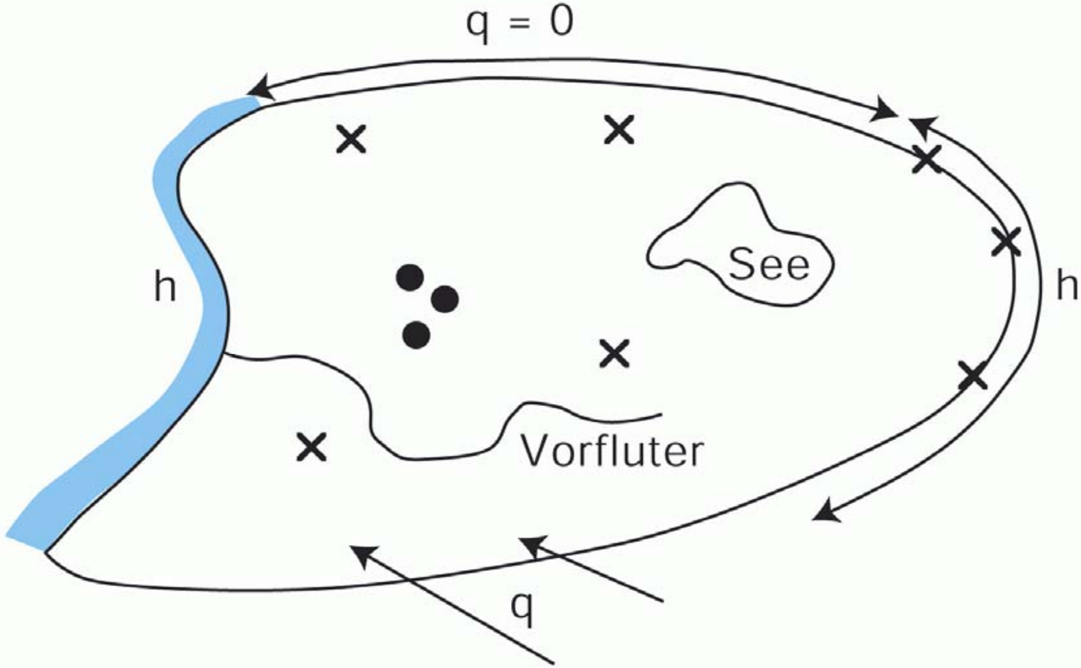
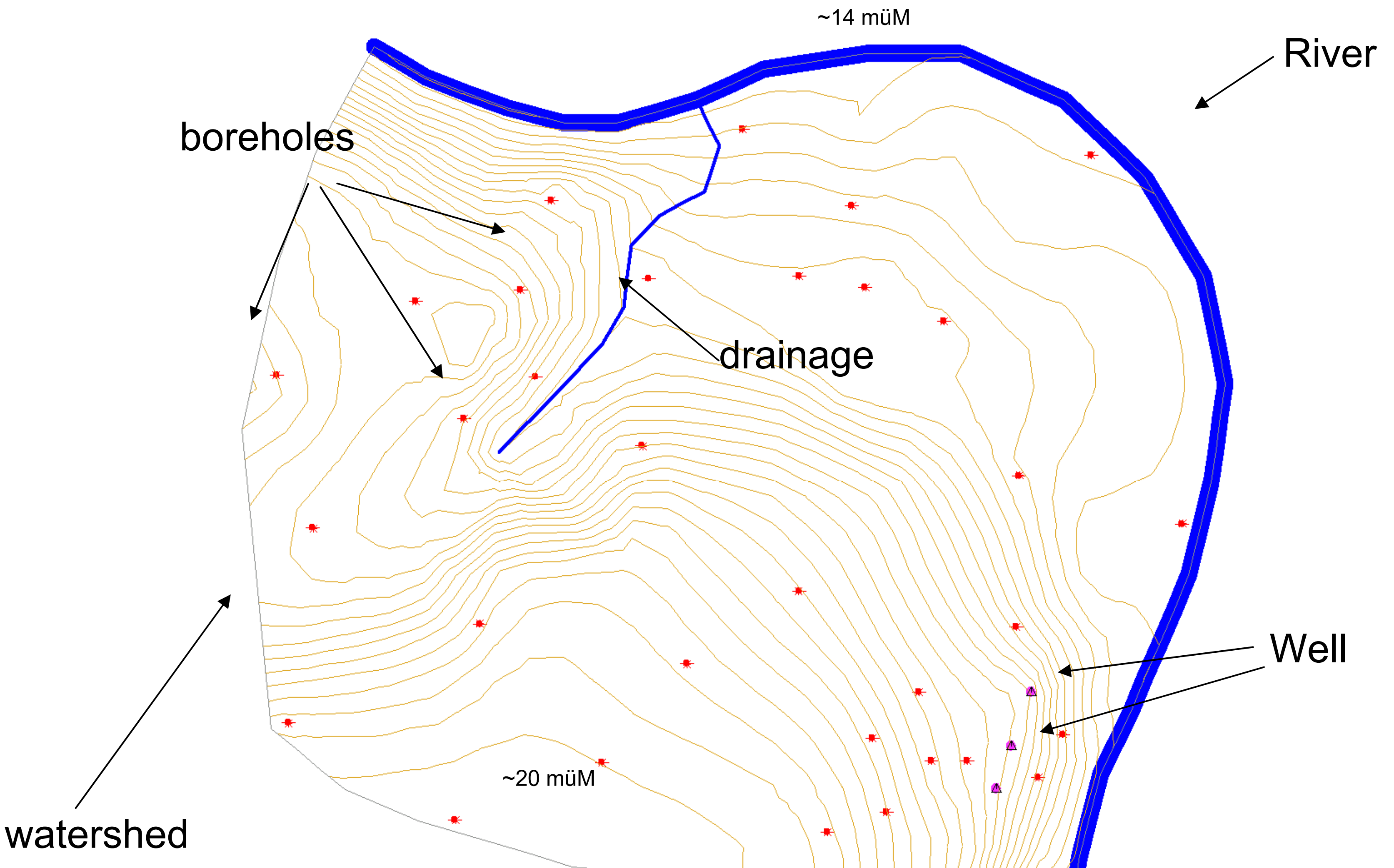
Boundary conditions and parameters




~14 müM
River
boreholes
drainage
Well
watershed
~20 müM

FE-Mesh

transient - 2D – 3D

boundary (POTE)

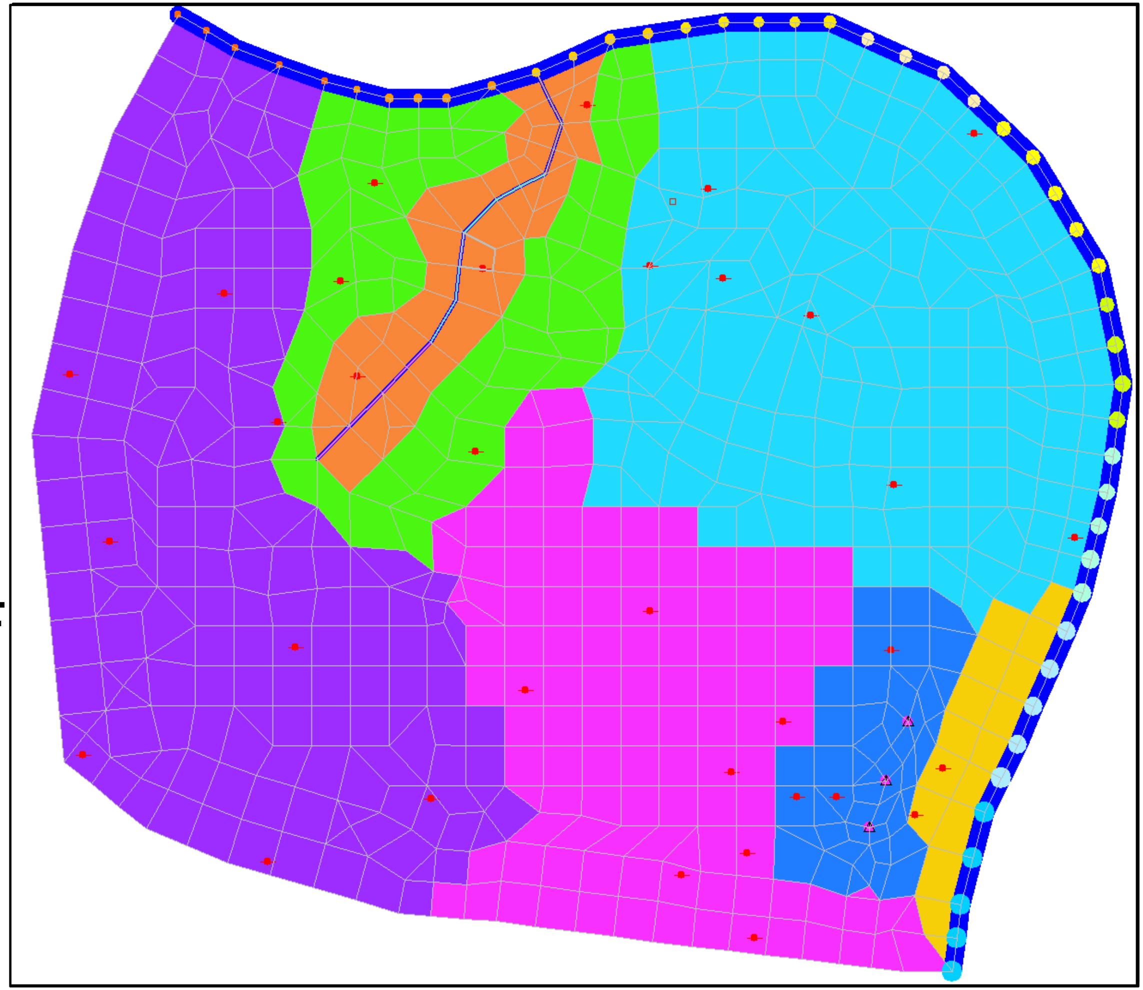
Well (KNOT)

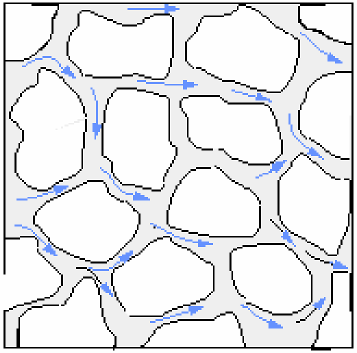
Leakage (LERA)

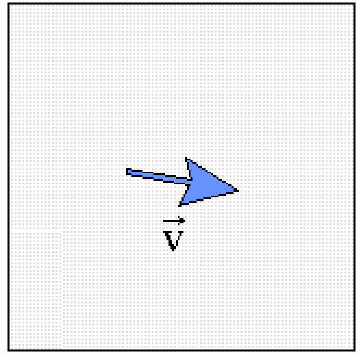
Stream level (VORF

Recharge (FLAE)

K-Values (KWER)







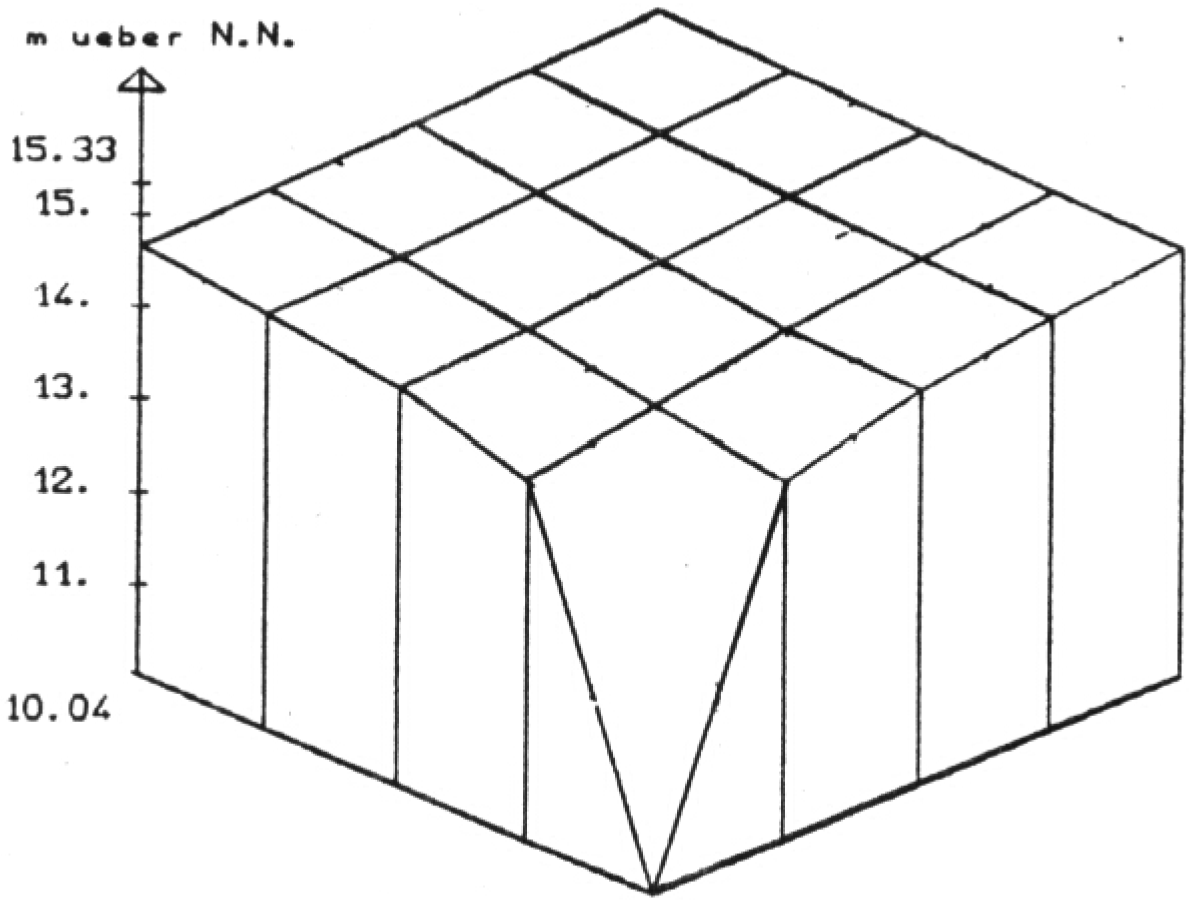
$$v_i = -K_{ij}\frac{k_{rel}}{\mu}\left[\frac{\partial}{\partial x_j}p - \varrho\,\vec{g}_j\right]$$

v_i	Darcy flow [m/s]
K_{ij}	Permeabilitätstensor [m^2]
ϱg	Density * Gravity [N/m^3]
μ	dynamical Viskosity [kg/ms]
k_{rel}	relative Permability [−]

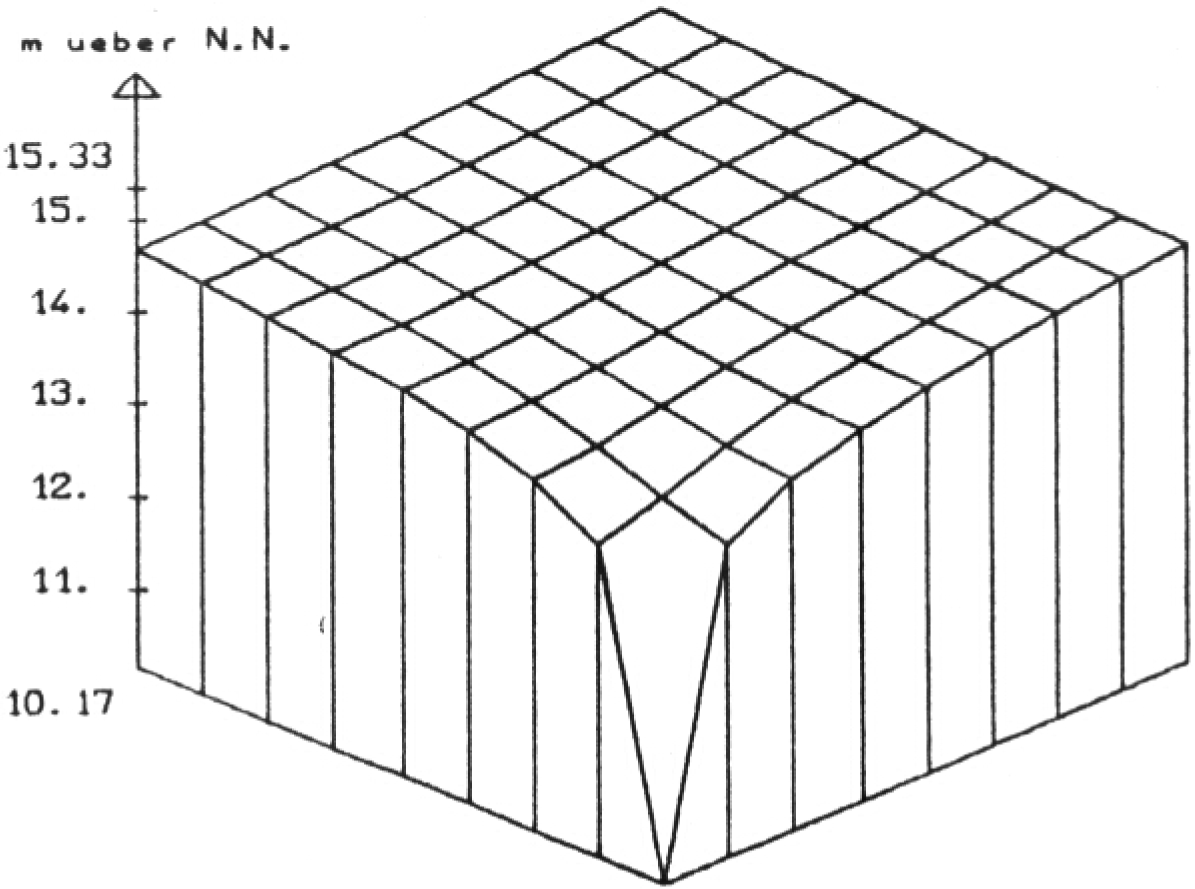
$$\varrho\left[S_w S_{op} + n\frac{\partial S_w}{\partial p}\right]\frac{\partial p}{\partial t} + \left[n S_w \frac{\partial \varrho}{\partial c}\right]\frac{\partial c}{\partial t} - \frac{\partial}{\partial x_i}\left[\varrho K_{ij}\frac{k_{rel}}{\mu}\left[\frac{\partial}{\partial x_j}p - \varrho\vec{g}_j\right]\right] = \varrho Q$$

