodynamic dispersion:

Due to the irregular velocity distribution of the water movement in soil pores and the different local velocities and flow paths .

Only active with water movement!!



longitudinal dispersion

transversal dispersion

Hydrodynamic dispersion:

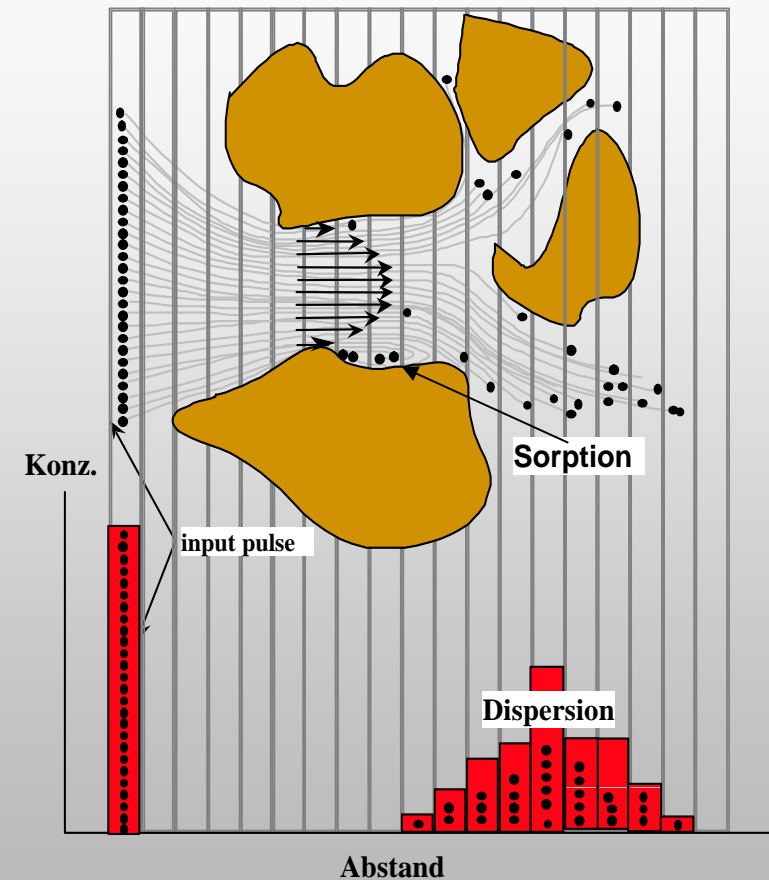
Dispersive flux in the soil solution :

$$J_{hd} = -D_{hd} \cdot \frac{\partial c}{\partial z} \quad \text{mg.cm}^{-2} \cdot \text{d}^{-1}$$

D_{hd} is a function of the mean porewater velocity :

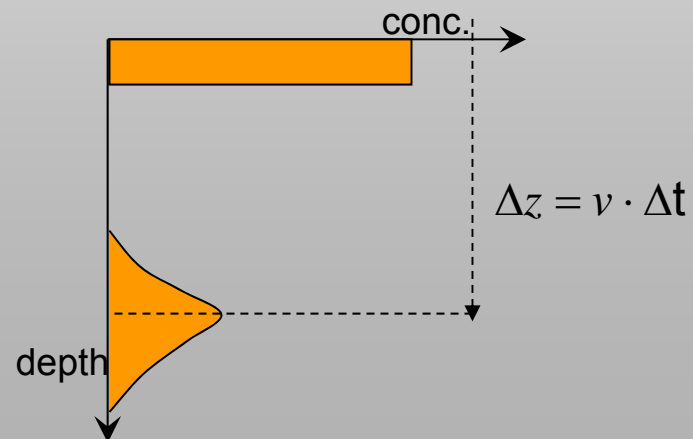
$$D_{hd} = \lambda \cdot v \quad \text{cm}^2 \cdot \text{d}^{-1}$$

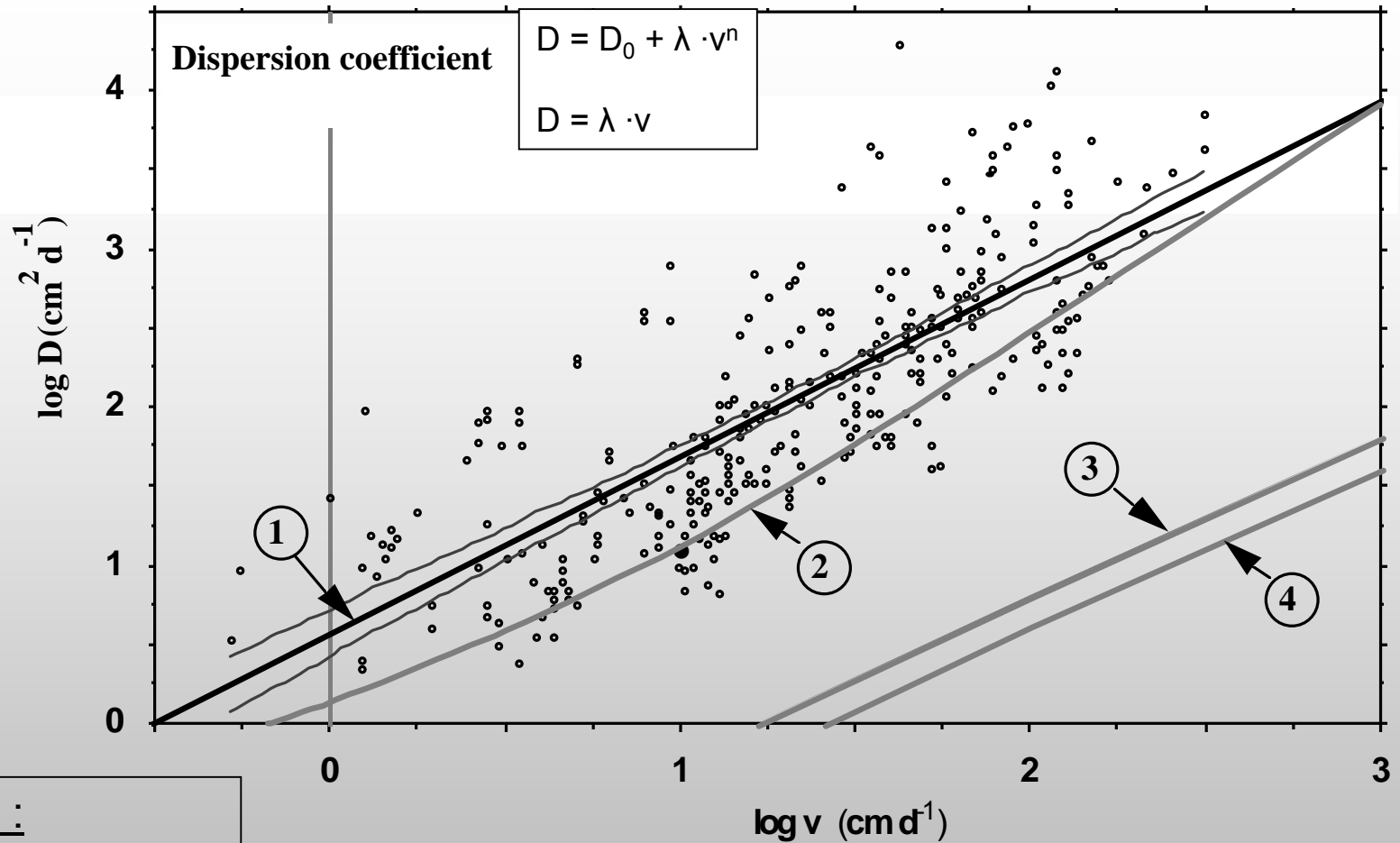
$$\lambda = \text{dispersivity} \quad [\text{cm}]$$