Storage density- massflow source/ sink

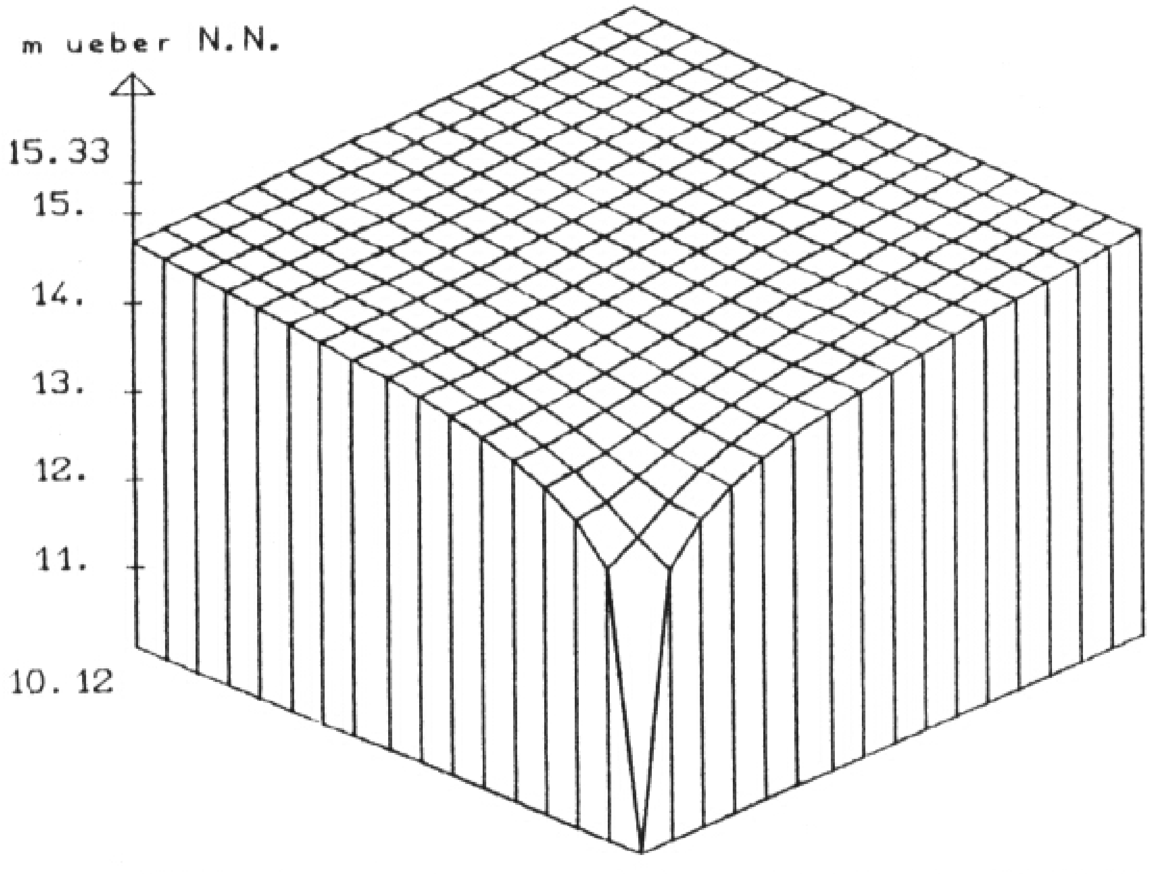
Well I



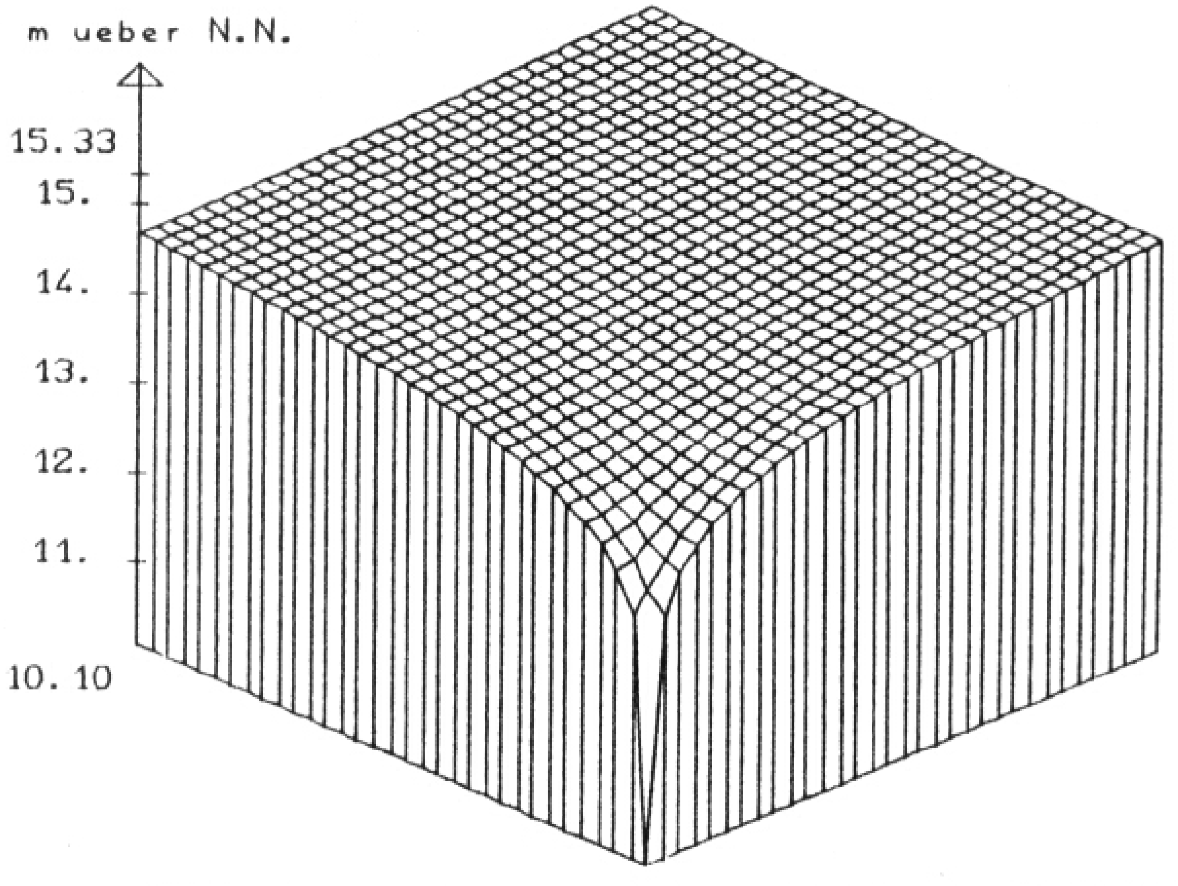
Well II



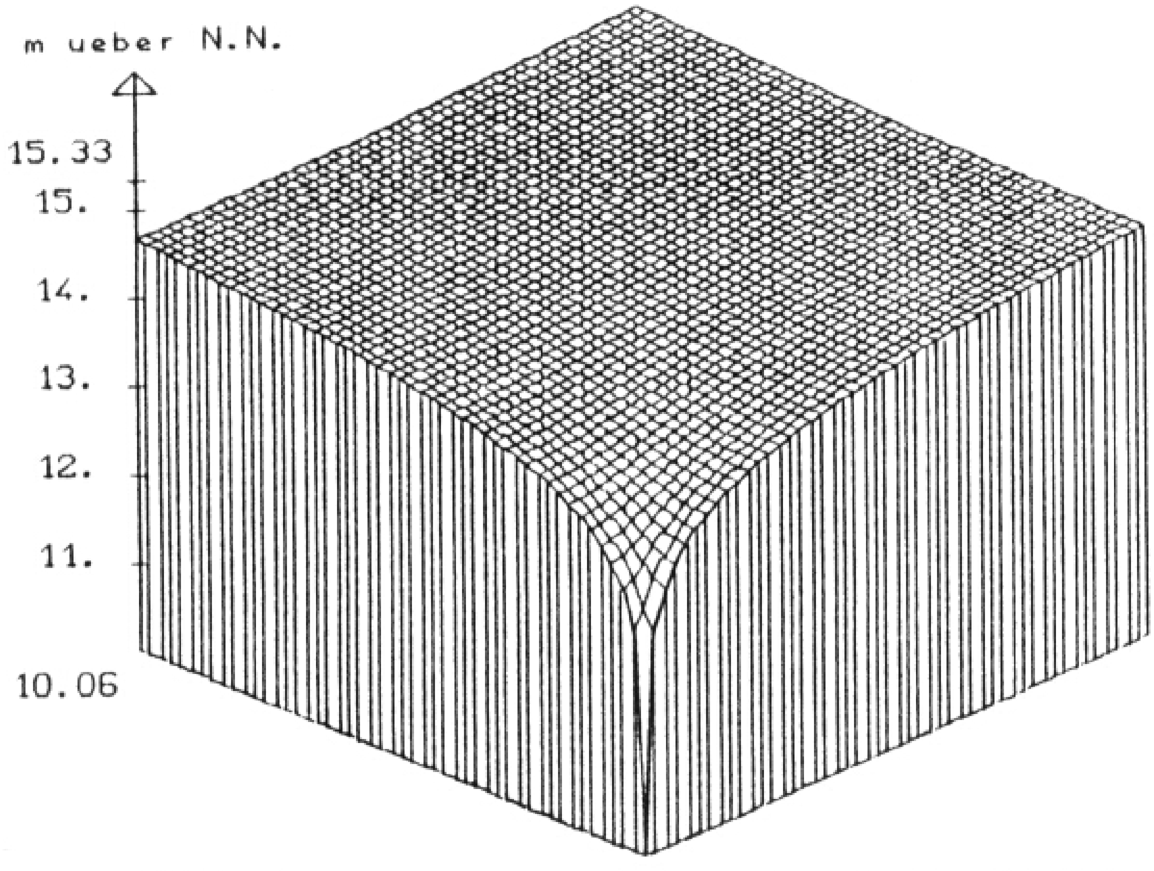
Well III



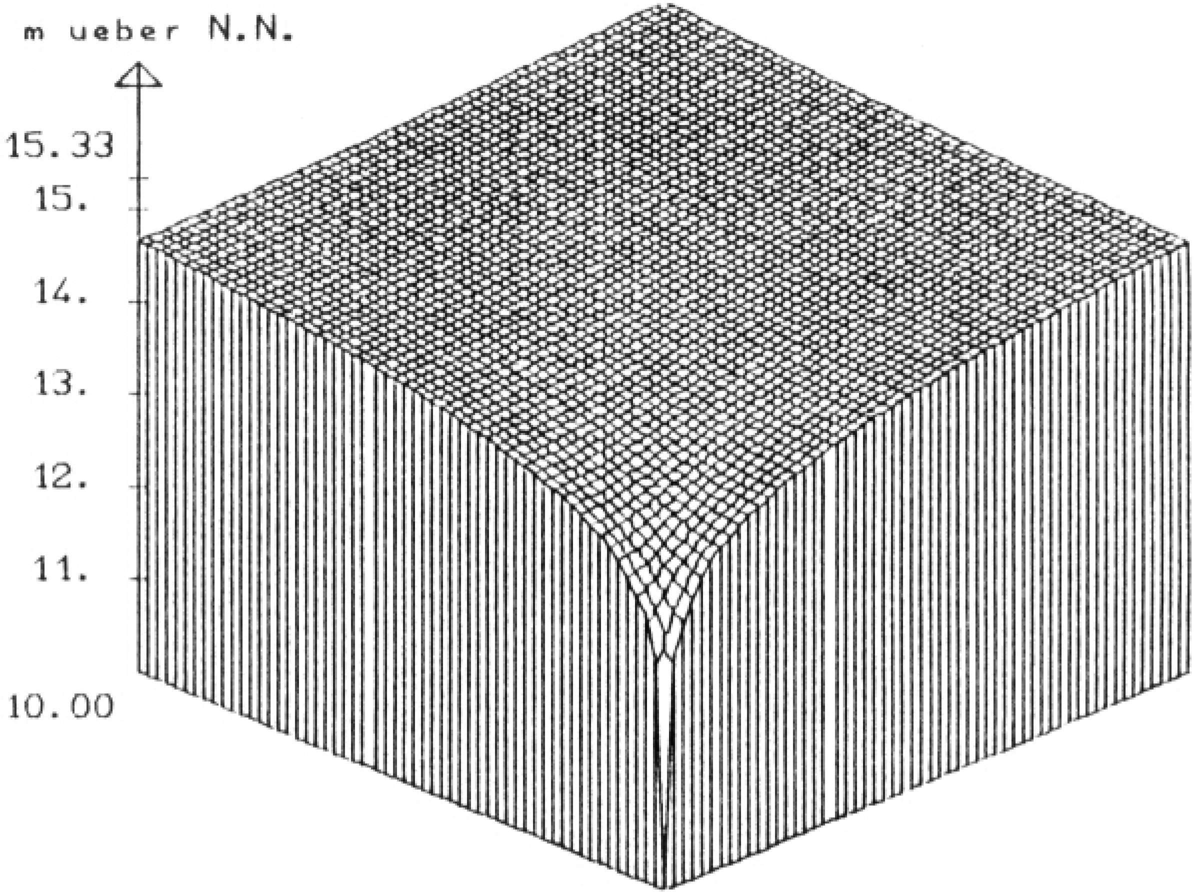
Well IV



Well V

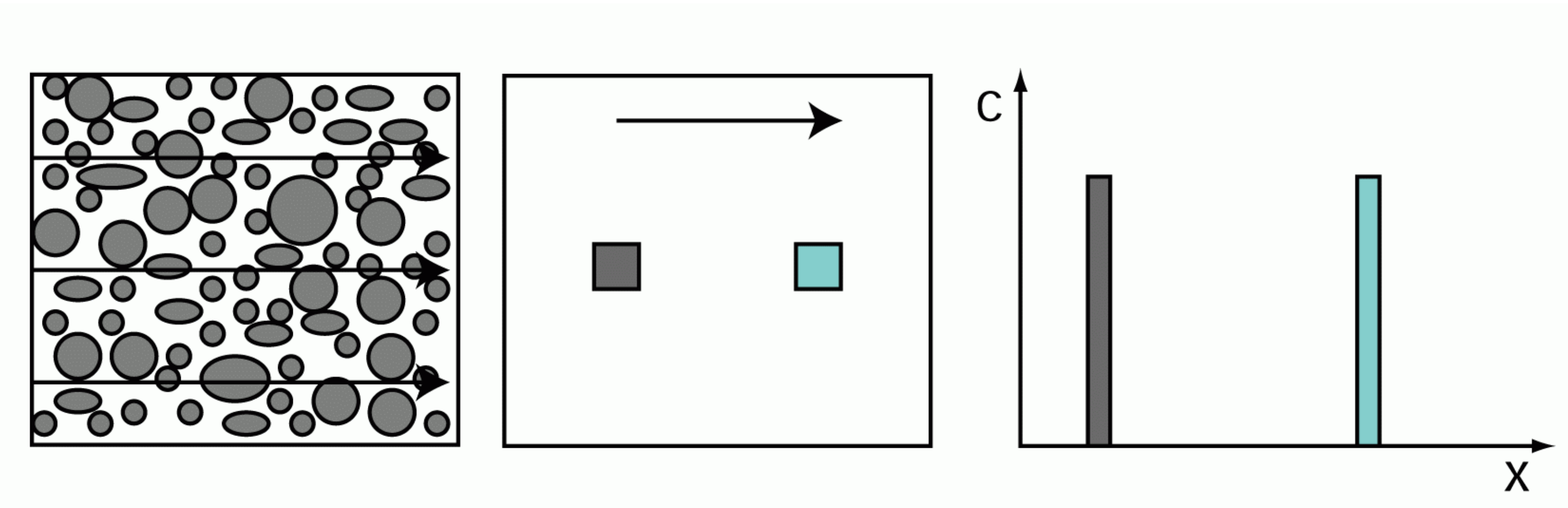


Well VI

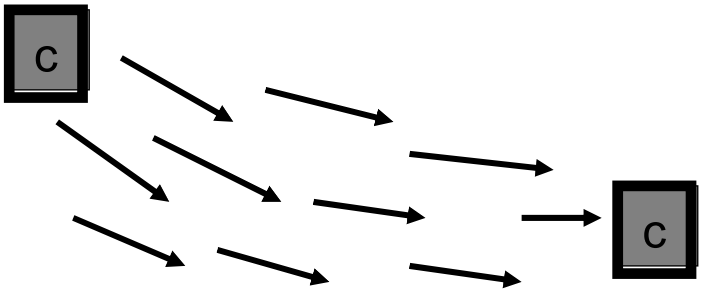


Transport processes

Advektion



Advection

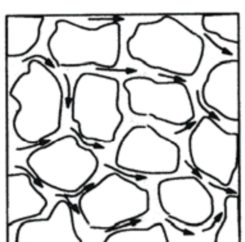


transport with groundwater flow

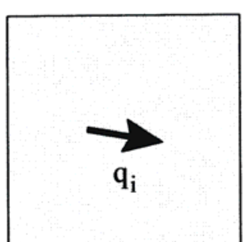
depends on the average particle velocity
of groundwater (distance velocity)

advectiv flux = particle velocity * concentration

$$j_i^a = u_i c$$



particle velocity



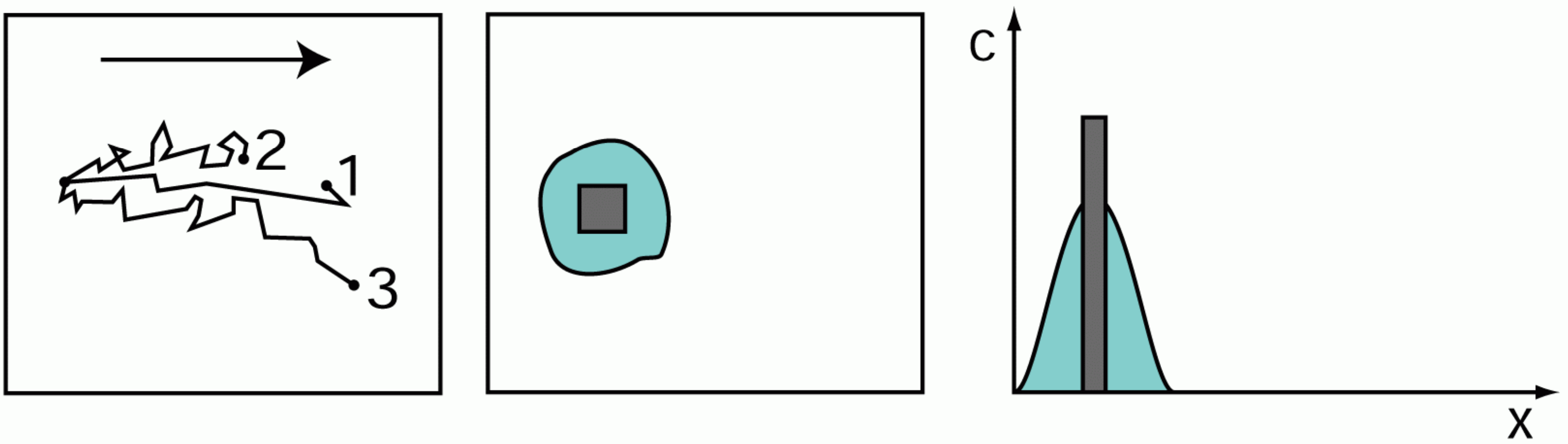
darcy velocity

average particle velocity (distance velocity) =
Darcy velocity / effective porosity

$$u_i = \frac{q_i}{n^{eff}}$$

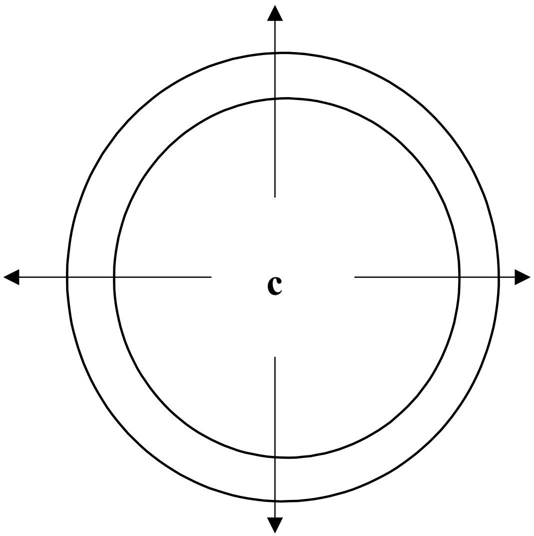
Transport processes

Diffusion



Diffusion

flux from higher to lower concentration



depends on:

- soil characteristics
- gradient of concentration

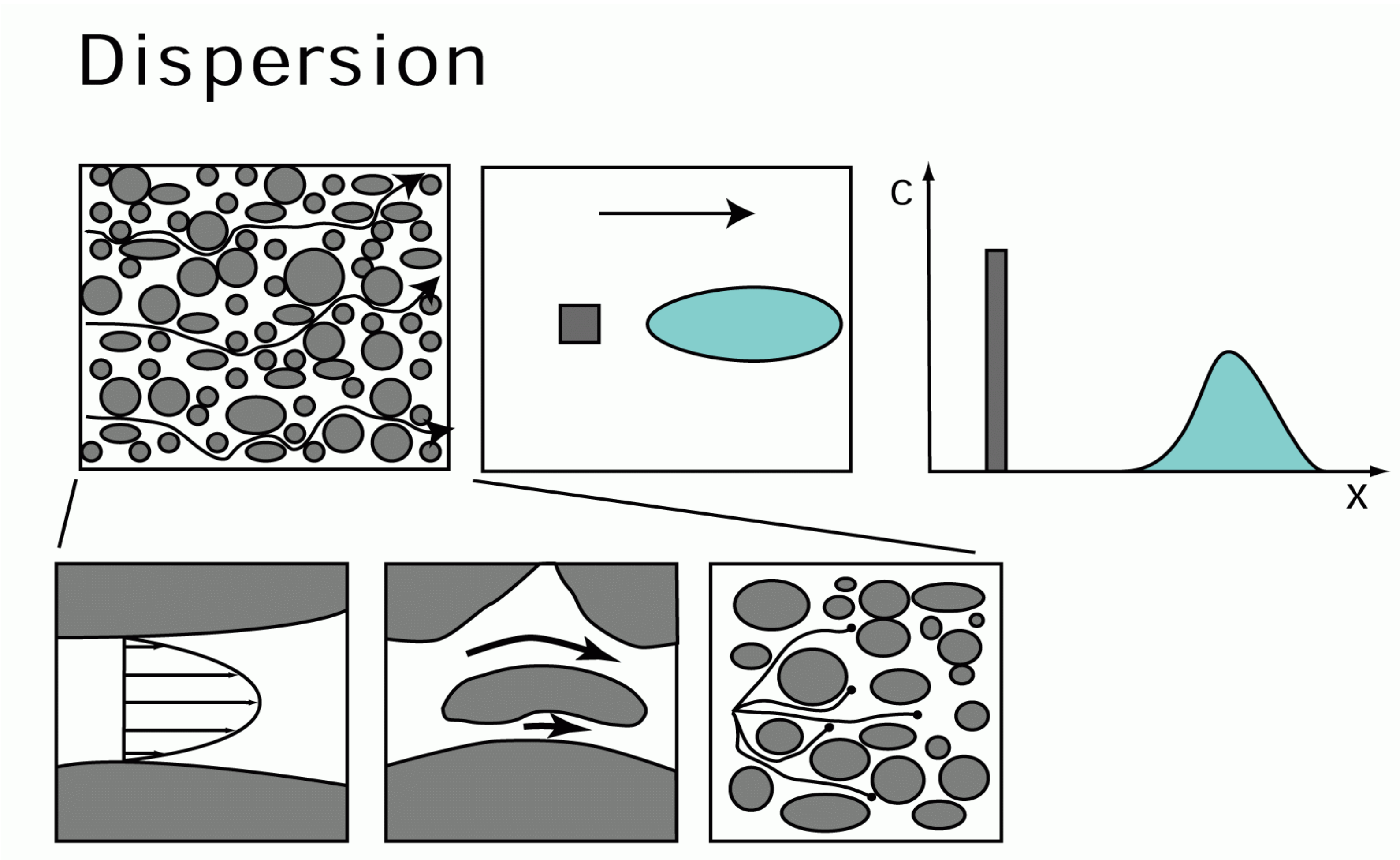
depends <u>not</u> on:

- groundwater flow !
- direction

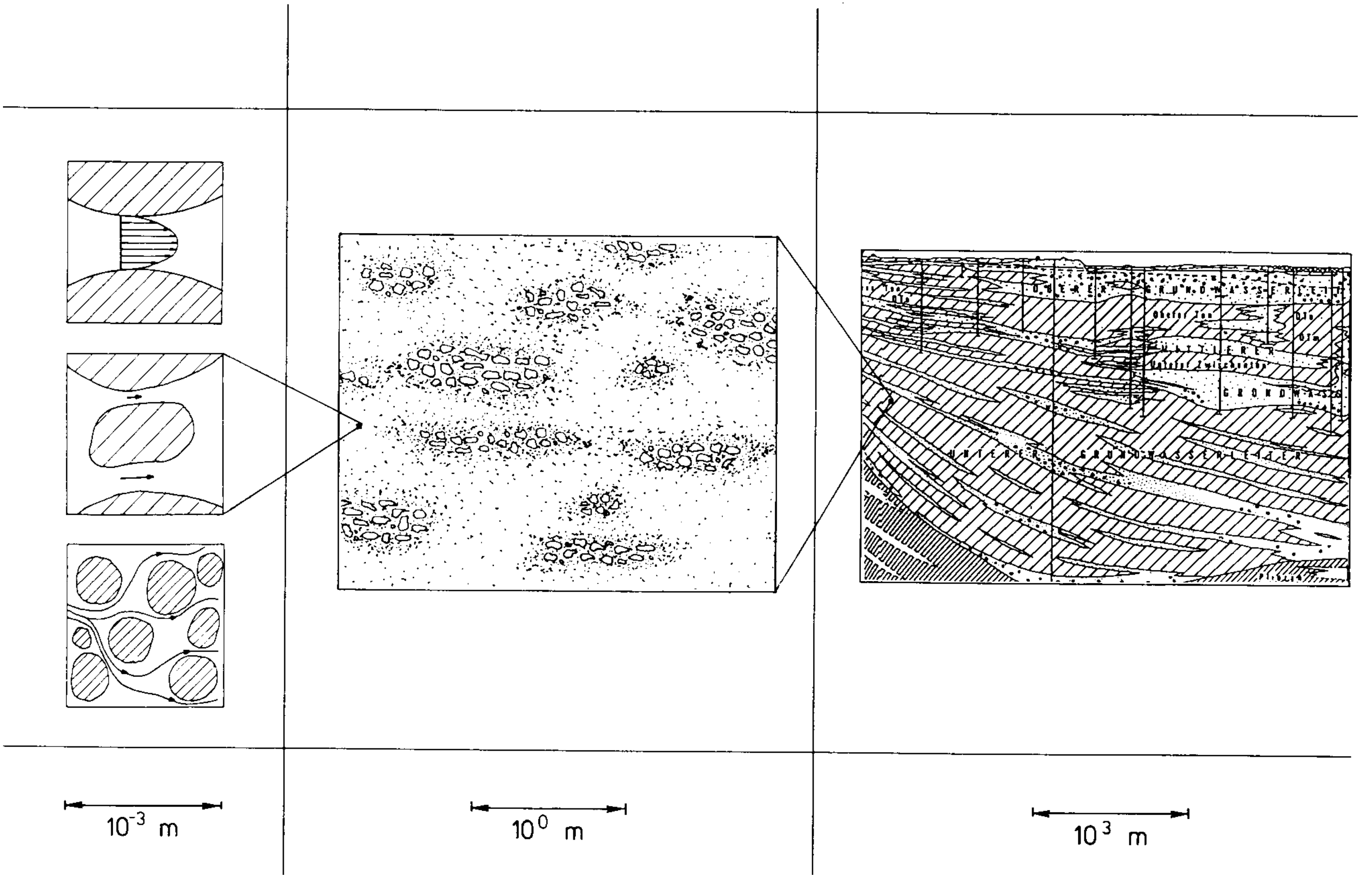
flux = diffusion coefficient * (- gradient of concentration)

$$\dot{j}_i^m = -D \frac{\partial c}{\partial x_i}$$

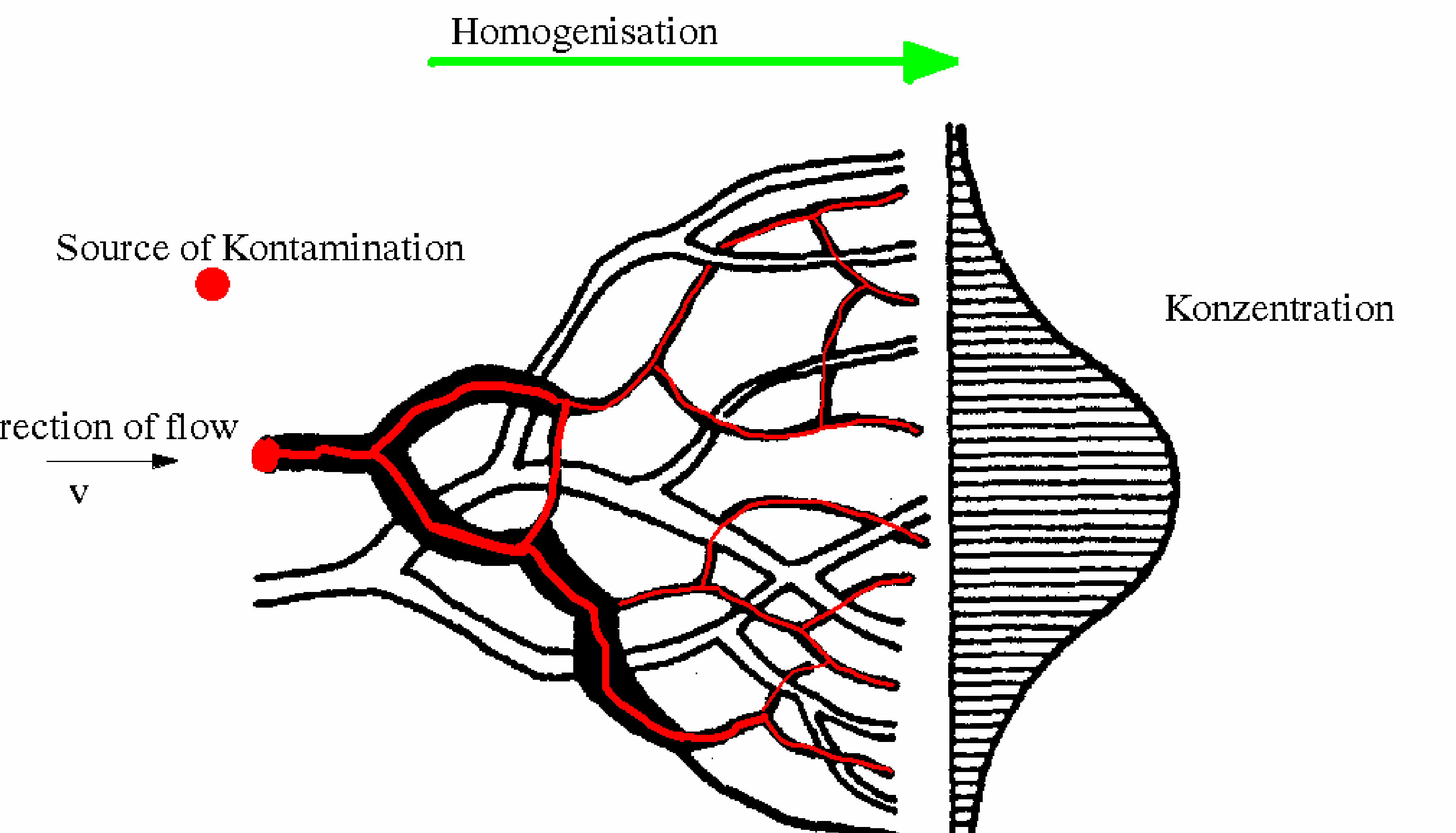
Transport processes 3



Scale

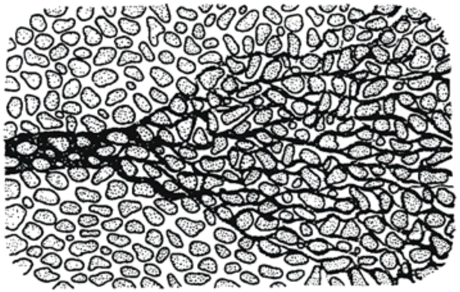


Makroskopic **Dispersion** because of mikroskopic Heterogenity



Hydromechanical Dispersion

Spreading of the transported substance due to the way around the grains and heterogenity of permeability in all scales



depends on:
- soil characteristics
- flow velocity
- model scale
- gradient of concentration

flux = dispersion tensor * (- gradient of concentration)

$$j_i^d = -D_{ij} \frac{\partial c}{\partial x_j}$$

$$D_{xx} = \alpha_L \frac{u_x^2}{|u|} + \alpha_{TH} \frac{u_y^2}{|u|} + \alpha_{TV} \frac{u_z^2}{|u|}$$

$$D_{xy} = D_{yx} = (\alpha_L - \alpha_{TH}) \frac{u_x u_y}{|u|}$$

$$D_{yy} = \alpha_{TH} \frac{u_x^2}{|u|} + \alpha_L \frac{u_y^2}{|u|} + \alpha_{TV} \frac{u_z^2}{|u|}$$

$$D_{xz} = D_{zx} = (\alpha_L - \alpha_{TV}) \frac{u_x u_z}{|u|}$$

$$D_{zz} = \alpha_{TV} \frac{u_x^2}{|u|} + \alpha_{TV} \frac{u_y^2}{|u|} + \alpha_L \frac{u_z^2}{|u|}$$

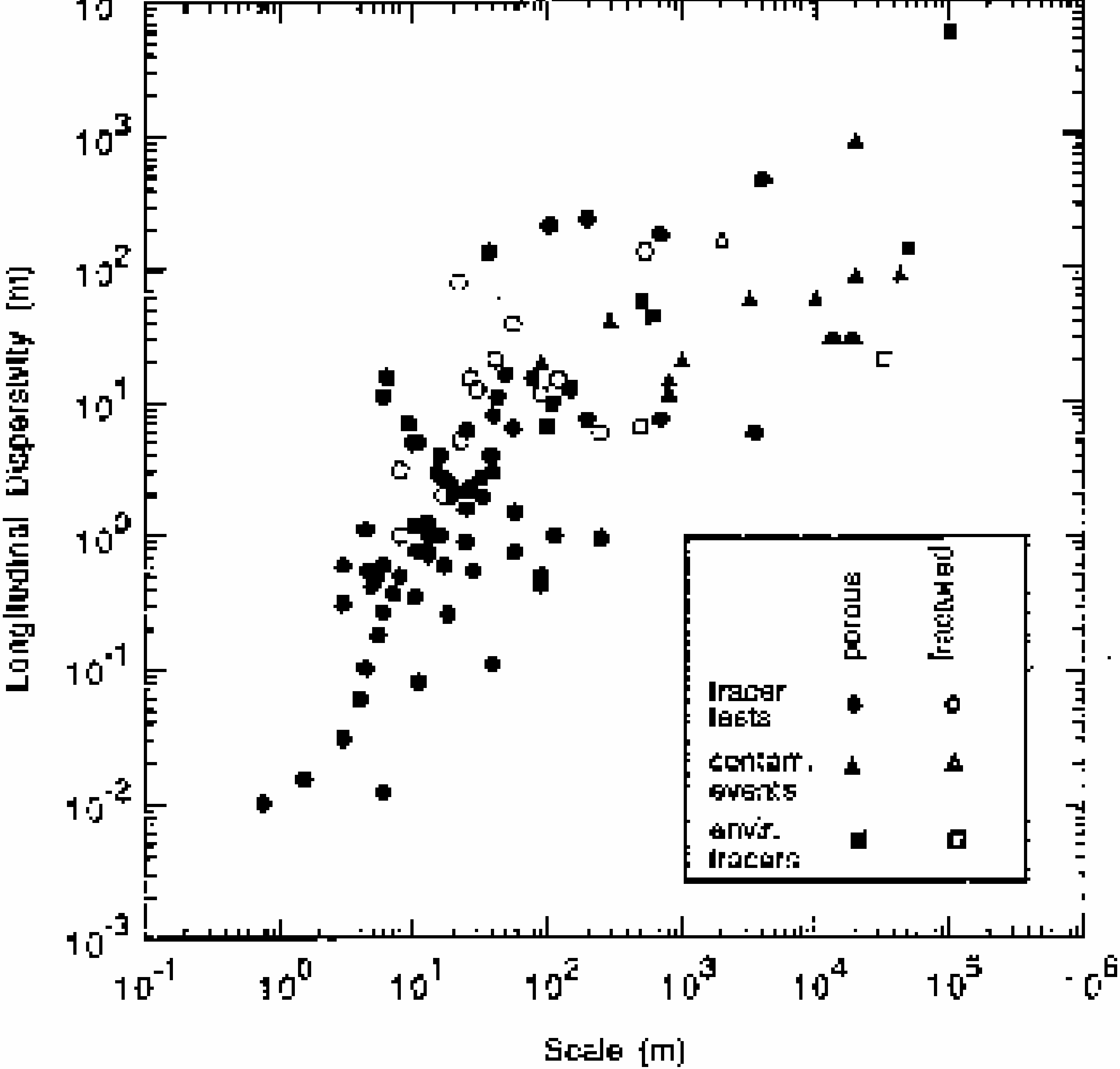
$$D_{yz} = D_{zy} = (\alpha_L - \alpha_{TV}) \frac{u_y u_z}{|u|}$$

mit: α_L longitudinal dispersion coefficient [m]

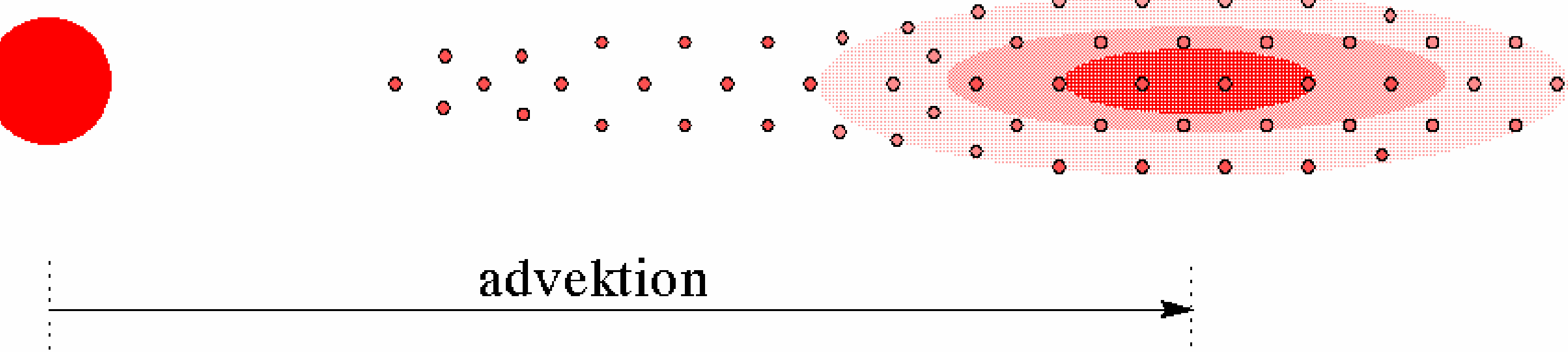
α_{TH} transversal horizontal dispersion coeff. [m]

α_{TV} transversaler vertical dispersion coeff. [m]

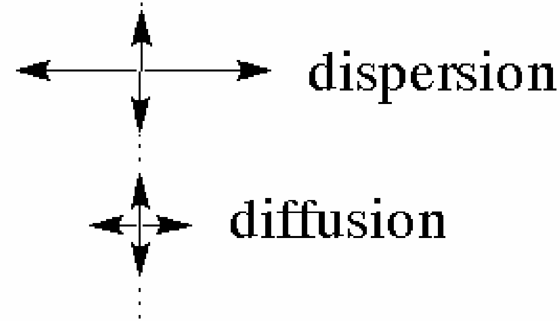
u_i distance velocity [m/s]



Longitudinal Dispersivity (m)
Scale (m)
porous
fractured
tracer tests
contam. events
envir. tracers



Transport



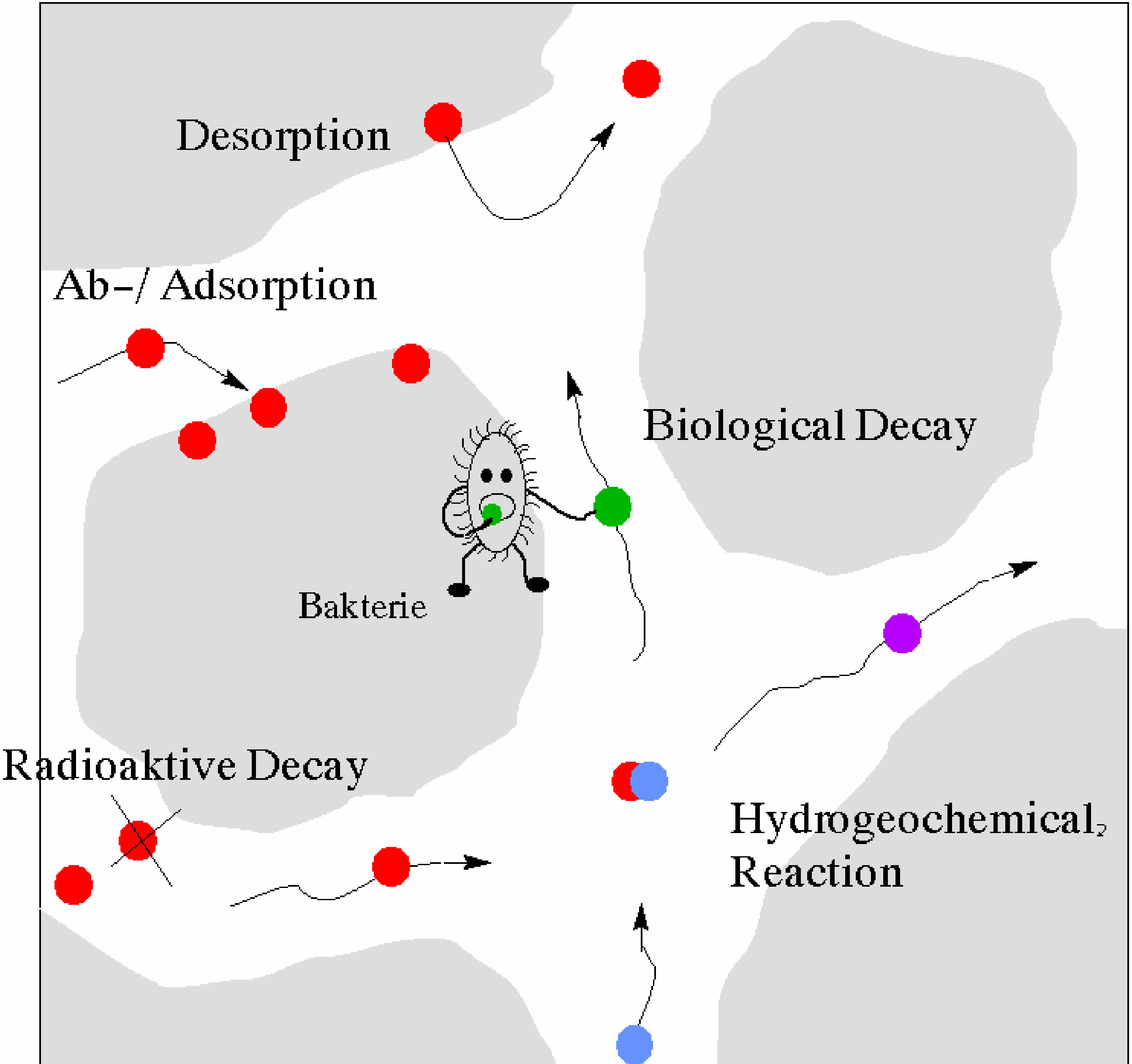
$$(nS_w \varrho)\frac{\partial c}{\partial t} + \varrho\, v_i \frac{\partial c}{\partial x_i} - \frac{\partial}{\partial x_i}(nS_w\, \varrho\left(D_{ij} + D_{mol}\,\delta_{ij}\right)\frac{\partial c}{\partial x_j}) = q(c^* - c)$$