Notation:

q	= filter velocity or darcy velocity	$\text{cm}^3 \cdot \text{cm}^{-2} \cdot \text{d}^{-1}$
v	= q/θ mean pore water velocity	$\text{cm} \cdot \text{d}^{-1}$
v_m	= q/θ_m effective pore water velocity	$\text{cm} \cdot \text{d}^{-1}$
θ	= water content (mit $\theta = \theta_m + \theta_{im}$)	$\text{cm}^3 \cdot \text{cm}^{-3}$
θ_m, θ_{im}	= mobile water content, resp. immobile water content	$\text{cm}^3 \cdot \text{cm}^{-3}$



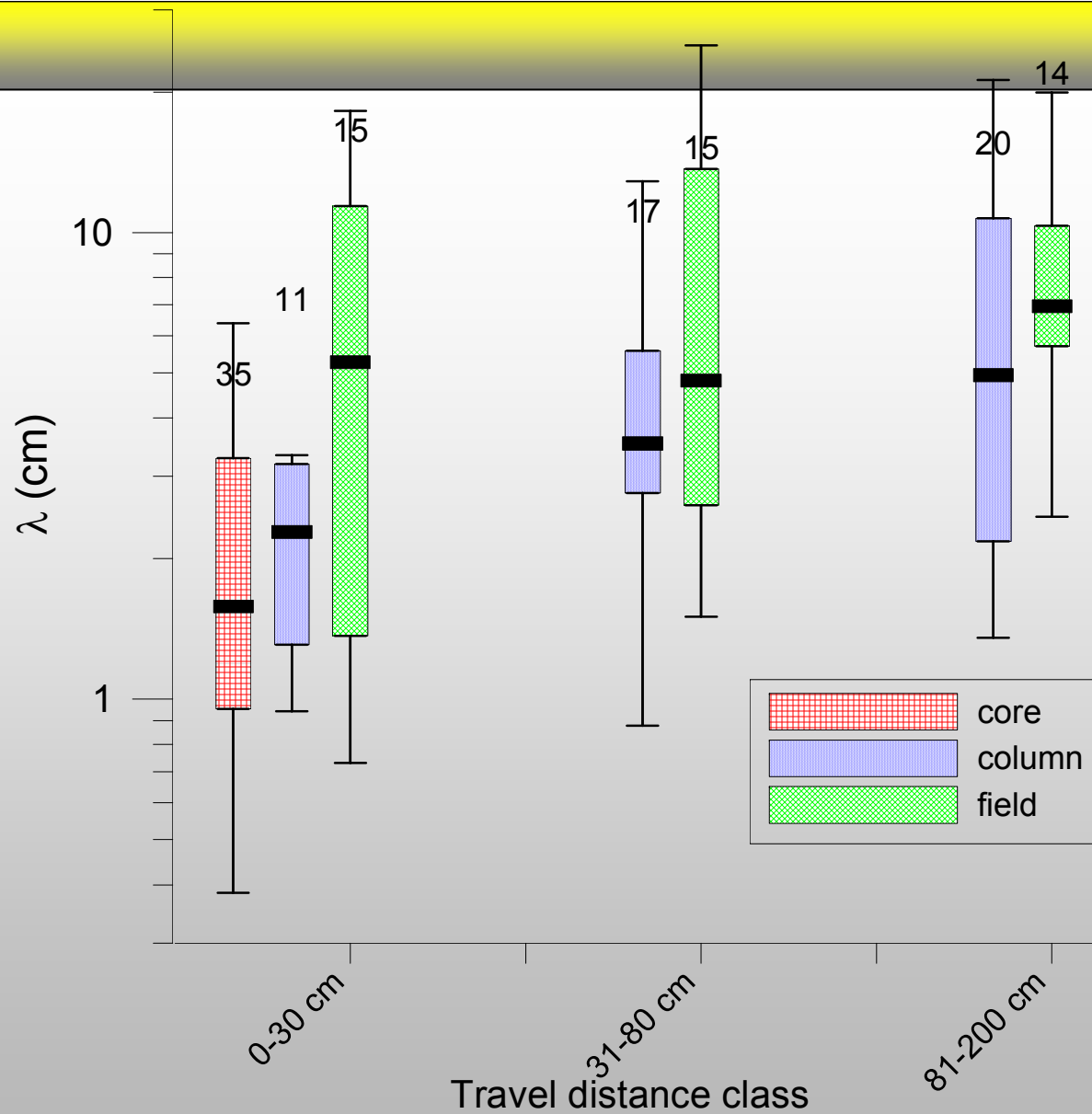


Dispersivity λ :

Lab column: 0.01-1.0 cm

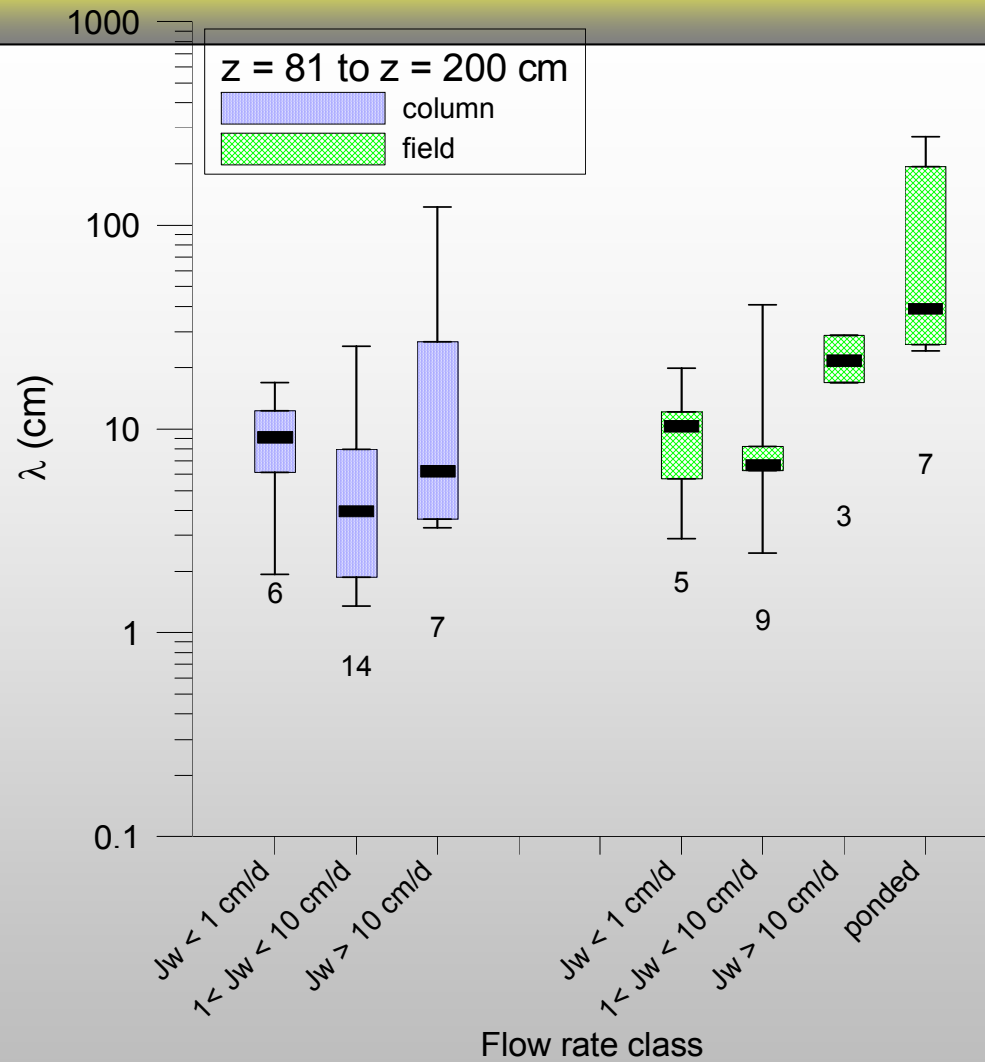
Field soils: 0.5 – 20 cm

- | | | |
|---------|--|-----------------------------|
| curve 1 | $D = 0.60 + 2.93 v^{1.11}$ (Nielsen et al. 1976) | } field experiments |
| curve 2 | $D = 0.62 + 0.545 v^{1.355}$ (Kirda et al. 1973) | |
| curve 3 | $D = 0.04 v$ (Bertsch et al. 1978) | } laboratory experiments 19 |
| curve 4 | $D = 0.063 v$ (Bertsch et al. 1978) | |