storage　　advektion　　dispersion & diffusion　　source

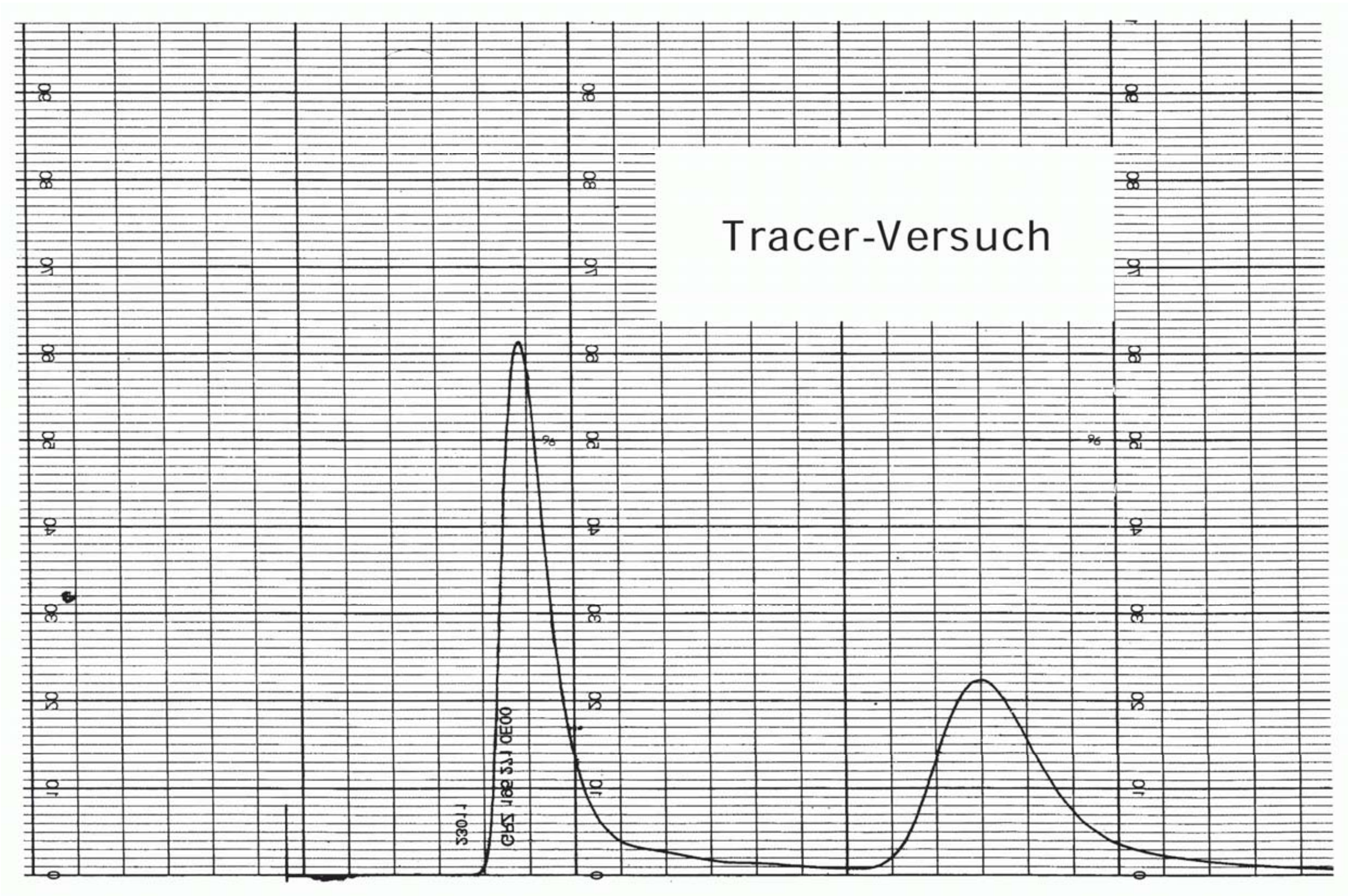
coupled　　$\varrho(c) = \varrho_0 + \frac{\partial \varrho}{\partial c} * c$　　or PHREEQC-2

$|\ f$

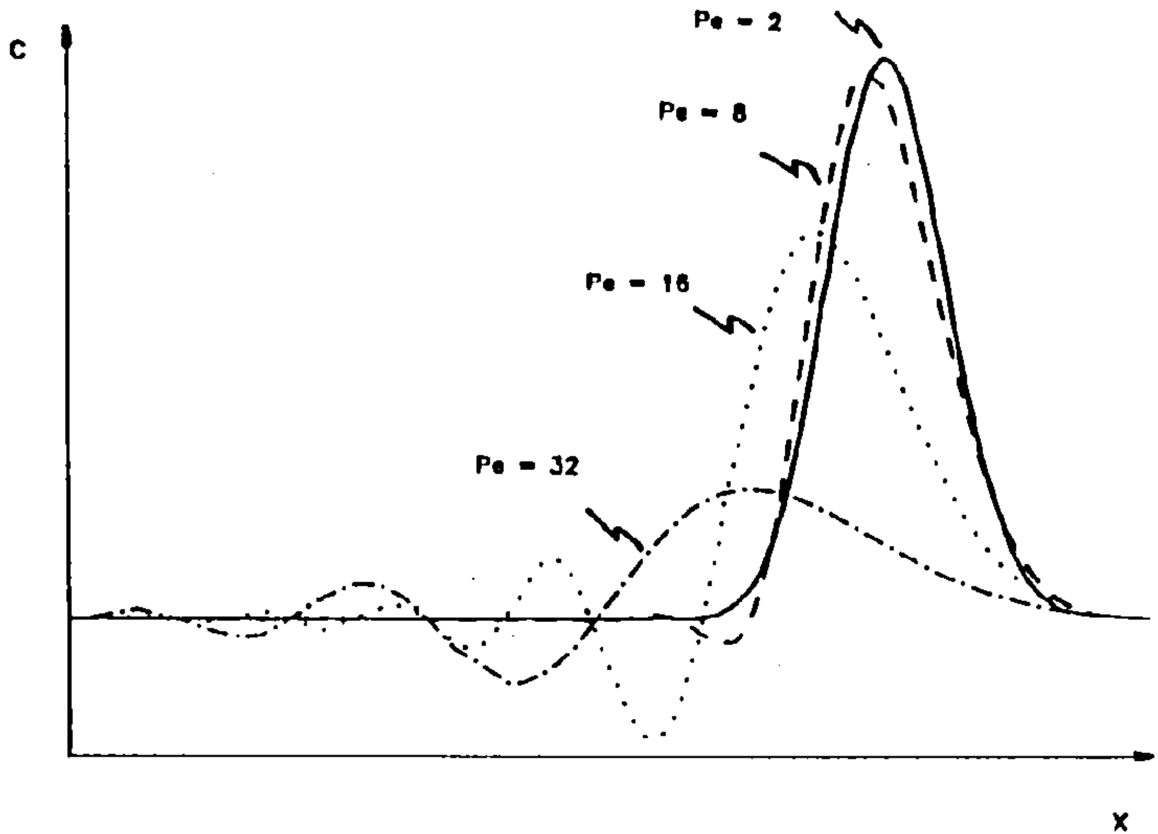
Nonkonservative Transport Processes



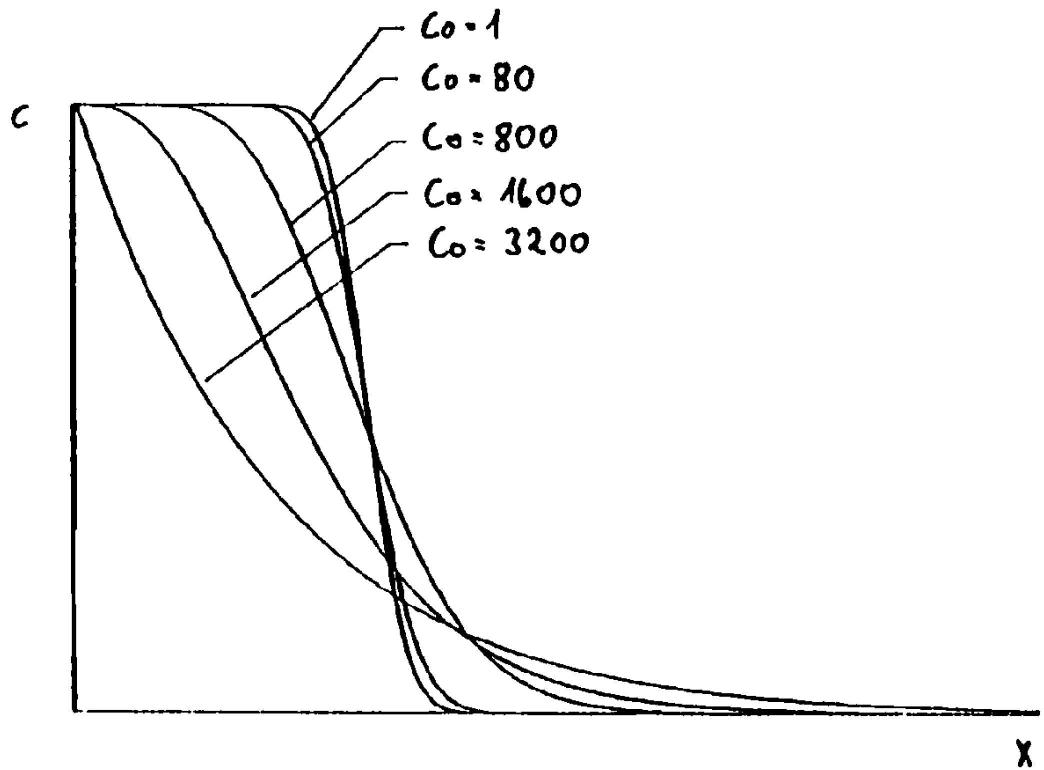
Tracer Porous Media



Influence of peclet number



Influence of courant criterion



⇒ transport equation: symmetric + stabilisation

- streamline upwind

⇒ solver

- SuperLU ⟶ $O(n^2)$
- PCG method ⟶ $O(n^{3/4})$

  preconditioning:

  ICC, SSOR, BlockSSOR, AMG
- Multigrid ⟶ $O(n)$

⇒ nonlinearity

- Leakage condition with limited mass flow rates
- Saturation
- Density
- Sorption ⟶ Picard iteration

$$\frac{\partial c}{\partial t} + A_1 c + A_2 c = f \qquad (4)$$

where

$$A_1 = -\, \boldsymbol{div}(\boldsymbol{D}\ \boldsymbol{grad}(\,)) + q(\,), \qquad (5)$$

$$A_2 = \boldsymbol{v}\boldsymbol{grad}(\,), \qquad (6)$$

$$f = qc^{*}\,. \qquad (7)$$

The time discretisation results in:

$$\frac{\Delta c}{\Delta t} + \Theta(A_1 + A_2)\Delta c = -(A_1 + A_2)c^n + f, \qquad (8)$$

where

$$c^{n+1} = c^n + \Delta c \qquad (9)$$

$0 \leq \Theta \leq 1.$

As a first step the term Δc is substituted by $'e'$ and equation (8) becomes:

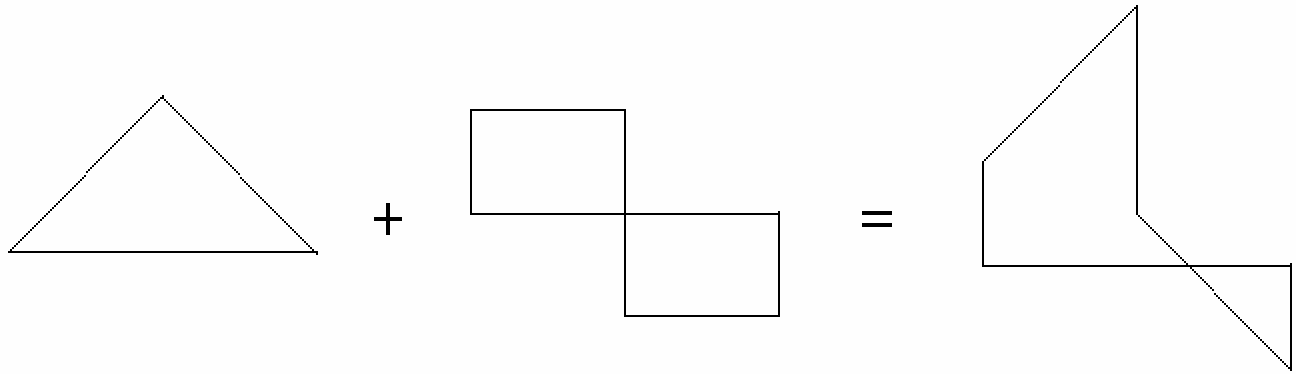
$$\frac{e}{\Delta t} + \Theta A_1 e = -(A_1 + A_2)c^n + f. \qquad (10)$$

In the second step $'g'$ is determined using $'e'$ previously obtained from equation (10)

$$\frac{g}{\Delta t} + \Theta A_2 g = \frac{e}{\Delta t}. \qquad (11)$$

The final solution for the time step n+1 is given by

$$c^{n+1} = c^n + g \qquad (12)$$



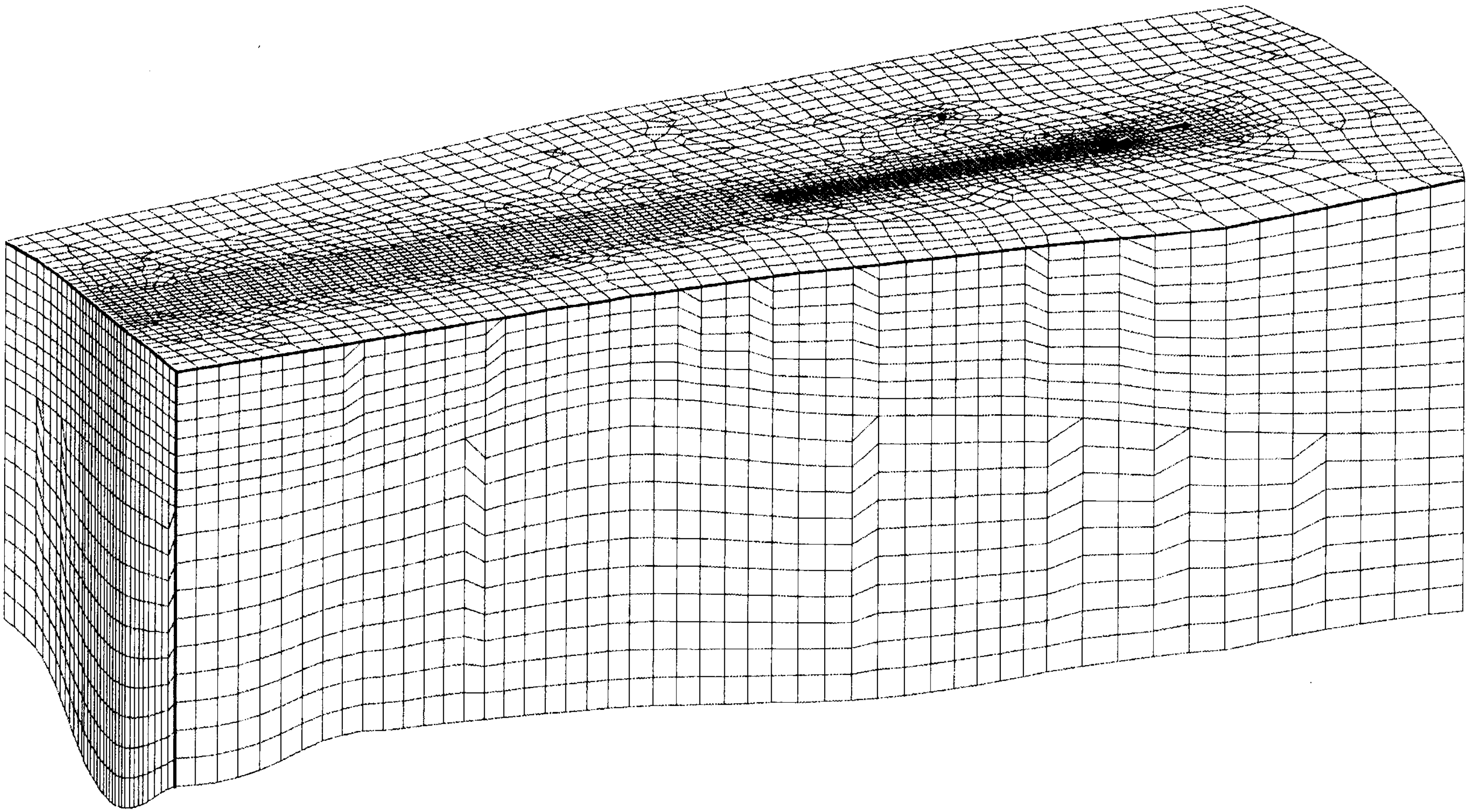
ϕ_i $\Theta \Delta t v_l \phi_{i,l}$ *upwind weighting*

Test function of the operator split

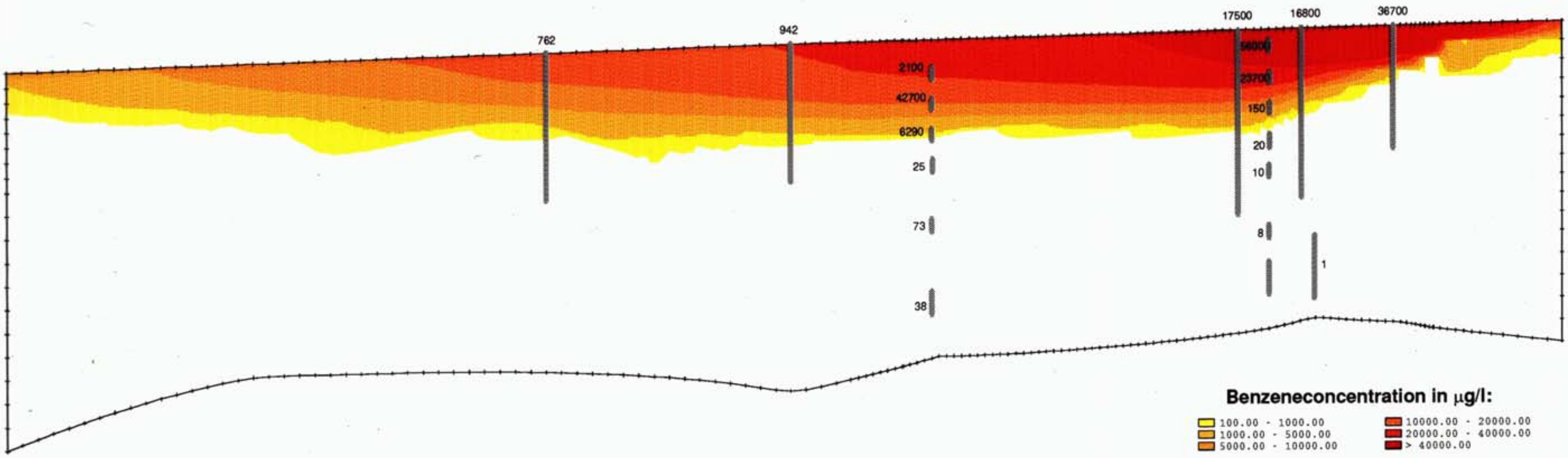
Testfunction of the secound step

$\Theta^2 \Delta t v_k v_l \phi_{i,l} \phi_{j,k}$

3D-Model Mesh

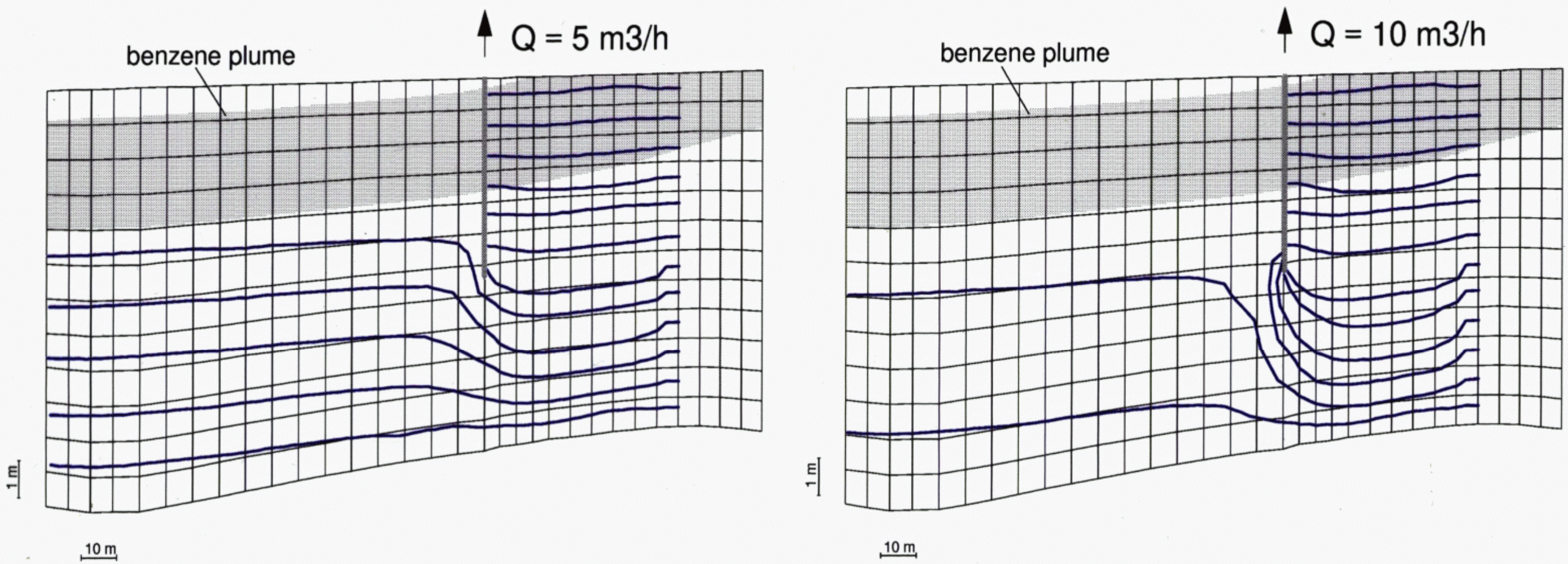


Calculated bencene plume

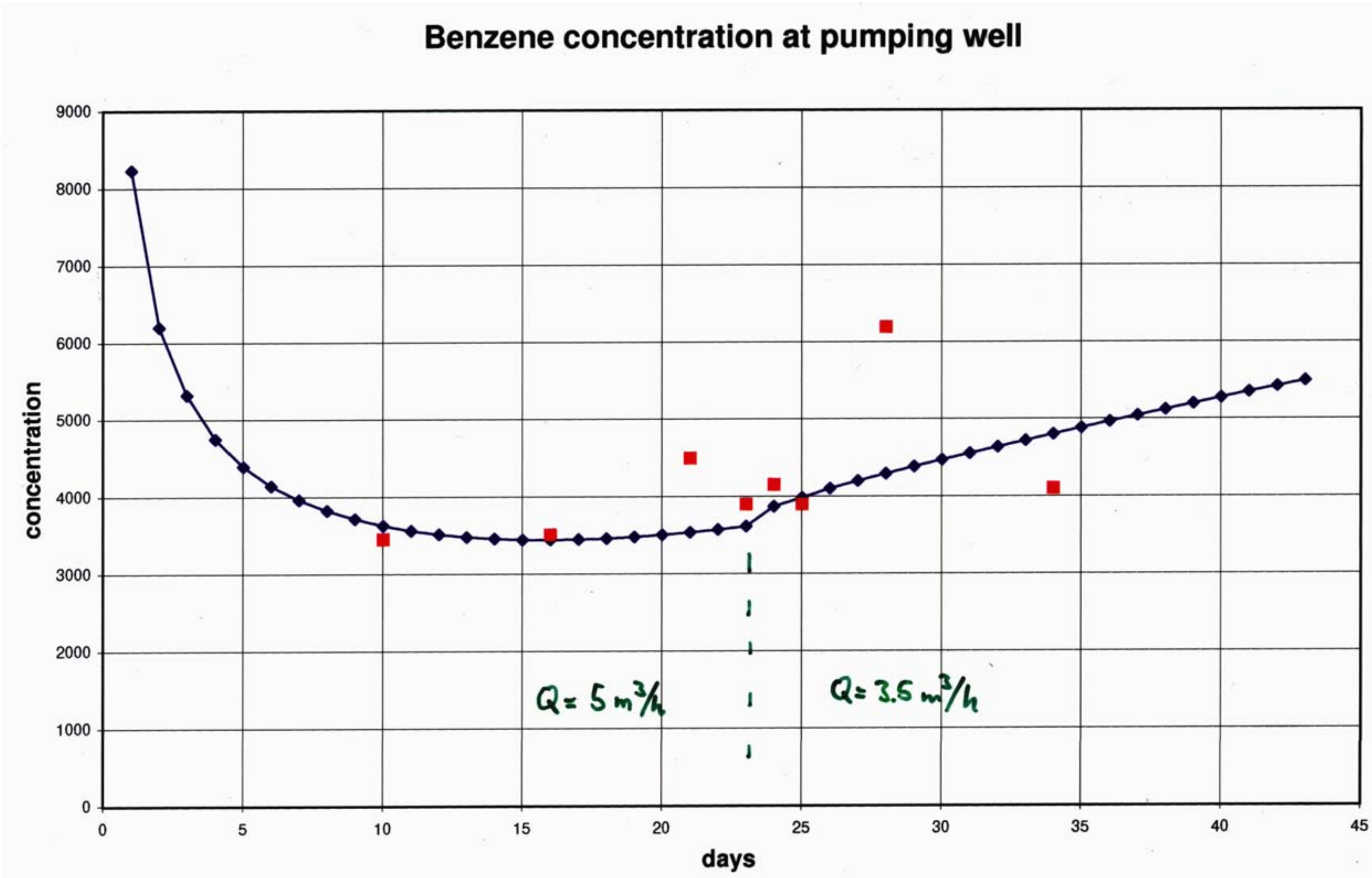


Calculated bencene plume and measured concentrations

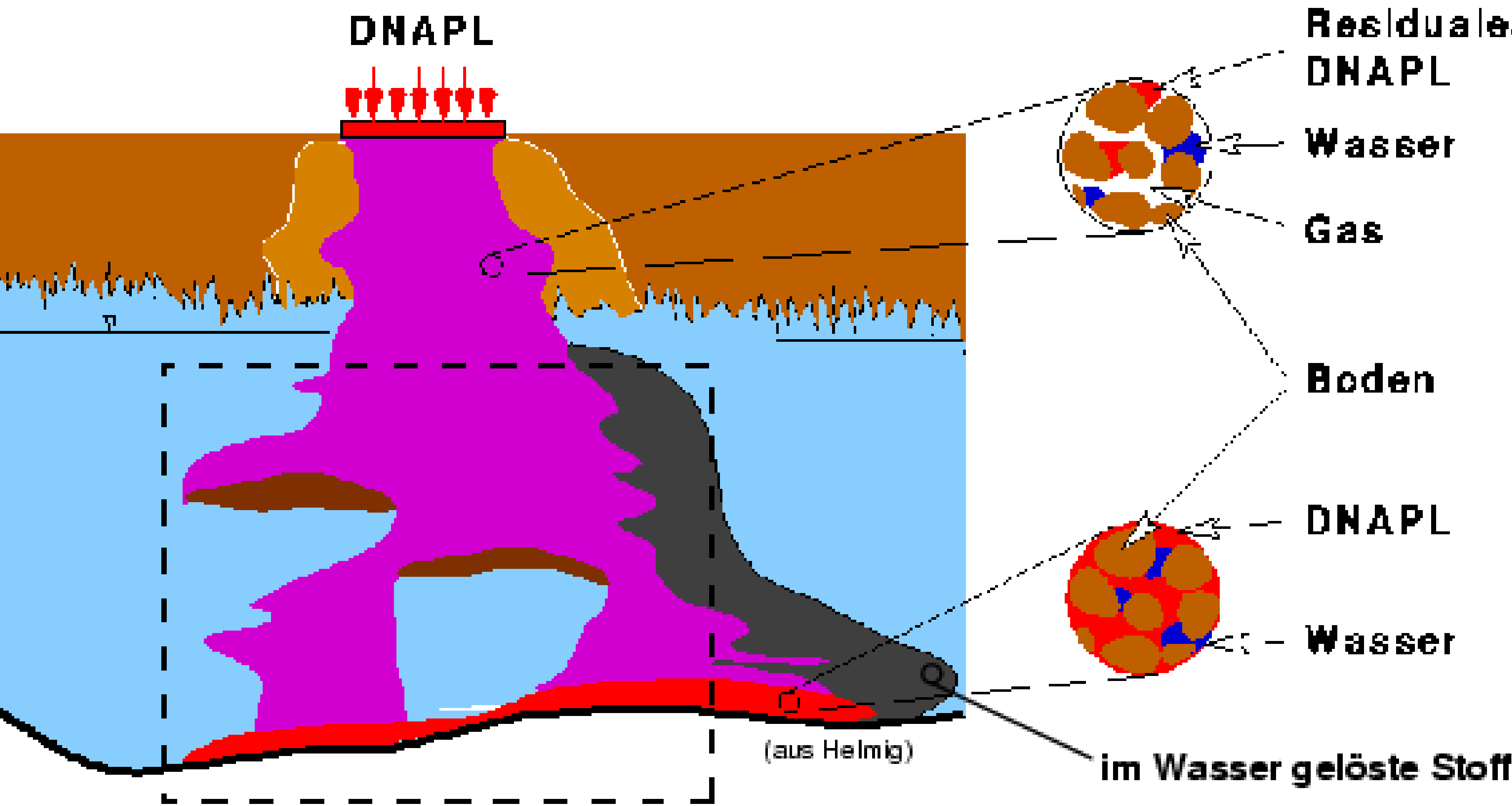
ertical catchment area of a partialy penetrating we



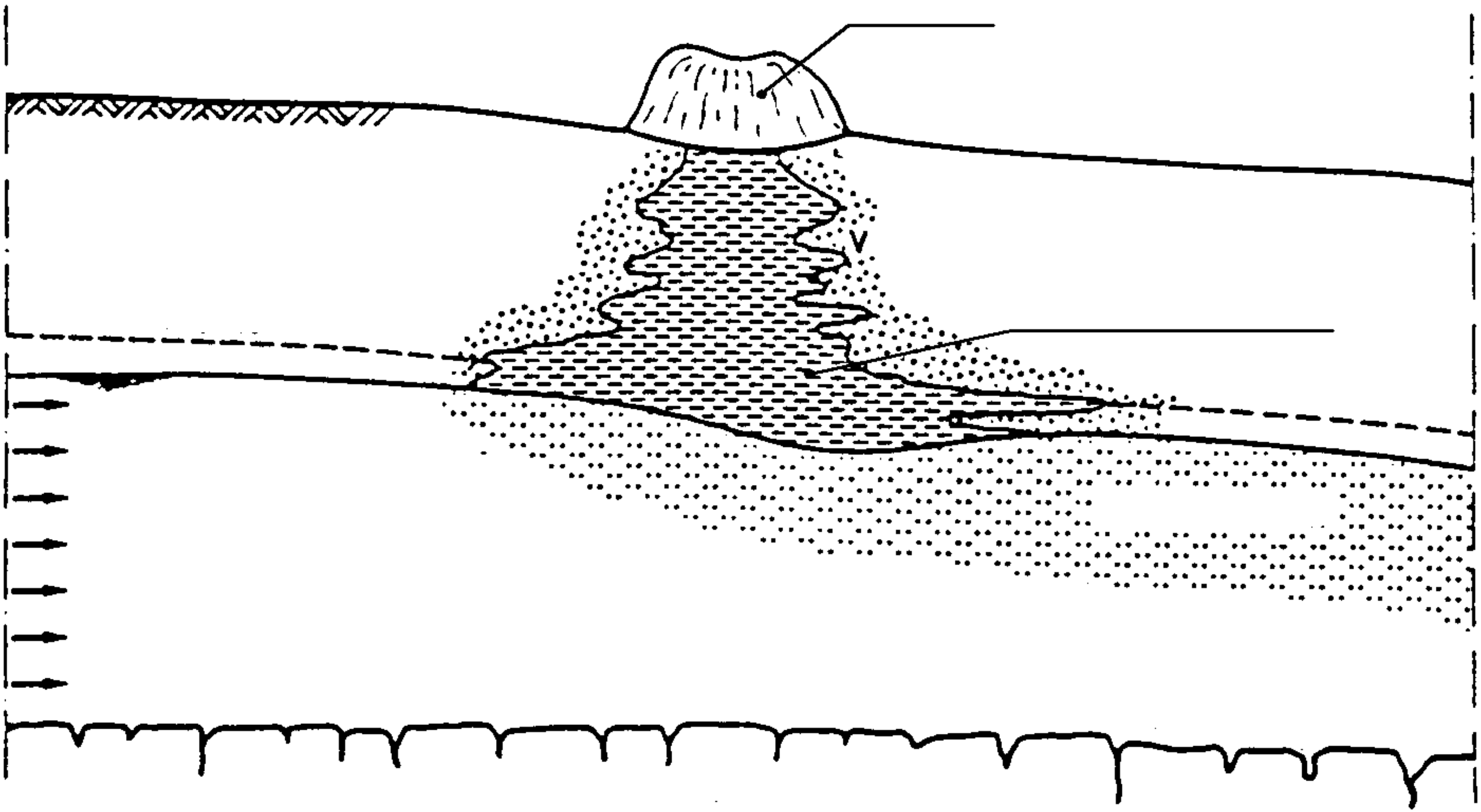
Vertical catchment area of a partialy penetrating well with pathlines


Benzene concentration at pumping well
concentration
days
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
0
5
10
15
20
25
30
35
40
45
Q= 5 m³/h
Q= 3.5 m³/h

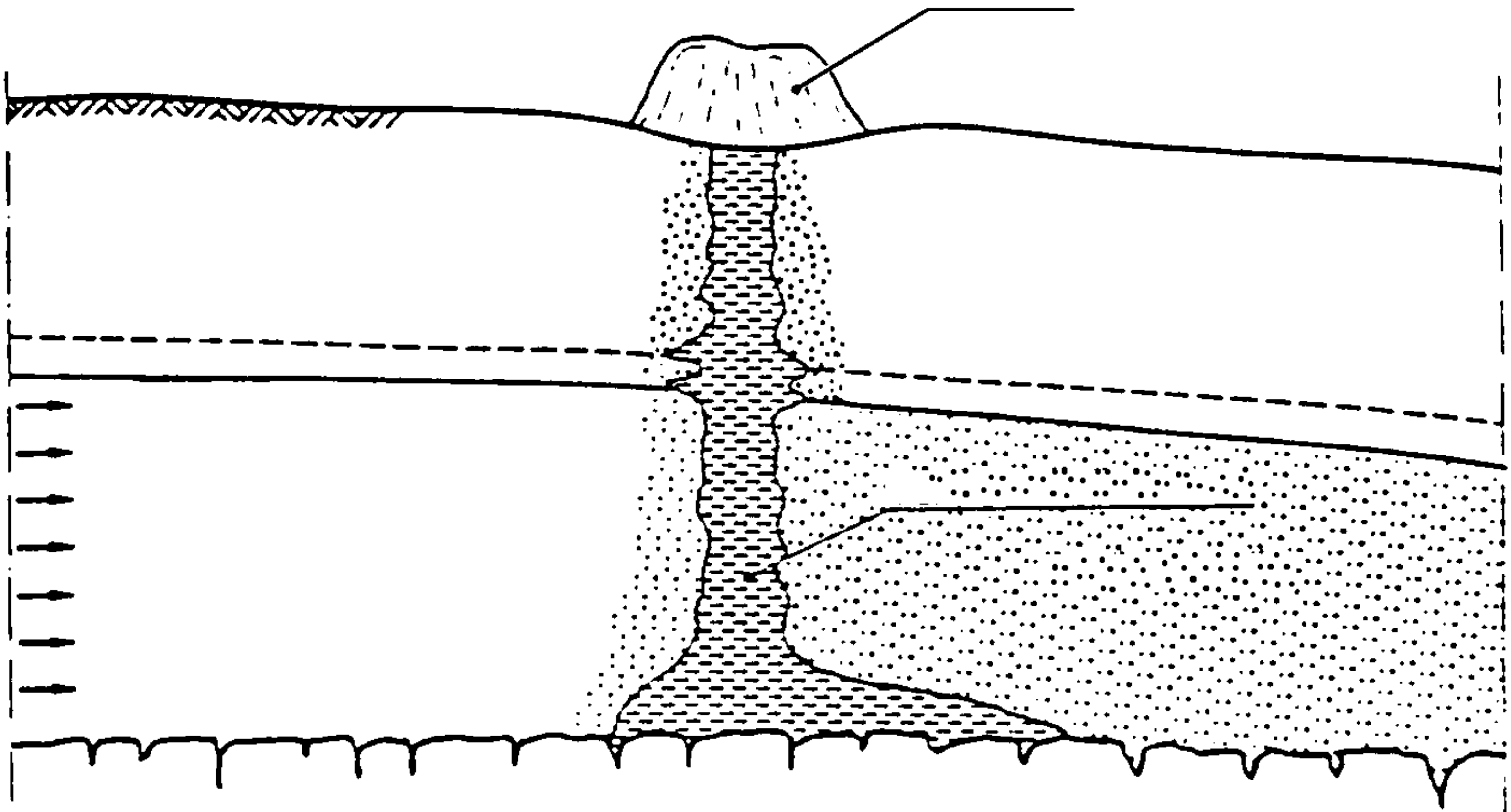
Multiphase Flow

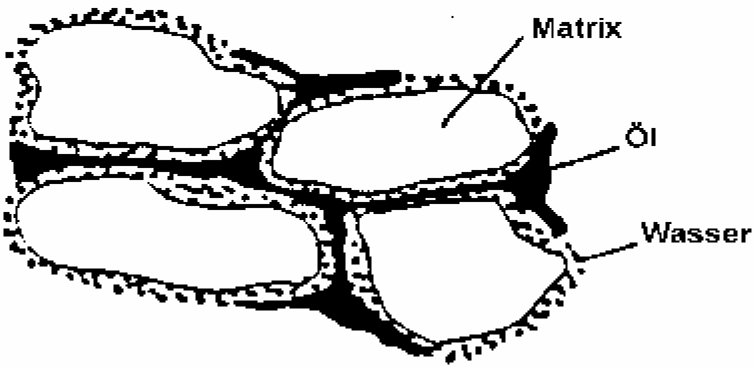


Multiphase Flow

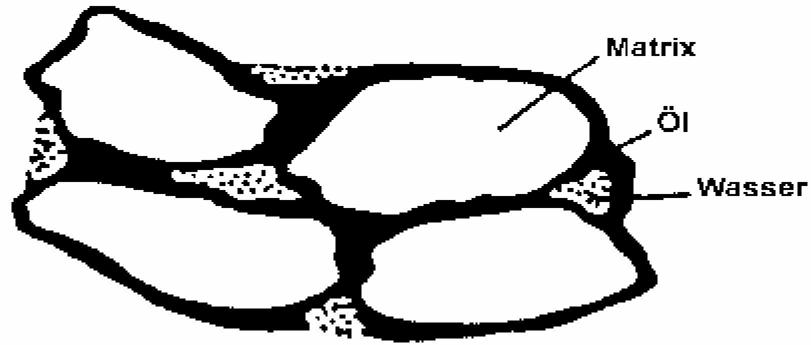


Multiphase Flow

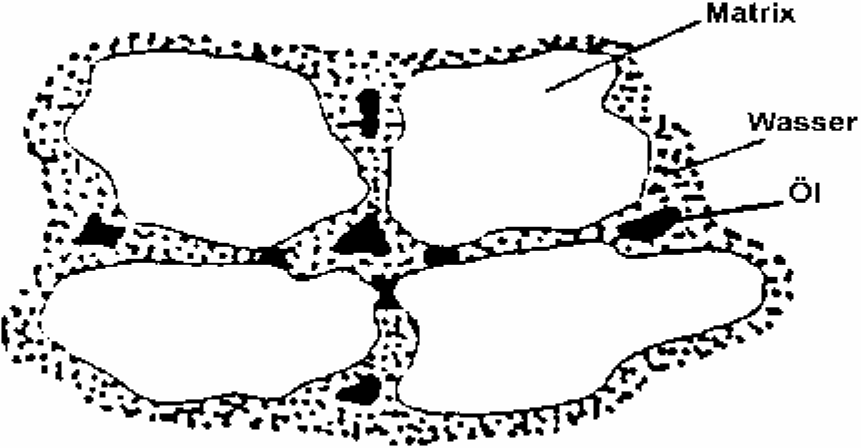




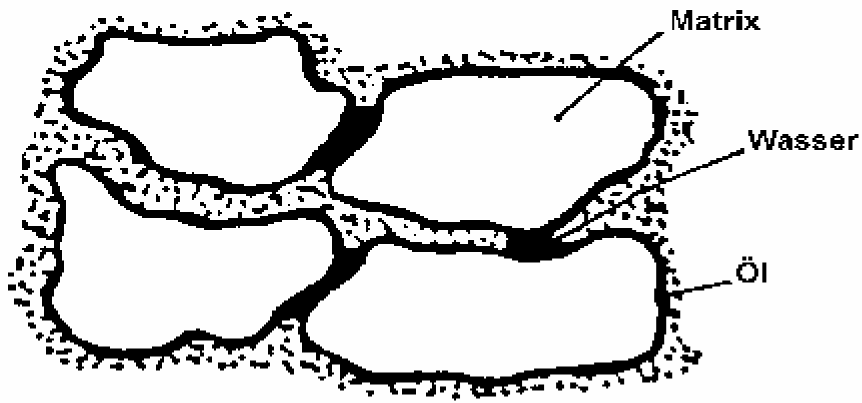
Funiculare Verteilung (Öl)
Benetzende Phase: Wasser