(Vanderborght & Vereecken, 2007)

The dispersivity λ as a function of the transport distance (0-30 cm, 30-81 cm and 81-200 cm) of core, column and field experiments



(Vanderborght & Vereecken, 2007)

The dispersivity λ as a function of 4 flow rate classes for a transport distance of 81 to 200 cm in column and field experiments

Apparent or effective dispersion coefficient

Diffusive and hydromechanical caused dispersive fluxes cannot be separated macroscopically and thus are taken together:

diffusive-dispersive flux in the soil:

$$J_{dd} = -(D_m + D_{hd}) \cdot \frac{\partial c}{\partial z} = -D_e \cdot \frac{\partial c}{\partial z} \quad \text{mg.cm}^{-2} \cdot \text{d}^{-1}$$

D_e = „effective“ or „apparent“ diffusion coefficient
or just „dispersion coefficient“

Convective- dispersive flux:

Total solute flux in the soil is the sum of the convective and the diffusive-dispersive flux:

$$J_{cd} = J_{dd} + J_c$$

$$J_{cd} = \underbrace{-(D_m + D_{hd}) \cdot \frac{\partial c}{\partial z}}_{\text{diffusive-dispersive}} + \underbrace{q \cdot c}_{\text{convective}} \quad \text{mg.cm}^{-2} \cdot \text{d}^{-1}$$

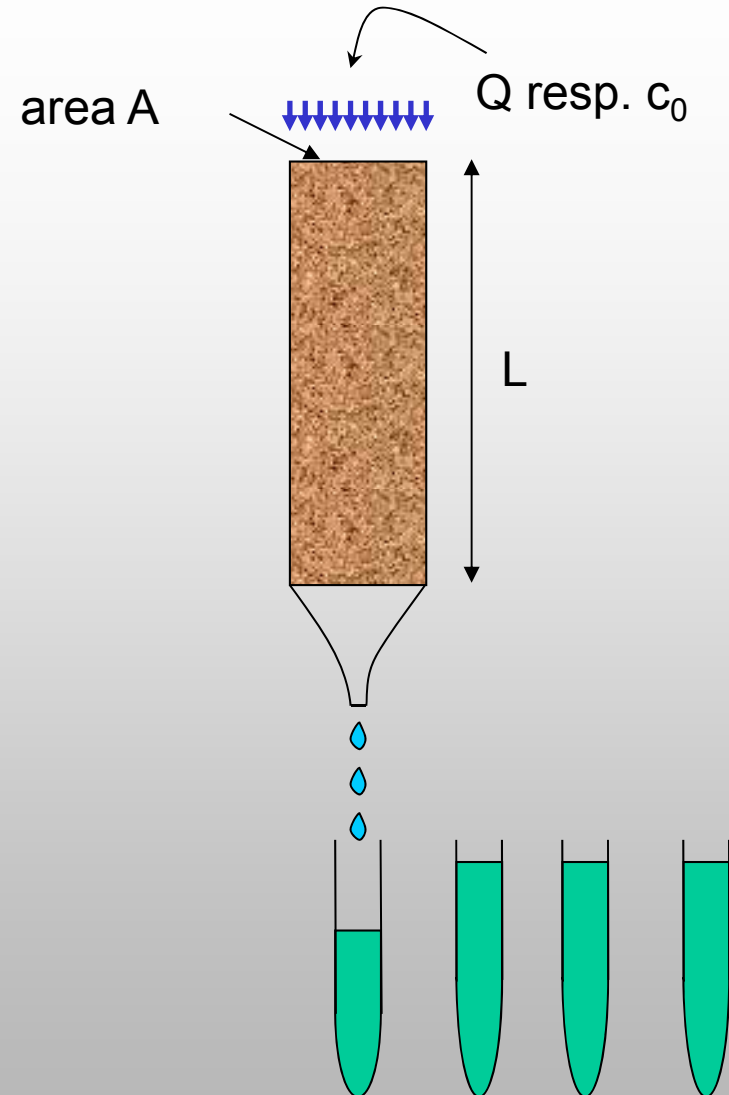
Solute transport in a soil column:

- volumetric water content θ $\text{cm}^3 \cdot \text{cm}^{-3}$
- colum length L cm
- column area A cm^2
- irrigation amount Q $\text{cm}^3 \cdot \text{d}^{-1}$
($Q = q \cdot A$)
- solute concentration c_0 $\text{mg} \cdot \text{cm}^{-3}$
- Pore water velocity v $\text{cm} \cdot \text{d}^{-1}$
($v = q/\theta$)

Definition of pore volume:

$$1 \text{ PV} = A \cdot L \cdot \theta \quad \text{cm}^3$$

The exchange of 1 PV takes t_{PV} days



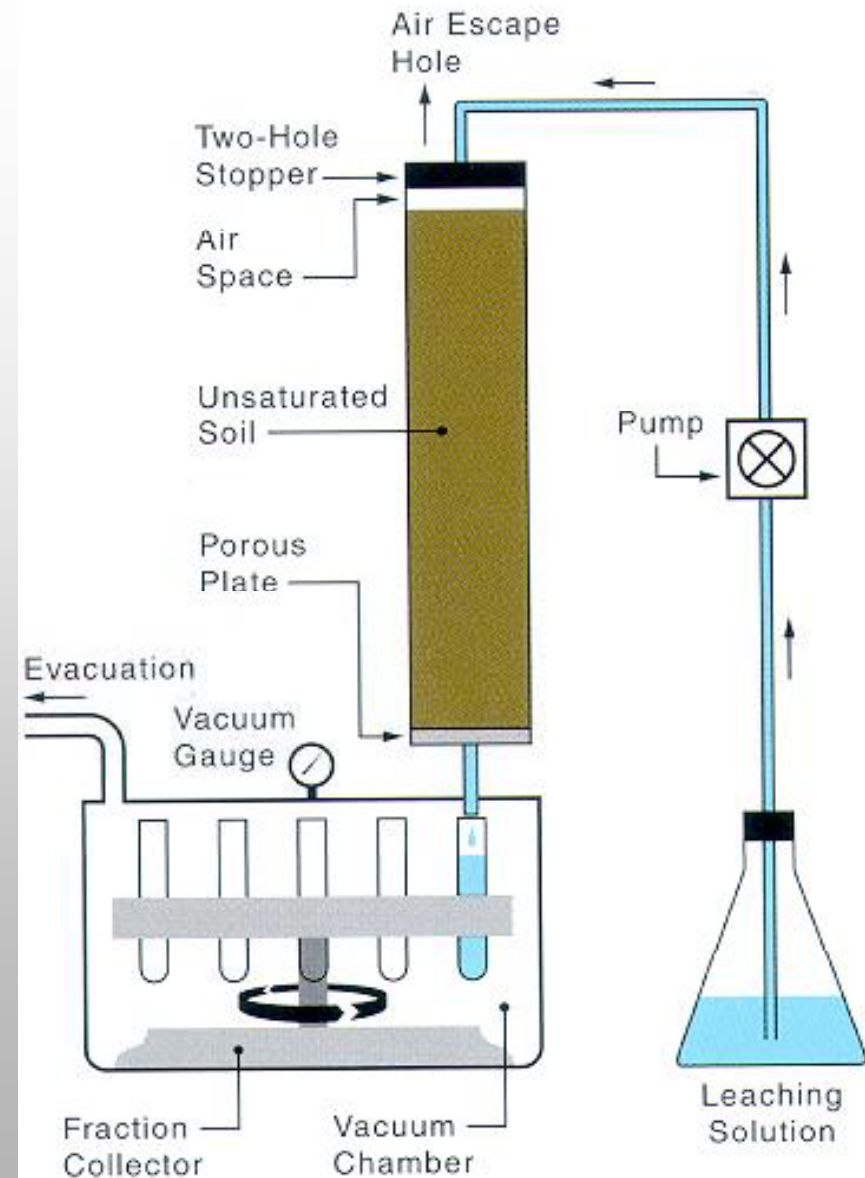
Break through curves:

= concentration in time

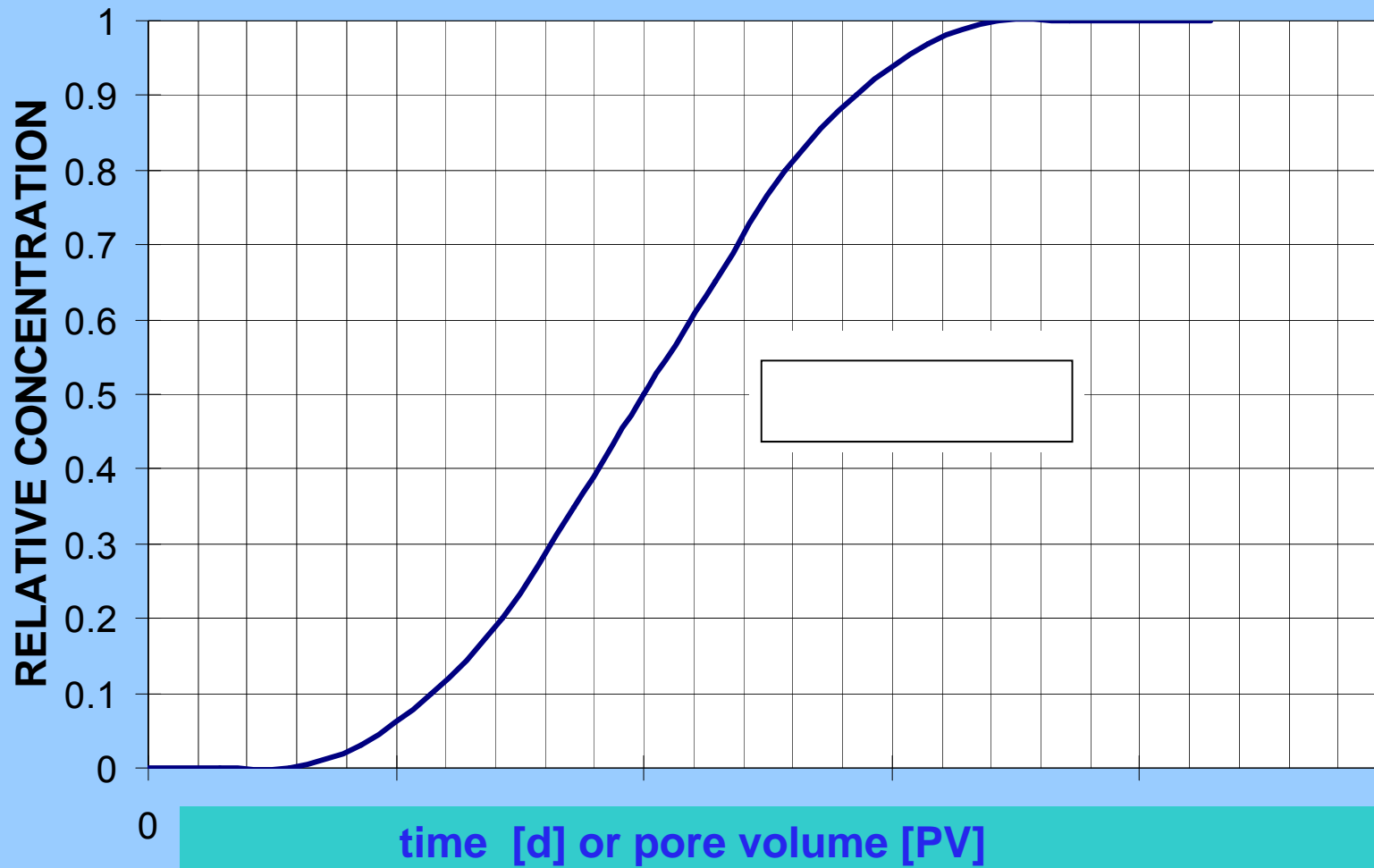
- at the end of a soil column

or

- in a chosen depth



Breakthrough curve : convection and diffusion-dispersion



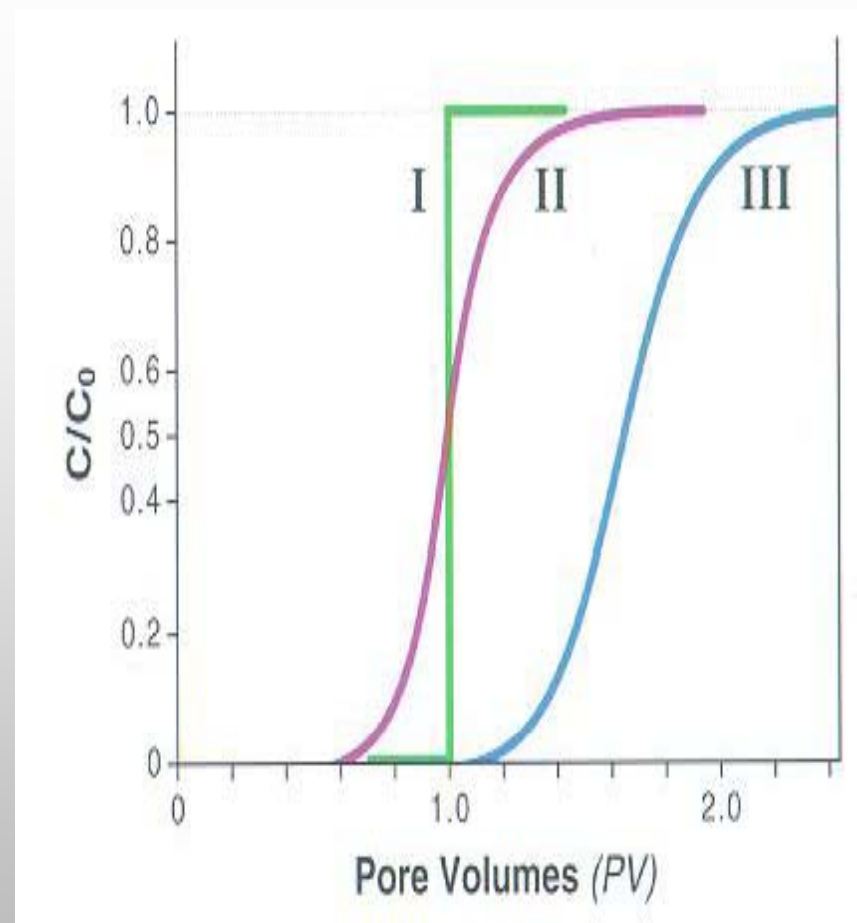
- relative concentration c/c_0

- Pore volume

(= dimensionless time)