Funiculare Verteilung (Öl)
Benetzende Phase: Öl



Insulare Verteilung / Residualöl
Benetzende Phase: Wasser



Pendulare Verteilung / Residualöl
Benetzende Phase: Öl

1. Phase

$$(\rho^{nw} S^{op,nw} (1 - S^{w}) \frac{\partial p^{c}}{\partial S^{w}} - n \rho^{nw}) \frac{\partial S^{w}}{\partial t} + \rho^{nw} S^{op,nw} (1 - S^{w}) \frac{\partial p^{w}}{\partial t}$$

$$- \frac{\partial}{\partial x_j} (\frac{\rho^{nw}}{\eta^{nw}} k^{r,nw} K_{ij} \frac{\partial}{\partial x_i} (\frac{dp^{c}}{dS^{w}} S^{w} + p^{w} + \rho^{nw} g z)) - \rho^{nw} q^{nw} =$$

2. Phase

$$\rho^{w} \frac{\partial S^{w}}{\partial t} + \rho^{w} S^{op,w} S^{w} \frac{\partial p^{w}}{\partial t} - \frac{\partial}{\partial x_j} (\frac{\rho^{w}}{\eta^{w}} k^{r,w} K_{ij} \frac{\partial}{\partial x_i} (p^{w} + \rho^{w} g z)) - \rho^{w} q^{w} =$$

Coupeling Condition

$$\sum S^{\alpha} = 1 \qquad\qquad p^{c} = p^{nw} - p^{w}$$

with

$$p^{c} = p^{c}(S^{w}) \qquad k^{r,w} = k^{r,w}(S^{w}) \qquad k^{r,nw} = k^{r,nw}(S^{w})$$

Boundary Condition

1. Art

$$S^{w} = \overline{S}^{w}(t)$$

$$p^{w} = \overline{p}^{w}(t) \quad \text{auf} \quad \Gamma_1 \subset \Gamma$$

2. Art

$$q^{w}\mathbf{n} = \overline{q}_{n}^{w}(t)$$

$$q^{nw}\mathbf{n} = \overline{q}_{n}^{nw}(t) \quad \text{auf} \quad \Gamma_2 \subset \Gamma$$

Initial Condition

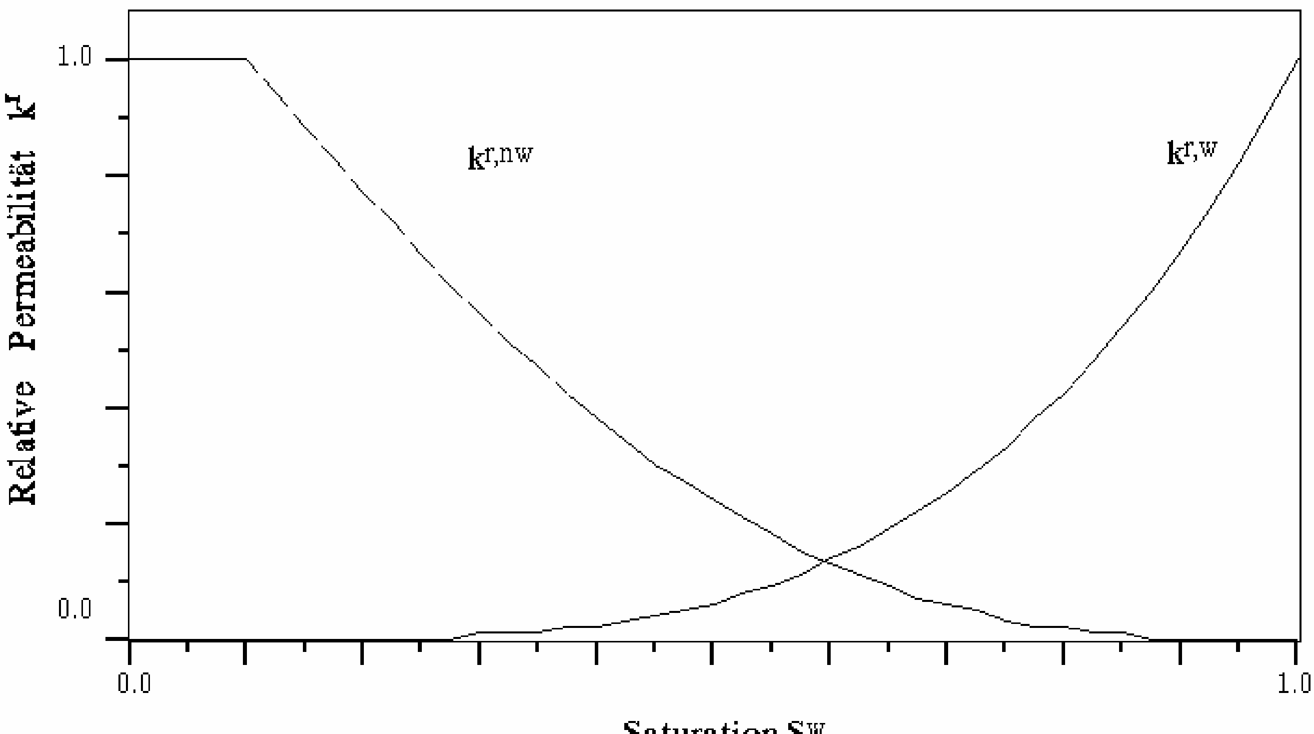
$$S^{w}(x, y, z, t_0) = \overline{S}^{w}$$

$$p^{w}(x, y, z, t_0) = \overline{p}^{w}$$

Relative Permeability - Saturation law from Brooks-Corey

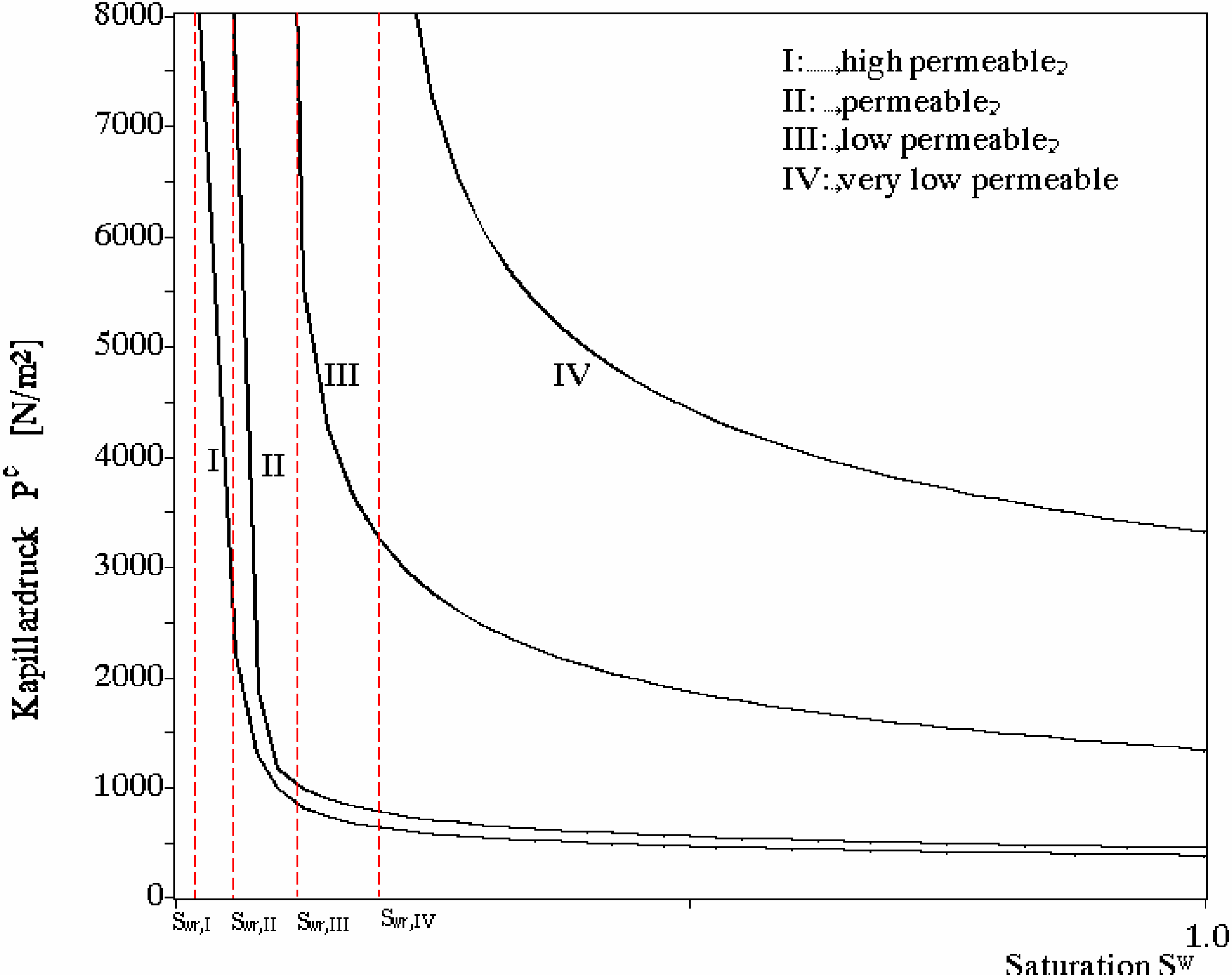
$$k^{r,w} = (S_e)^{\frac{2+3\lambda}{\lambda}}$$

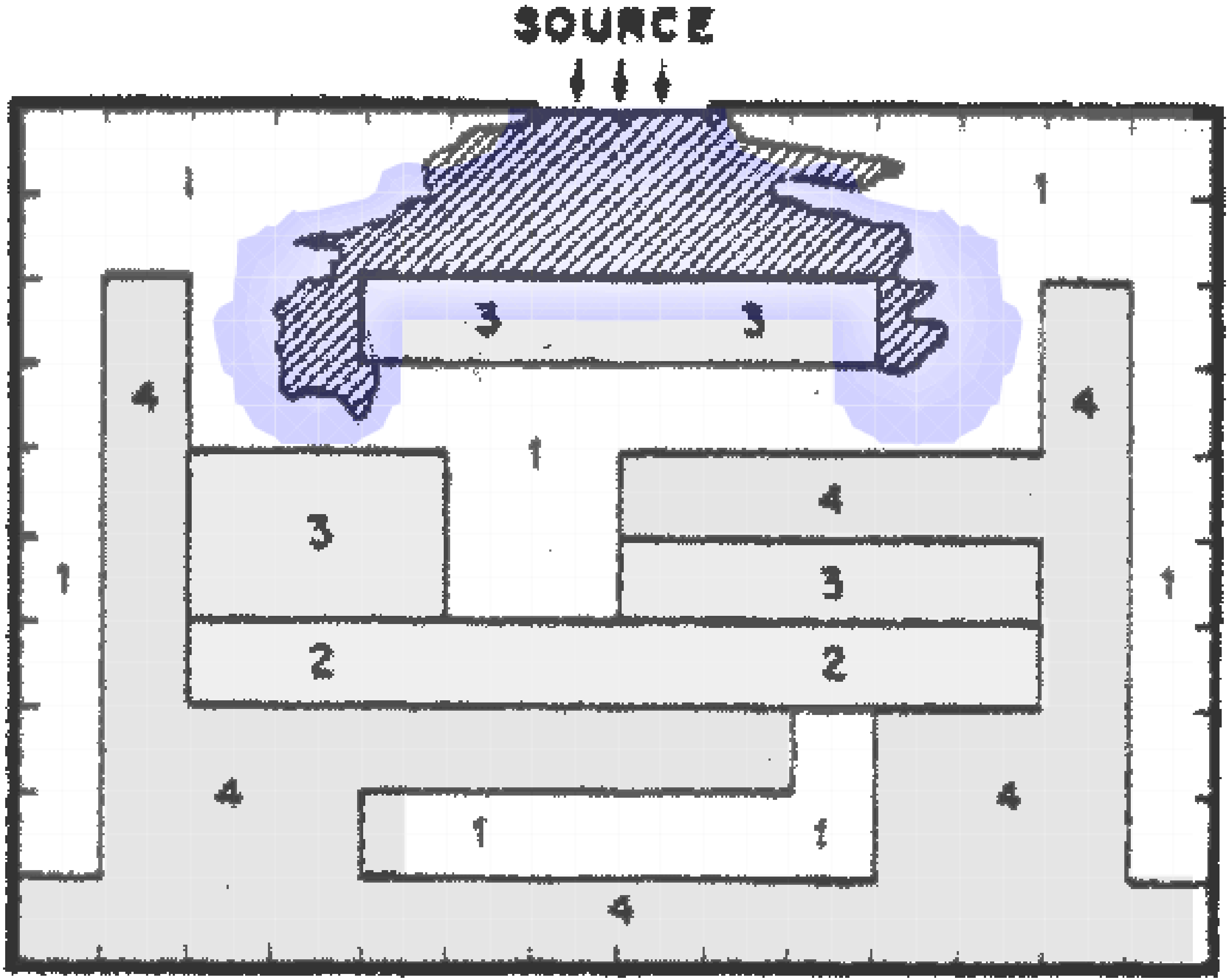
$$k^{r,nw} = (1 - S_e)^2\left[1 - S_e^{\frac{2+\lambda}{\lambda}}\right] \qquad \text{with} \qquad S^e = \frac{S^w - S^{wr}}{1 - S^{wr}}.$$

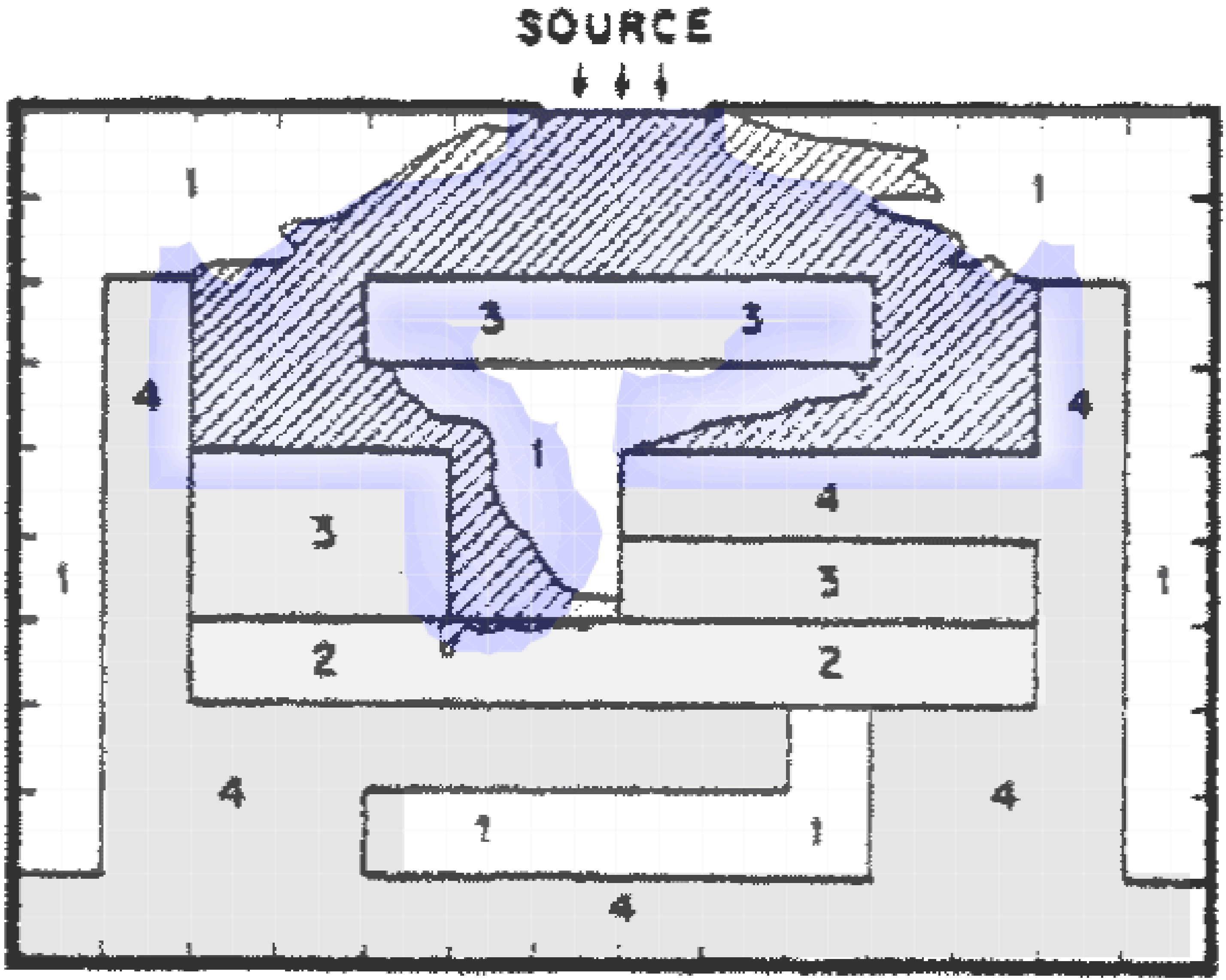


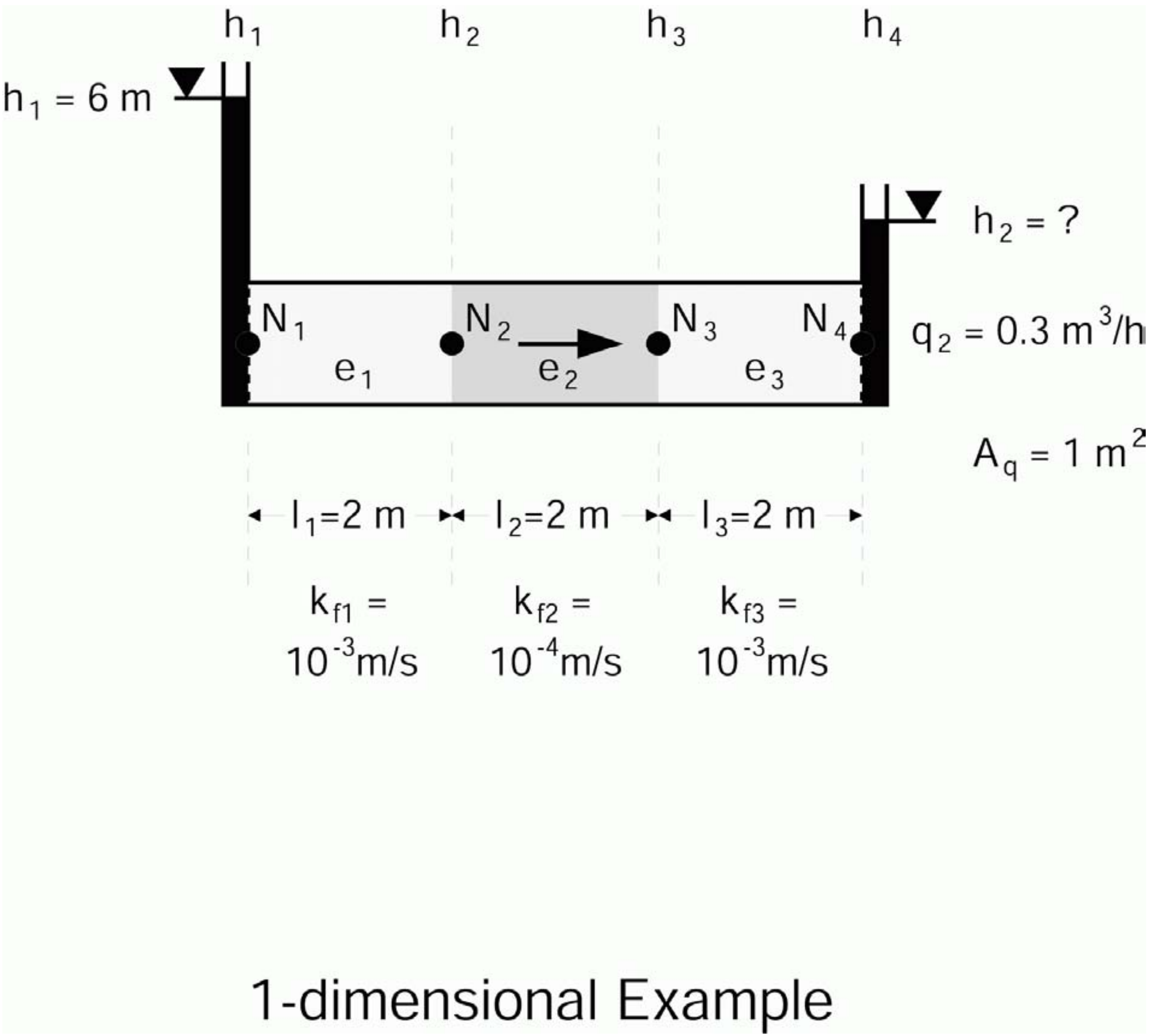
Capillary-Pressure-Saturation law from Brooks-Corey

$$p^c = p^b \left(\frac{S^w - S^{wr}}{1 - S^{wr}} \right)^{-\frac{1}{\lambda}}, \qquad p^c \geq p^b.$$




SOURCE
1
1
3
3
4
4
1
3
4
1
3
1
2
2
4
4
1
1
4


SOURCE
1
1
3
3
4
4
1
3
4
3
1
1
2
2
4
4
1
1
4


h1
h2
h3
h4
h1 = 6 m
h2 = ?
N1
N2
N3
N4
e1
e2
e3
q2 = 0.3 m3/h
Aq = 1 m2
l1=2 m
l2=2 m
l3=2 m
kf1 = 10-3m/s
kf2 = 10-4m/s
kf3 = 10-3m/s
1-dimensional Example

General Transport Equation:

$$
\left(\mathrm{n}\,S_r\varsigma\right)\frac{\partial c}{\partial t}+\left(\left(1-\mathrm{n}_{\mathrm{a}}\right)\varsigma_s\right)\frac{\partial c_s}{\partial t}+\left(\mathrm{n}S_r\varsigma\right)\mathbf{v}\nabla c-\nabla\left(\mathrm{n}\,S_r\varsigma\left(d_m\mathbf{I}+\mathbf{D}\right)\nabla c\right)
$$

$$
=q(c^{in}-c\ )+q_c+\left(\mathrm{n}S_r\varsigma\right)f\ (c)+\left(\left(1-\mathrm{n}_{\mathrm{a}}\right)\varsigma_s\right)f_s(c_s)+\sum q^j
$$

with:

- *c = concentration of material in fluid [kg/kg]*
- *c_s = adsorbed concentration of material in matrix [kg/kg]*
- *c^{in} = input concentration of material [kg/kg]*
- *q_c = predetermined in-/output of material [kg/m³/s]*
- *q^j = in-/output of material from reactions*

General Transport Equation:

$$\left(\mathrm{n}\,S_r\varsigma\right)\frac{\partial c}{\partial t}+\left(\left(1-\mathrm{n_a}\right)\varsigma_s\right)\frac{\partial c_s}{\partial t}+\left(\mathrm{n}S_r\varsigma\right)\mathbf{v}\nabla c-\nabla\left(\mathrm{n}\,S_r\varsigma\left(d_m\mathbf{I}+\mathbf{D}\right)\nabla c\right)$$

$$=q(c^{in}-c\ )+q_c+\left(\mathrm{n}S_r\varsigma\right)f\ (c)+\left(\left(1-\mathrm{n_a}\right)\varsigma_s\right)f_s(c_s)+\sum q^j$$

Parameters:

- n = discharge-effective porosity of aquifer [-]
- n_a = total porosity of aquifer [-]
- S_r = saturation level [-]
- ς = density of fluid [kg/m³]
- ς = density of matrix [kg/m³]
- q = fluid source/depression term
- v = distance velocity [m/s] ; $v = v_f/n$; v_f = filter velocity [m/s]
- d_m = molecular diffusion coefficient [m²/s]
- D = symmetric dispersion tensor [m²/s]
- f = source/depression term built by production-/reduction-/degradation-processes of the material in the fluid [kg/kg/s]
- f_s = source/depression term built by production-/reduction-/degradation-processes of the adsorber in the fluid/matrix [kg/kg/s]

Adsorption Models

- Calculation without adsorption (non-adsorption)
- Linear adsorption model (Henry):

  k_d = Henry-isotherme of material [m³/kg]

$$c_s = (k_d \varsigma_0) c$$

- Freundlich-adsorption:

  k_1 = 1st Freundlich-isotherme of material [m³/kg] and
  k_2 = 2nd Freundlich-isotherme of material [-]

$$c_s = k_1 \left(\varsigma_0 c_i \right)^{1/k_2}$$

- Langmuir-adsorption:

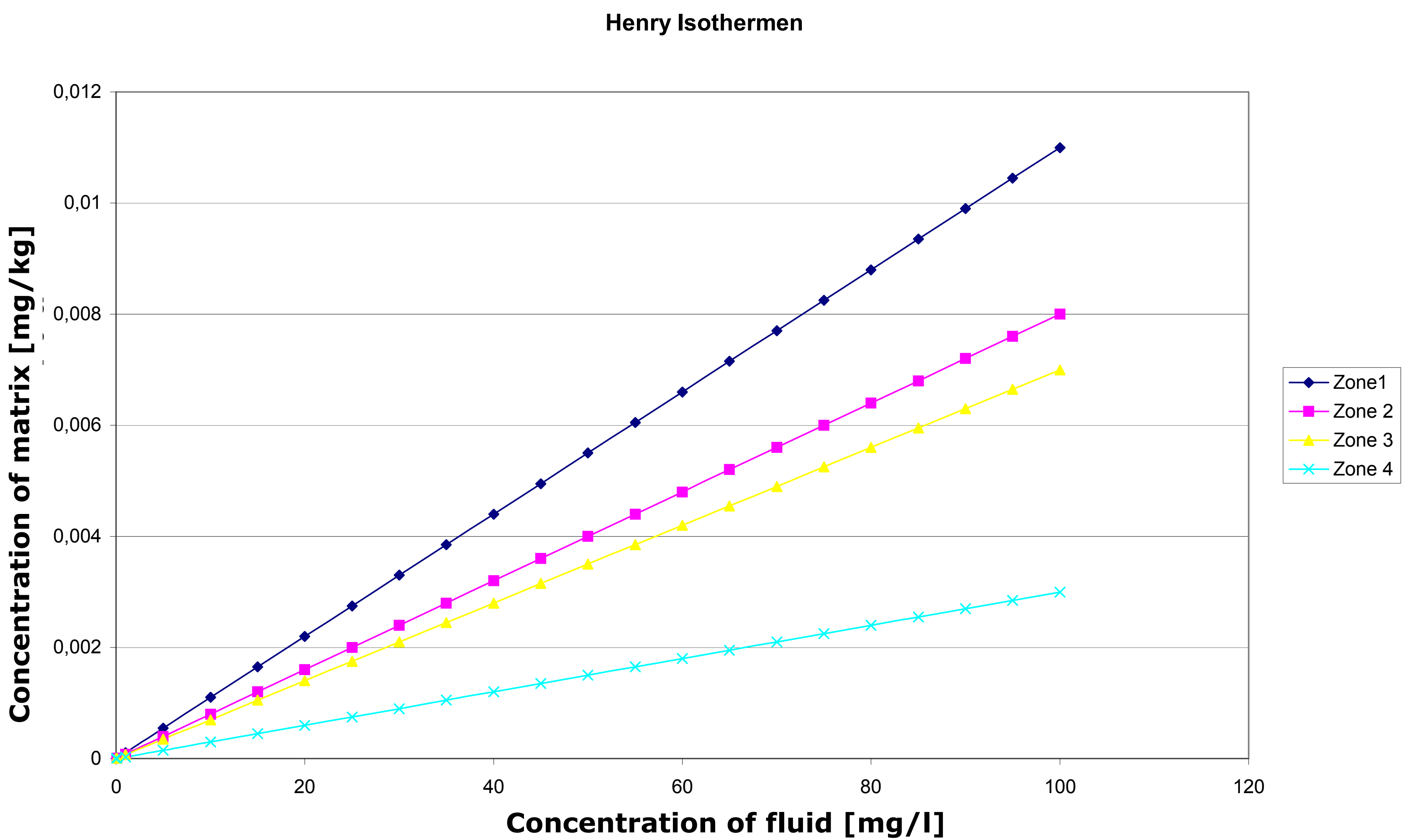
  k_1 = 1st Langmuir-isotherme of material [m³/kg] and
  k_2 = 2nd Langmuir-isotherme of material [m³/kg]

$$c_s = k_1 \left(\varsigma_0 c \right) / \left(1 + k_2 \varsigma_0 \right.$$

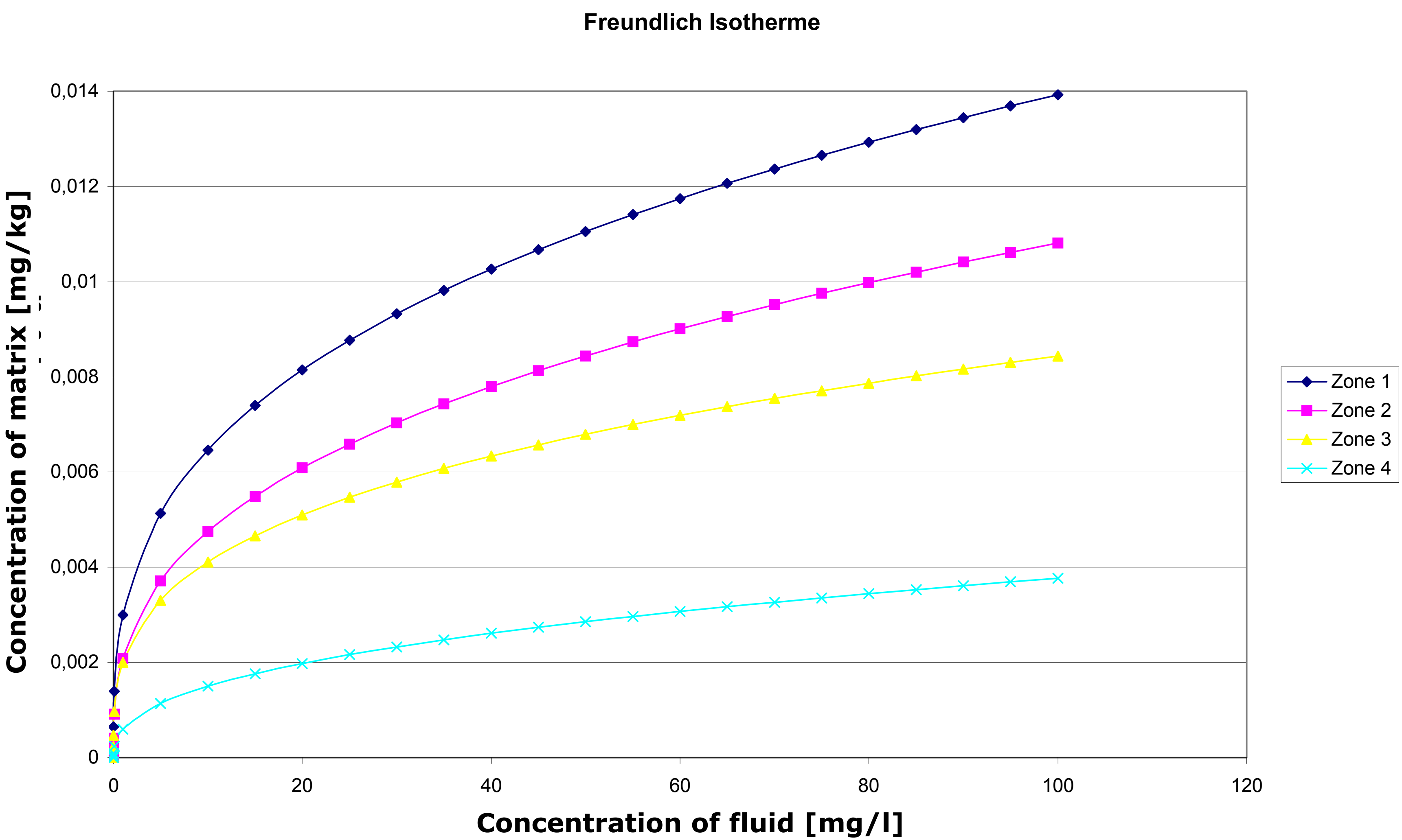
Individual zone-and material specifications can be defined