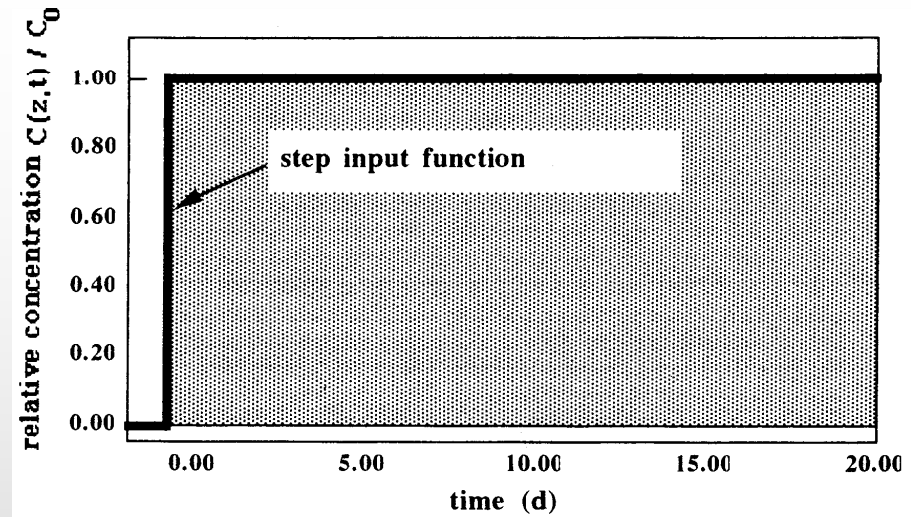
= time definition in multiple times
needed to exchange one pore volume
of soil solution

$$PV = t / t_{PV} = \frac{t}{L/v} = \frac{vt}{L}$$



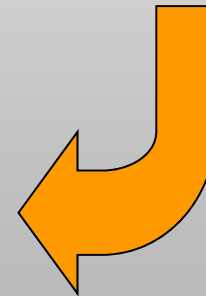
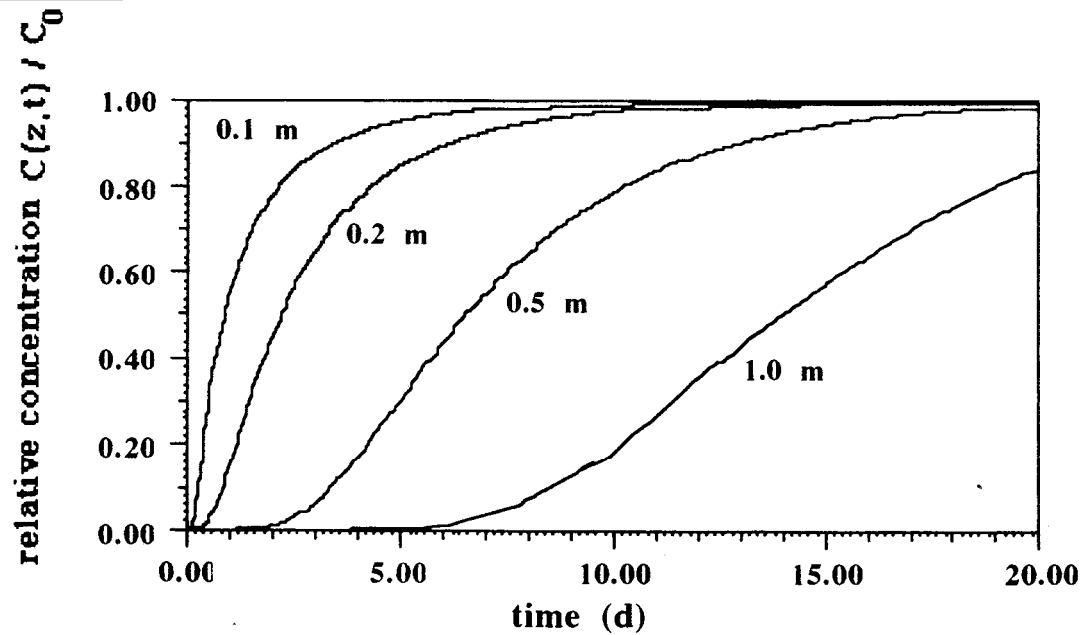
Break through curves: I : only convection („piston flow“)
II : convection and diffusion-dispersion
III : convection and diffusion-dispersion and retardation

Breakthrough curves in different depths for a step input:



$$q = 0.02 \text{ m d}^{-1} \quad \theta = 0.30 \text{ m}^3 \text{ m}^{-3} \quad D = 0.005 \text{ m}^2 \text{ d}^{-1}$$

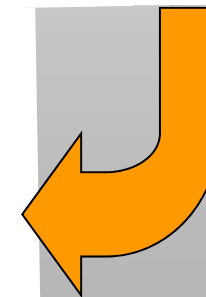
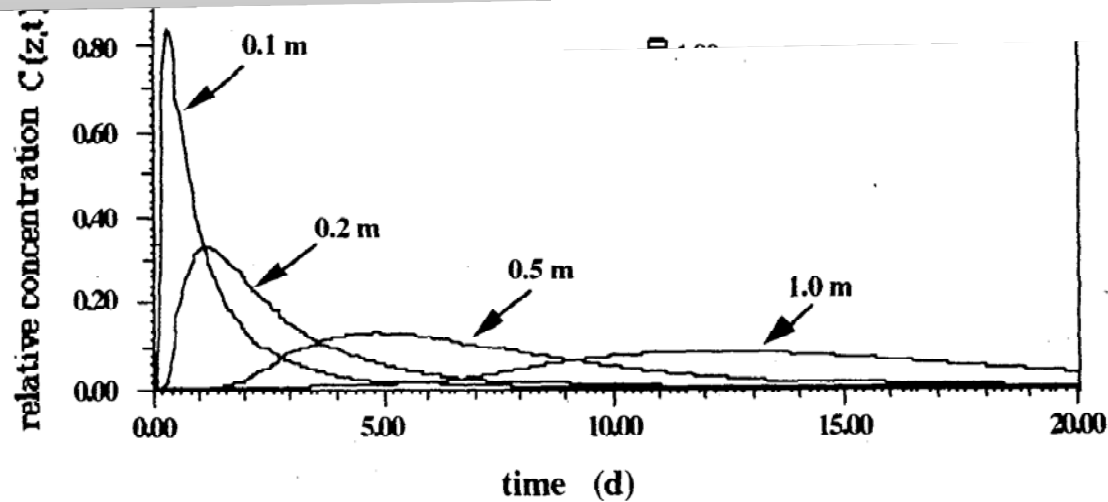
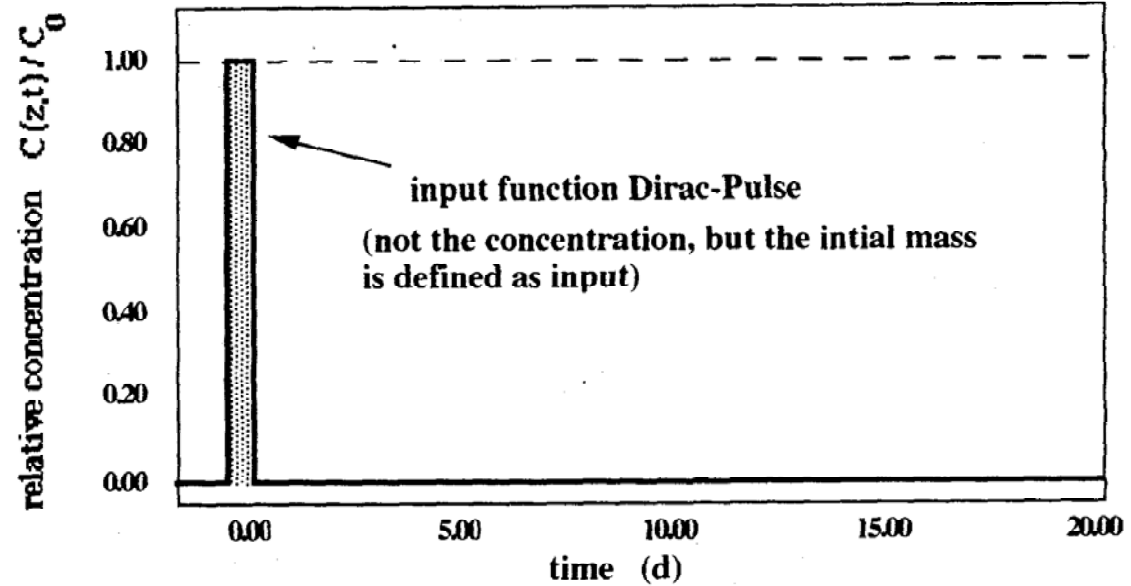
$$v = 0.067 \text{ m d}^{-1} \quad \lambda = D/v = 0.075 \text{ m}$$