Typical runs of isothermal curves

Henry

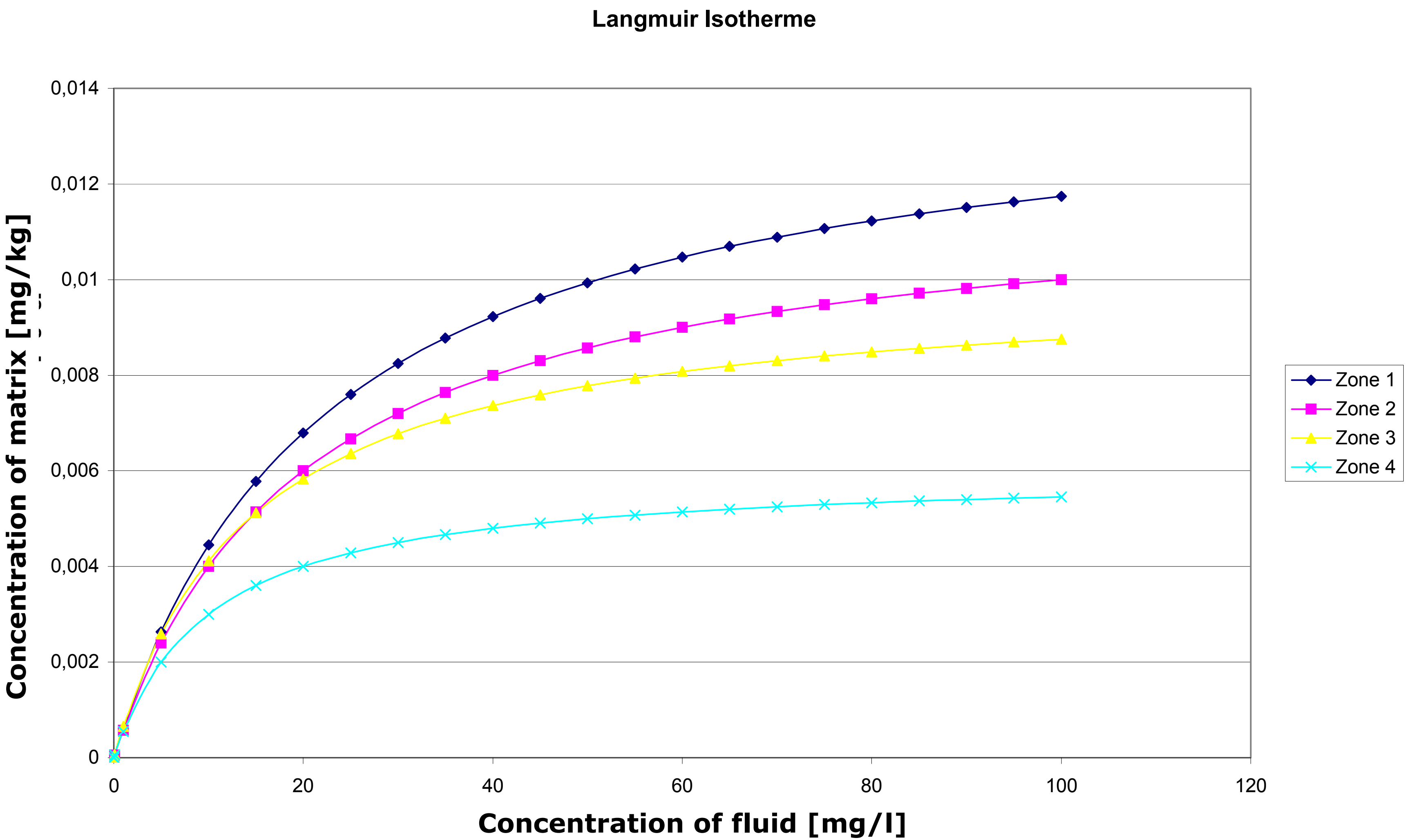


Typical runs of isothermal curves Freundlich

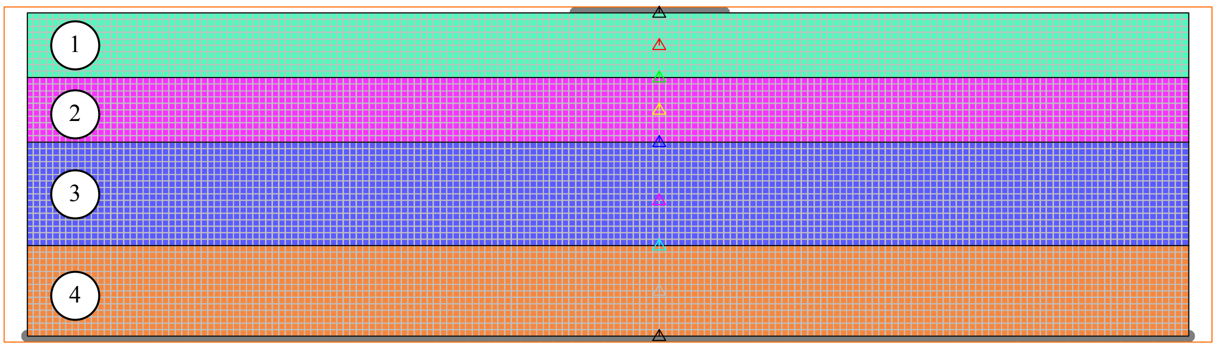


Typical runs of isothermal curves

Langmuir

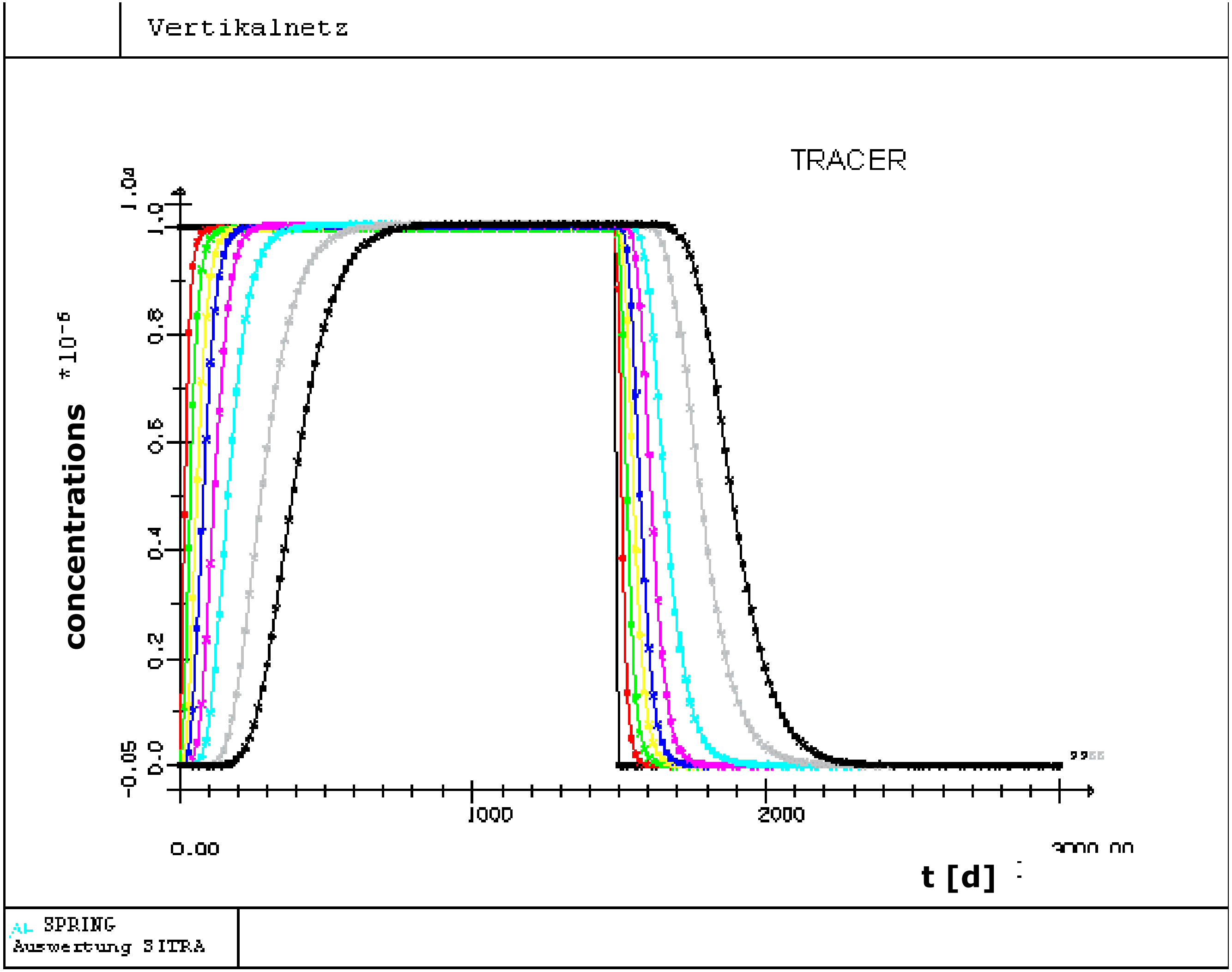


Conditions



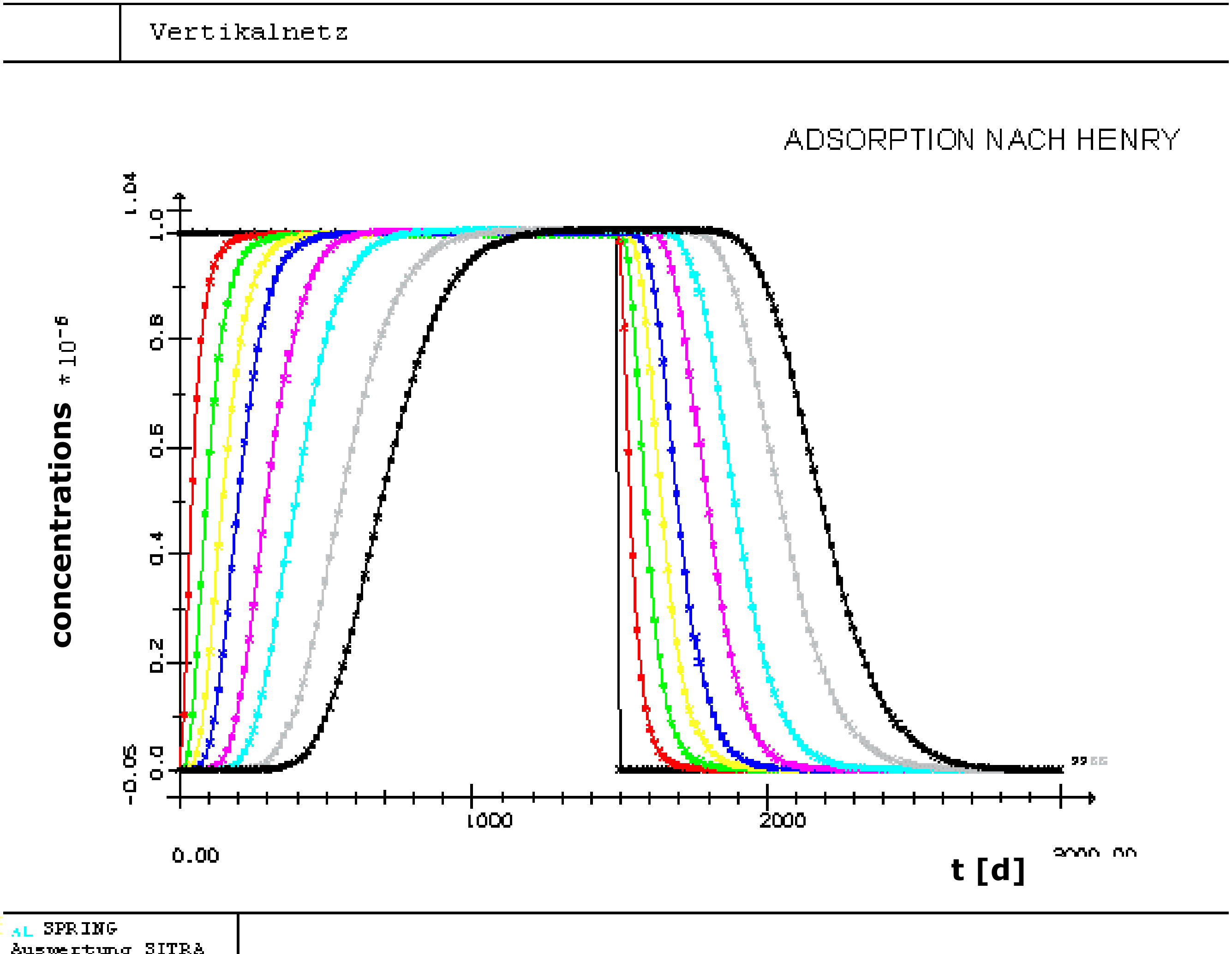
Layer Nr.	1	2	3	4
KWER [m/s]	8.9e-6	3.8e-7	1.5e-6	2.1e-4
PORO	0.04900	0.05200	0.05400	0.21000
DISP	0.08000	0.08000	0.08000	0.08000

Adsorption parameter: None - TRACER



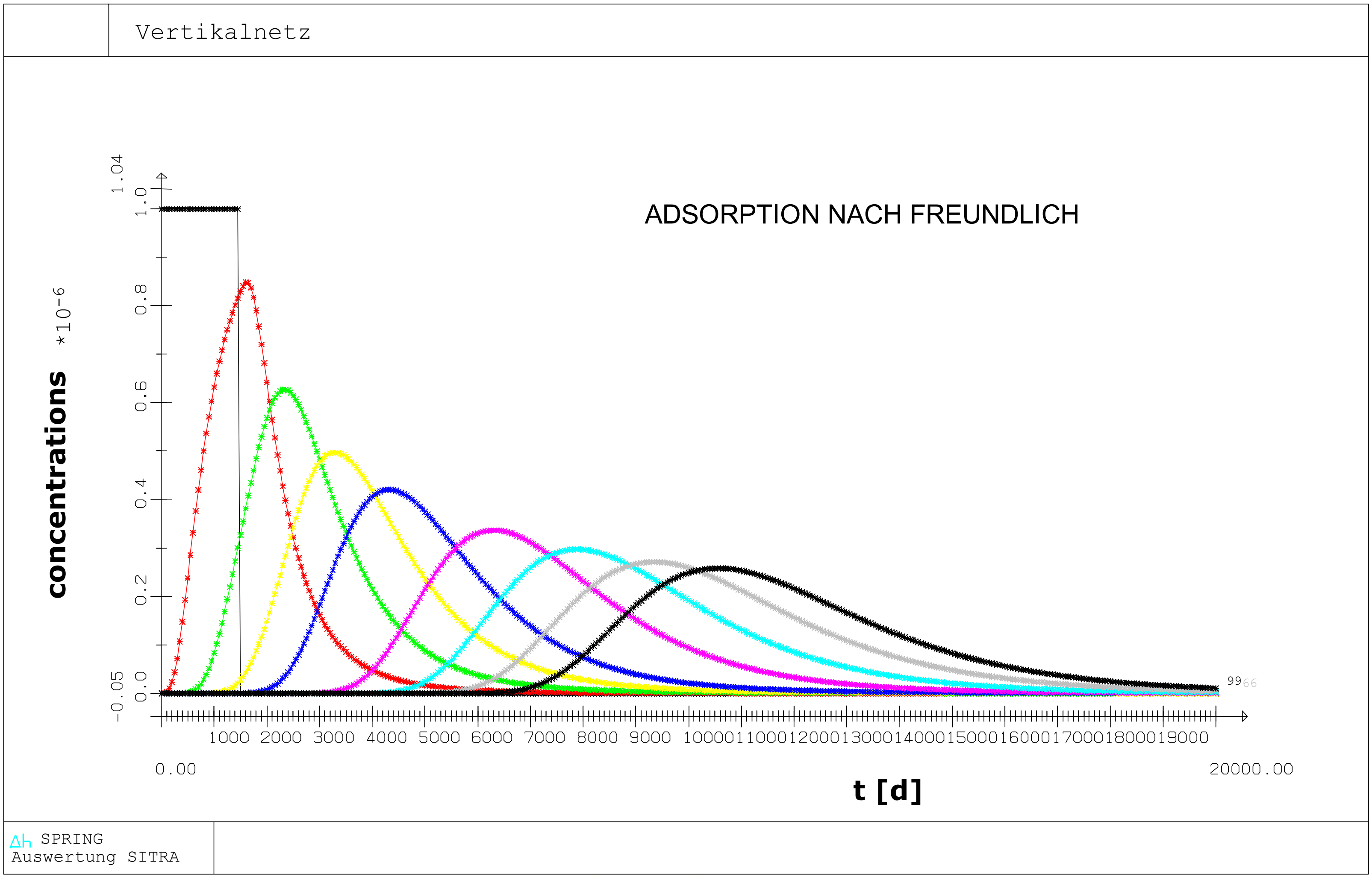
Examples

Henry: χ_1=0.00003 Equation: $C_s = \chi_1 \cdot \rho \cdot C$



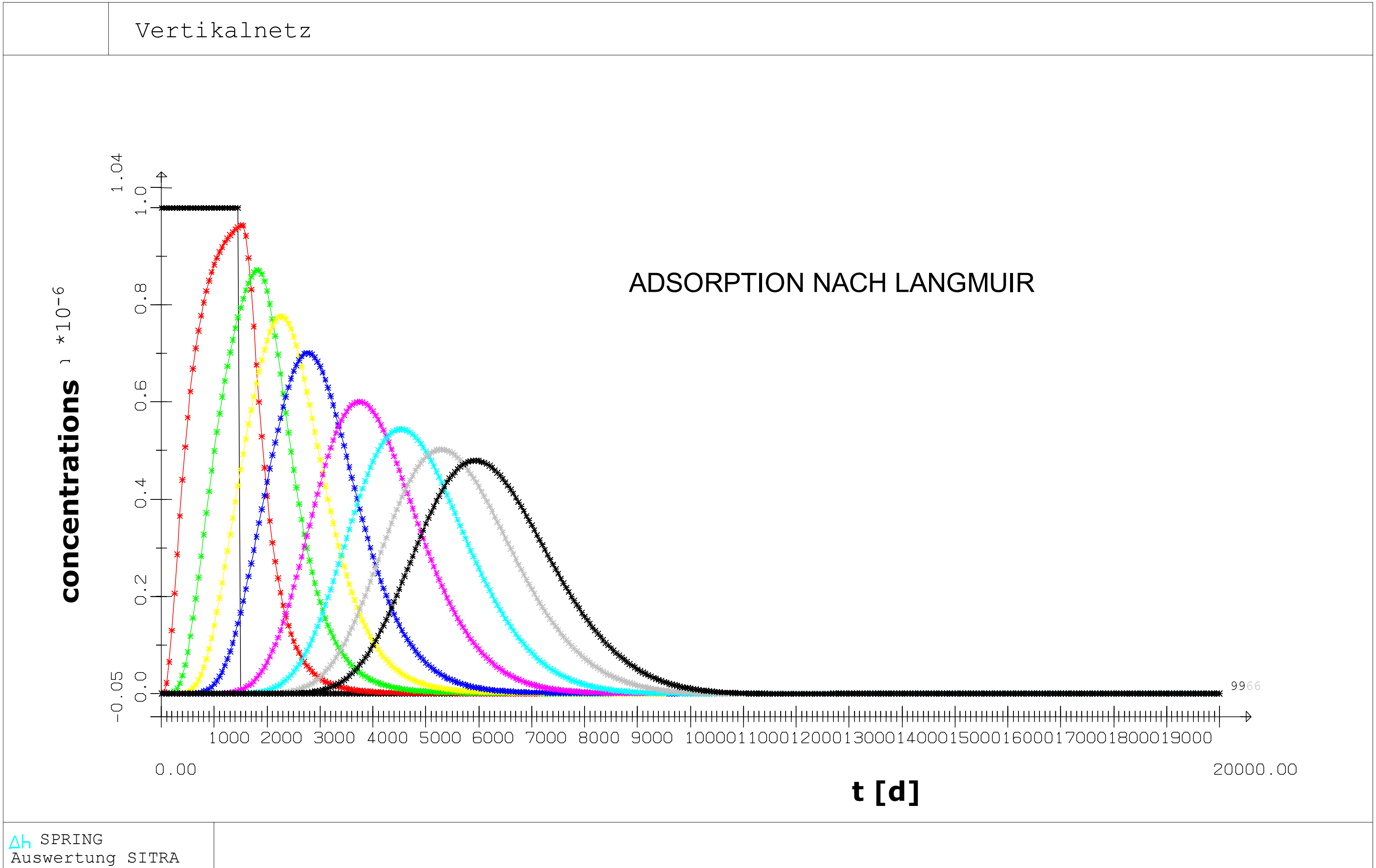
Examples

Freundlich: χ_1=0.0005, χ_2=1.1 Equation: $C_s = \chi_1 \cdot (\rho \cdot C)^{\frac{1}{\chi_2}}$



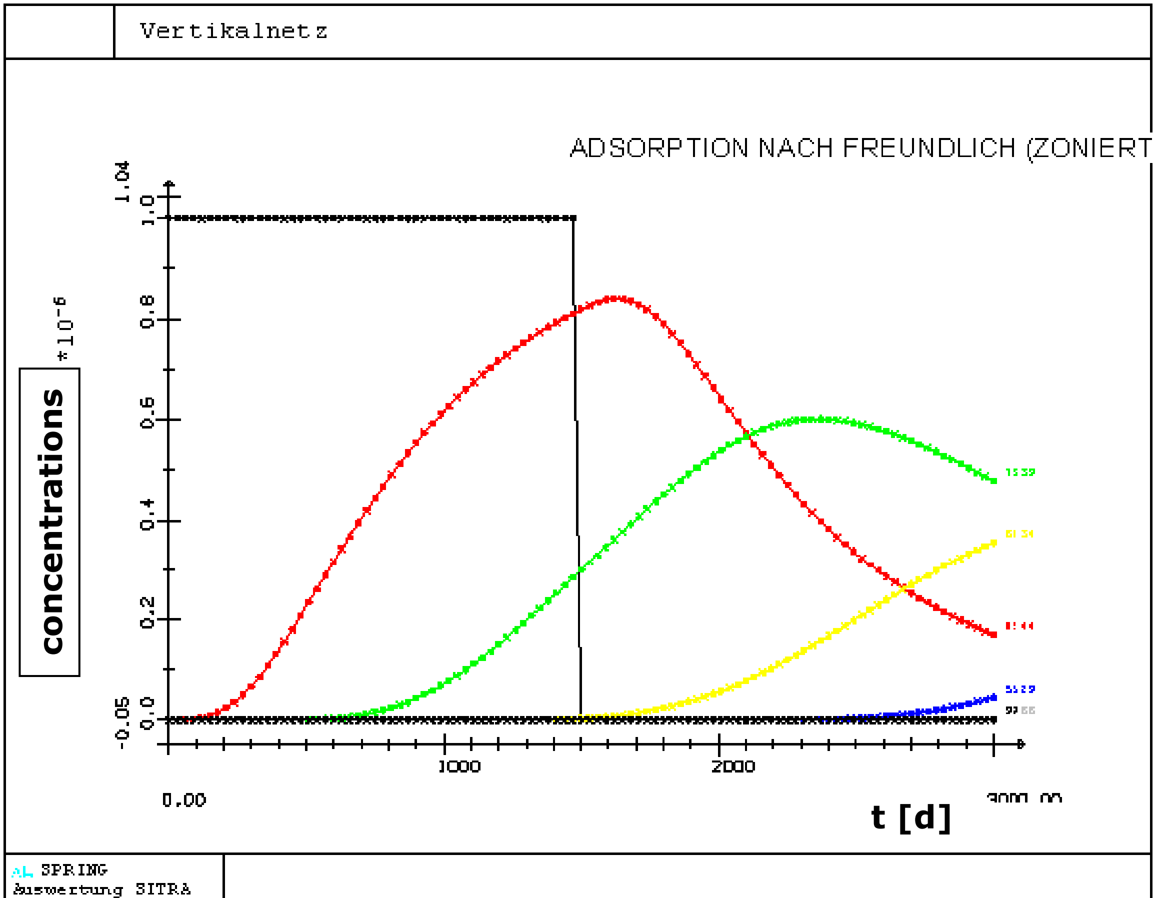
Examples

Langmuir: $\chi_1=0.0005$, $\chi_2=1.1$ Equation: $C_s = \dfrac{\chi_1 \cdot \rho \cdot C}{1+\chi_2 \cdot \rho \cdot C}$



Zone-specified Adsorptionparameters

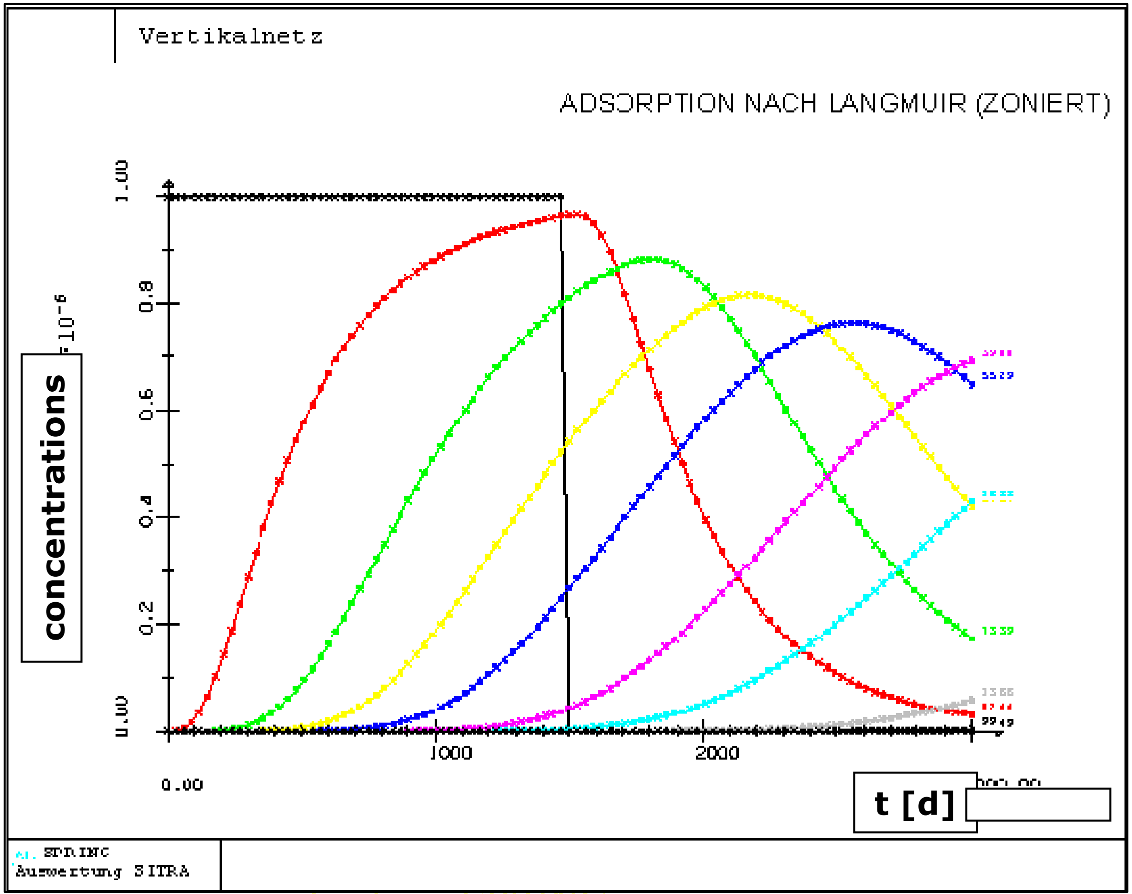
Layer Nr.	1	2	3	4
Freundlich	$\chi1=0.0005,\ \chi2=1.1$	$\chi_1=0.0004,\ \chi_2=1.2$	$\chi_1=0.0003,\ \chi_2=1.1$	$\chi_1=0.0010,\ \chi_2=1.1$



Examples

Zone-specified Adsorptionparameters

Layer Nr.	1	2	3	4
Langmuir	χ_1=0.0005, χ_2=1.1	χ_1=0.0004, χ_2=1.2	χ_1=0.0003, χ_2=1.1	χ_1=0.0010, χ_2=1.1



Zone-specified Adsorptionparameters

Layer Nr.	1	2	3	4
Linear	χ_1=0.00013	χ_1=0.00003	χ_1=0.00009	χ_1=0.000002