Breakthrough curves in different depths :

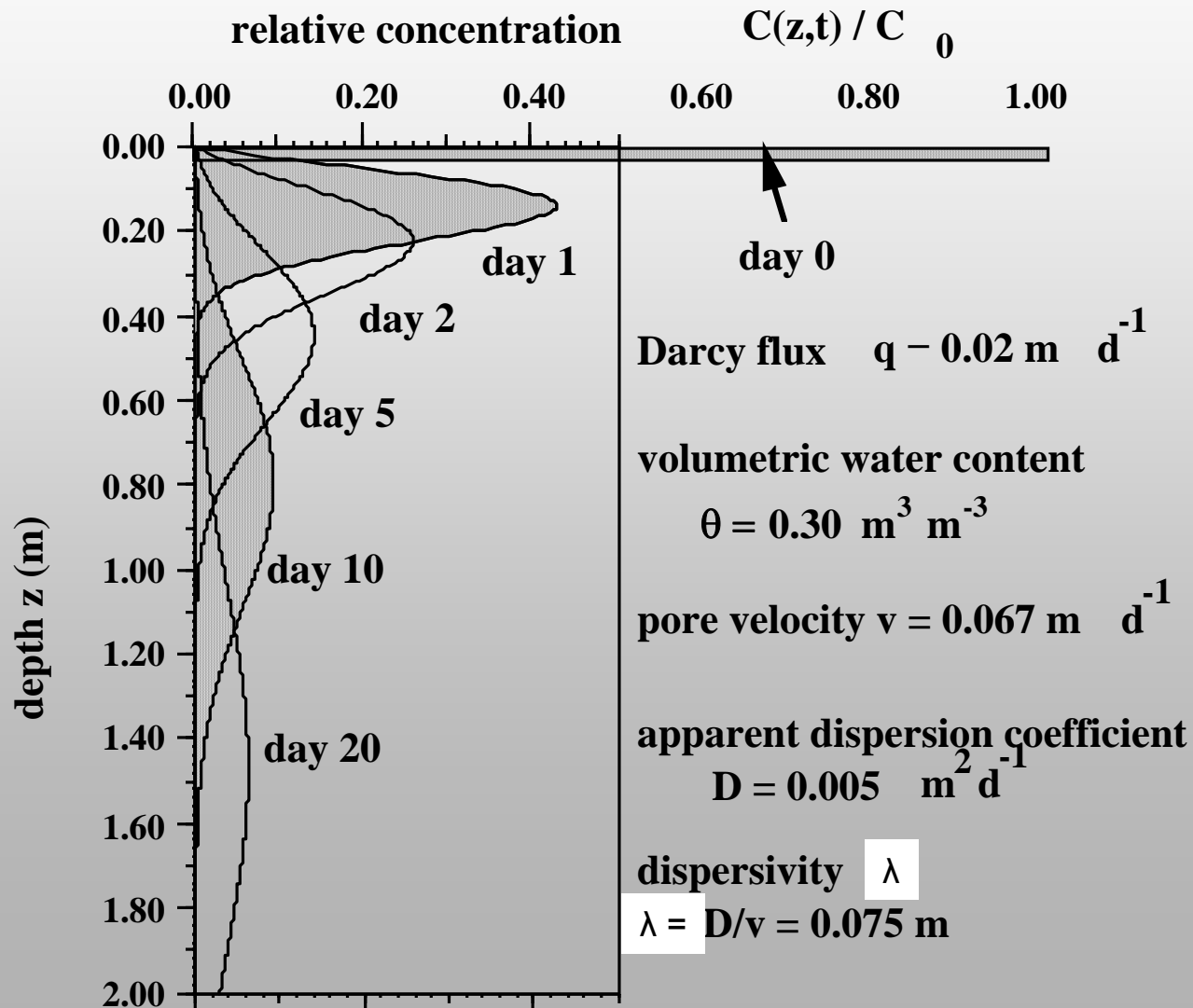
$$q = 0.02 \text{ m d}^{-1} \quad \theta = 0.30 \text{ m}^3 \text{ m}^{-3} \quad D = 0.005 \text{ m}^2 \text{ d}^{-1}$$

$$v = 0.067 \text{ m d}^{-1} \quad \lambda = D/v = 0.075 \text{ m}$$

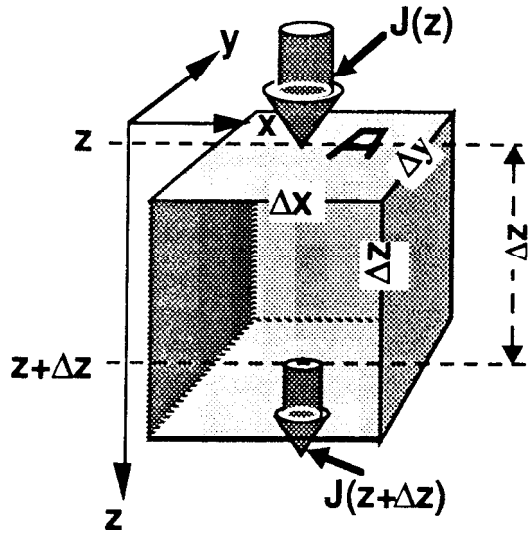


displacement of a solute pulse $C_t(z)$

concentration profiles



Derivation of the partial differential equation for solute transport in soils :



solute content in the soil : $C_{tot} = \theta \cdot c + \rho \cdot S$

- θ = volumetric water content $\text{cm}^3 \cdot \text{cm}^{-3}$
- c = concentration in the soil solution $\text{mg} \cdot \text{cm}^{-3}$
- ρ = bulk density of the soil $\text{g} \cdot \text{cm}^{-3}$
- S = adsorbed solute amount $\text{mg} \cdot \text{g}^{-1}$

Mass balance : Mass conservation

solute inflow – outflow = Change in solute content

$$J_{in} = J_z \cdot \Delta x \cdot \Delta y \cdot \Delta t$$

$$J_{out} = J_{z+\Delta z} \cdot \Delta x \cdot \Delta y \cdot \Delta t$$

in solution: $\Delta(\theta \cdot c) \cdot \Delta x \cdot \Delta y \cdot \Delta z$

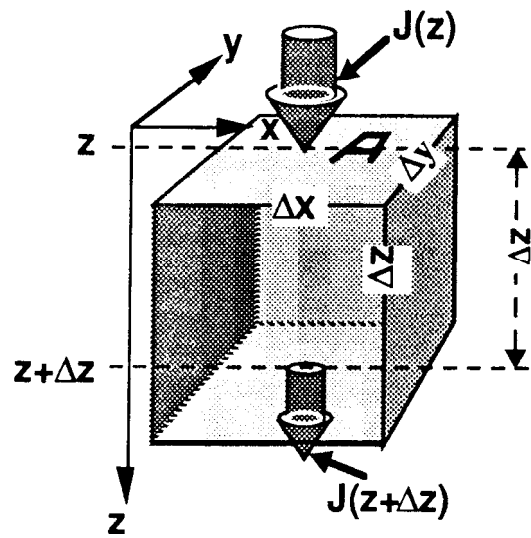
at the soil matrix: $\Delta(\rho \cdot S) \cdot \Delta x \cdot \Delta y \cdot \Delta z$

$$\frac{\Delta C_{tot}}{\Delta t} = - \frac{\Delta J}{\Delta z}$$



$$\frac{\partial C_{tot}}{\partial t} = - \frac{\partial J}{\partial z}$$

partial Differential equation for solute transport in soils :



θ = volumetric water content $\text{cm}^3 \cdot \text{cm}^{-3}$
 c = concentration in the soil solution $\text{mg} \cdot \text{cm}^{-3}$
 ρ = bulk density of the soil $\text{g} \cdot \text{cm}^{-3}$
 S = adsorbed solute amount $\text{mg} \cdot \text{g}^{-1}$

$$\frac{\partial C_{tot}}{\partial t} = - \frac{\partial J}{\partial z} \quad (1)$$

$$C_{tot} = \theta \cdot c + \rho \cdot S \quad (2)$$

$$J = -(D_m + D_{hd}) \cdot \frac{\partial c}{\partial z} + q \cdot c \quad \text{mg} \cdot \text{cm}^{-2} \cdot \text{d}^{-1} \quad (3)$$

(2) and (3) in (1): ➔

$$\frac{\partial \theta c}{\partial t} + \frac{\partial \rho S}{\partial t} = \frac{\partial}{\partial z} \left(D_e \frac{\partial c}{\partial z} \right) - \frac{\partial qc}{\partial z} \quad 32$$

Additional processes:

uptake by plants :

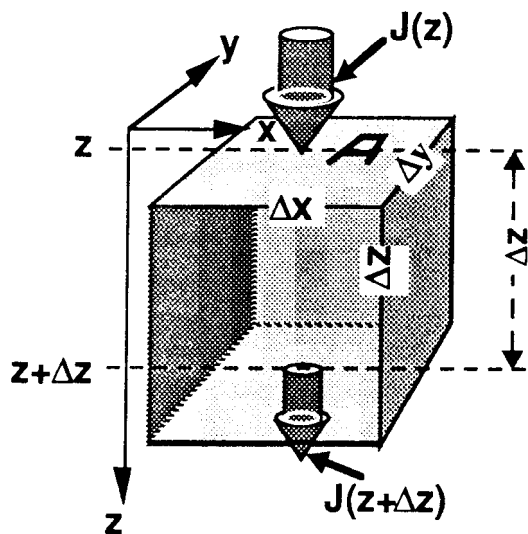
$$\frac{\partial \theta c}{\partial t} + \frac{\partial \rho S}{\partial t} = \frac{\partial}{\partial z} \left(D_e \frac{\partial c}{\partial z} \right) - \frac{\partial qc}{\partial z} - Q_{\text{uptake}}$$

decay/production

$$\frac{\partial \theta c}{\partial t} + \frac{\partial \rho S}{\partial t} = \frac{\partial}{\partial z} \left(D_e \frac{\partial c}{\partial z} \right) - \frac{\partial qc}{\partial z} - \underbrace{\mu_w \cdot \theta \cdot c - \mu_s \cdot \rho \cdot S}_{\text{1. order decay}}$$

1. order decay

Mobile-immobile



partial differential equation in soils:

$$\frac{\partial \theta c}{\partial t} + \frac{\partial \rho S}{\partial t} = \frac{\partial}{\partial z} \left(D_e \frac{\partial c}{\partial z} \right) - \frac{\partial qc}{\partial z} + Q - \mu_w \cdot \theta \cdot c - \mu_s \cdot \rho \cdot S + \gamma_w \cdot \theta + \gamma_s \cdot \rho$$

θ	= volumetric water content	$\text{cm}^3 \cdot \text{cm}^{-3}$
c	= concentration in the soil solution	$\text{mg} \cdot \text{cm}^{-3}$
ρ	= bulk density of the soil	$\text{g} \cdot \text{cm}^{-3}$
S	= adsorbed solute amount	$\text{mg} \cdot \text{g}^{-1}$
D_e	= Dispersion coefficient	$\text{cm}^2 \cdot \text{d}^{-1}$
q	= Darcy-Water flux	$\text{cm} \cdot \text{d}^{-1}$
μ	= 1. order decay rate	d^{-1}
γ	= 0. order produktion rate	$\text{mg} \cdot \text{cm}^{-3} \cdot \text{d}^{-1}$
Q	= sources/sinks	$\text{mg} \cdot \text{cm}^{-3} \cdot \text{d}^{-1}$
z	= depth	cm
t	= time	d

Sorption

- linear $\frac{\partial S}{\partial C} = \text{const.}$

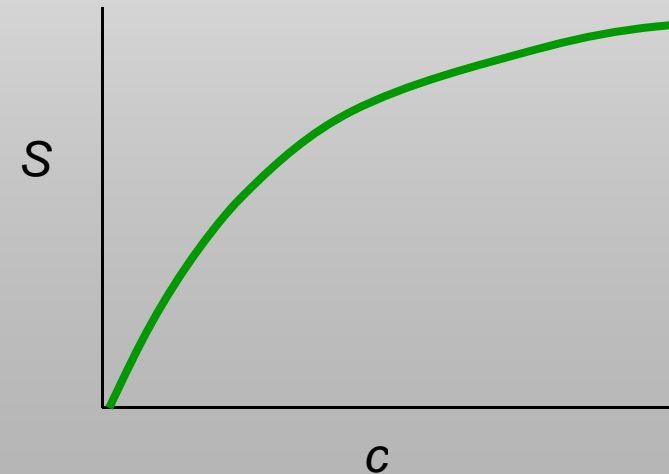
$$S = k \cdot c$$



- non linear $\frac{\partial S}{\partial C} = f(C)$

e.g.. Freundlich

$$S = k \cdot c^n$$



Stationary flow: - $q(z,t) = \text{constant}$
 - $\theta(z,t) = \text{constant}$

and

- no production or decay
- no sources and sinks
- linear sorption : $S = k \cdot c$ [mg.g⁻¹]

$$\theta \frac{\partial c}{\partial t} + \rho k \frac{\partial c}{\partial t} = \frac{\partial}{\partial z} \left(D_e \frac{\partial c}{\partial z} \right) - q \frac{\partial c}{\partial z} \quad \text{with } D = \frac{D_e}{\theta}$$

$$\left(1 + \frac{\rho k}{\theta}\right) \frac{\partial c}{\partial t} = D \left(\frac{\partial^2 c}{\partial z^2} \right) - \frac{q}{\theta} \cdot \frac{\partial c}{\partial z} \quad R \cdot \frac{\partial c}{\partial t} = D \left(\frac{\partial^2 c}{\partial z^2} \right) - v \cdot \frac{\partial c}{\partial z}$$

Example: $k = 2$
 $\rho = 1.5$
 $\theta = 0.4$

$R = \text{retardation factor} = 1 + \frac{\rho k}{\theta} \quad [-]$

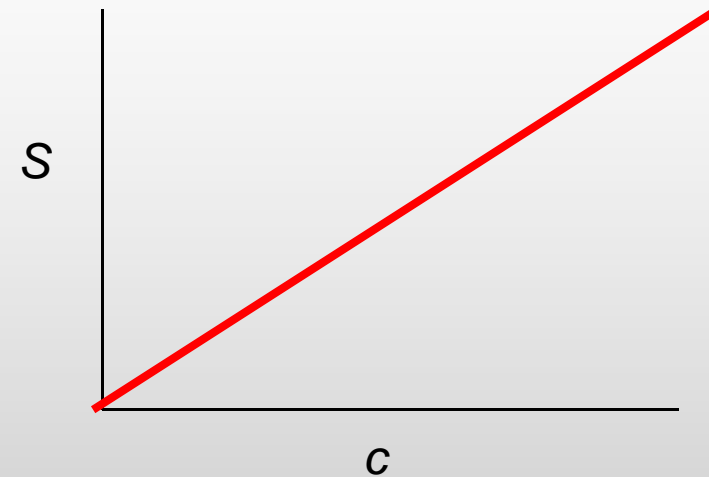
$v = \text{pore water velocity} \quad 36 [\text{cm.d}^{-1}]$

Sorption: general expression

$$S = \frac{k \cdot c^n}{1 + \eta c}$$

- linear $\frac{\partial S}{\partial C} = \text{const.}$

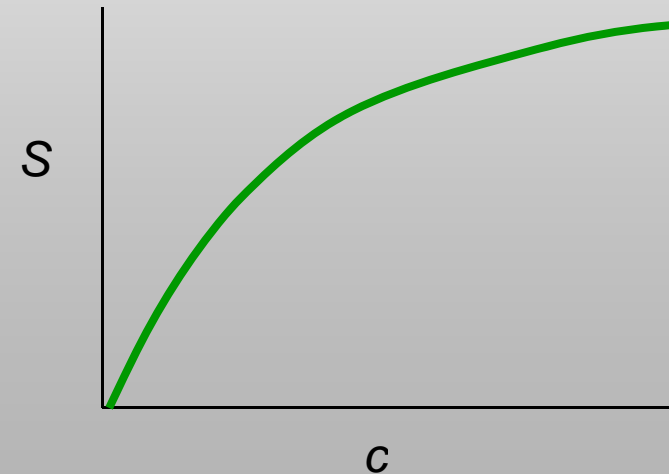
$$S = k \cdot c$$



- non linear $\frac{\partial S}{\partial C} = f(C)$

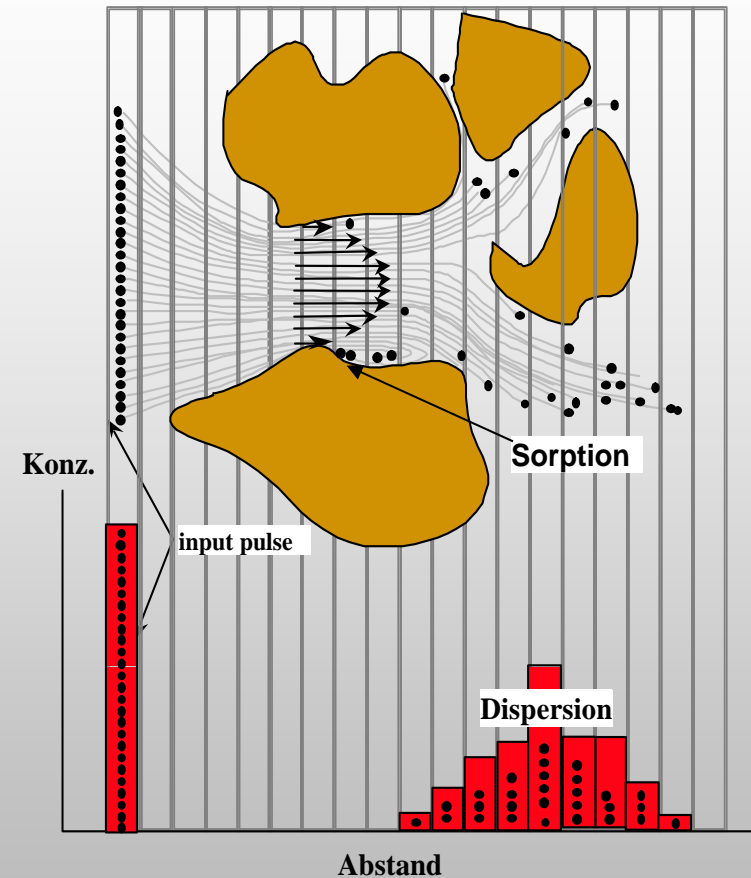
e.g.. Freundlich

$$S = k \cdot c^n$$



Important transport processes

- Konvektion: gelöste Moleküle werden mit dem *Wasser* transportiert
- Diffusion: Brown'sche Bewegung
- Hydrodynamische Dispersion: Unterschiedliche lokale Fließgeschwindigkeiten
- Sorption an der Bodenmatrix
- Abbau (mikrobiell)
- Lösung/Fällung



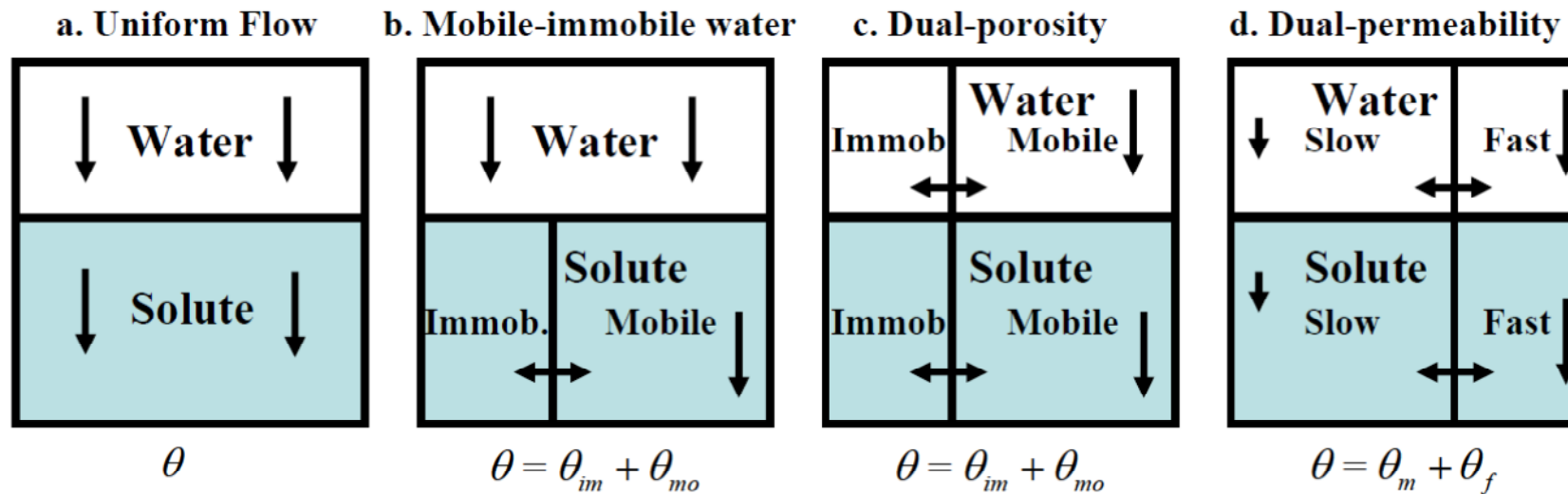


Figure 22.10. Conceptual models of water flow and solute transport (θ is the water content, θ_{mo} and θ_{im} in (b) and (c) are water contents in the mobile and immobile flow regions, respectively, and θ_m and θ_f in (d) are water contents in the matrix and macropore (fracture) regions, respectively).

(Simunek and Van Genuchten, 2006)

Nonequilibrium Two-Site Adsorption Model

$$S = S^e + S^k$$

s^e Type-1 sites with instantaneous sorption

s^k Type-2 sites with kinetic sorption

$$\frac{\partial s^k}{\partial t} = \alpha[(1 - f)K_d c - s^k]$$

f fraction of exchange sites assumed to be at equilibrium

