An Introduction to
Groundwater Modeling Techniques

- Motivation
- Abstraction and simplification
- Basic Ideas in Groundwater Modeling
- Characteristics of a Porous - Fractured Aquifer
- Basics in Contaminant Transport Modeling
- Problems in Contaminant Transport
- Modeling
- Examples

Literature

Bear, Jacob: Hydraulics of Groundwater, McGraw-Hill Inc., New York 1979

Harr, M. E.: Groundwater and Seepage. McGraw-Hill Inc., New York 1962

Kinzelbach, W. & Rausch, R.: Grundwassermodellierung. Borntraeger, Berlin 1995

Kinzelbach, W.: Numerische Methoden zur Modellierung des Transports von Schadstoffen im Grundwasser, R. Oldenburg Verlag, München 1987

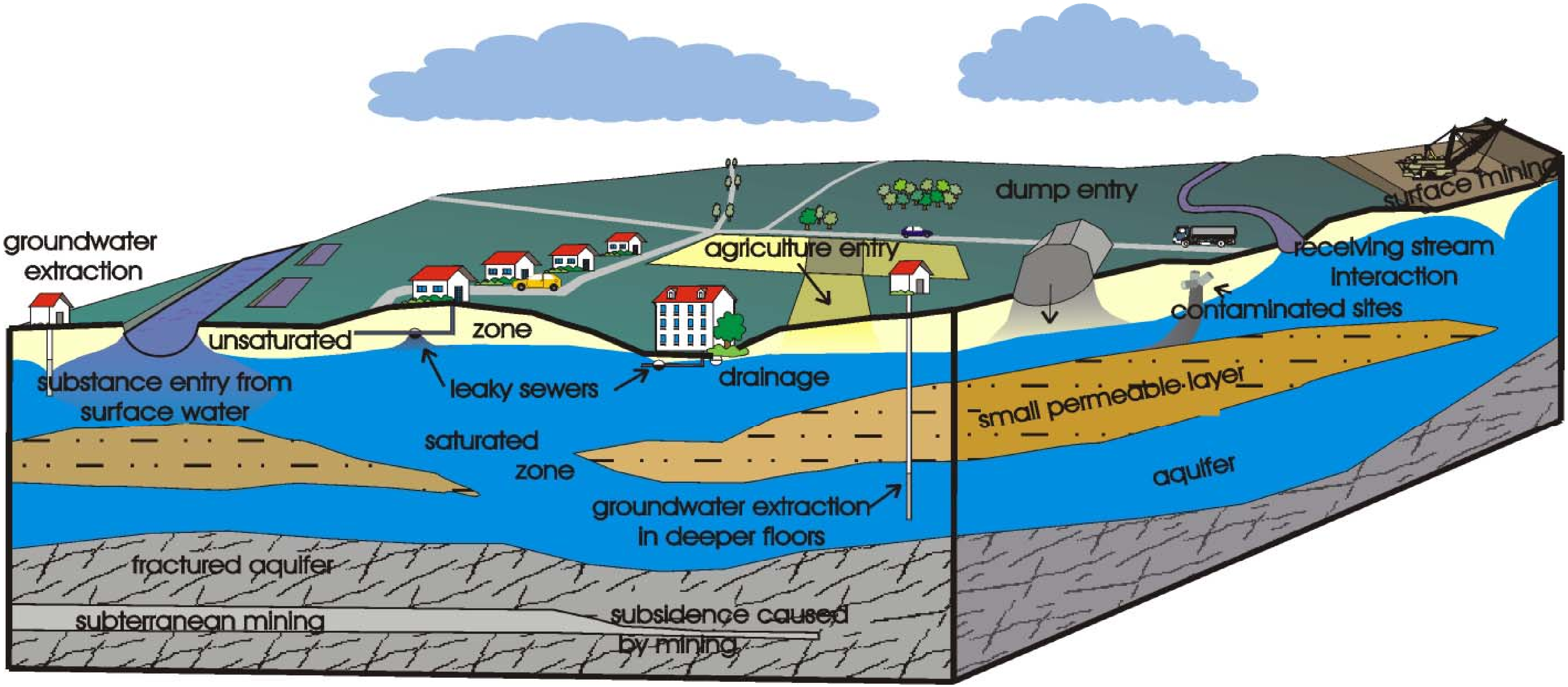
Verruijt, A.: Theory of Groundwater Flow, The Macmillan Press Ltd., London 1982

Huyakorn, P. S. & Pinder, G. F.: Computational Methods in Subsurface Flow. Academic Press, San Diego 1983

Wang, H. F. & Anderson, M. P.: Introduction to Groundwater Modelling. W. H. Freeman and Company, New York 1982

Bathe, H.-J.: Finite Element Methods, New York 1990

Definition of the Problem



Deformation Equation

external variables

operator

$L(u_i) = F_i$

deformation

u_i

load

F_i

compatibility

$\varepsilon_{ii} = ½(u_{i,j} + u_{i,j})$

equilibrium

$\sigma_{ij,i} = F_i$

strain

ε_{ii}

stress

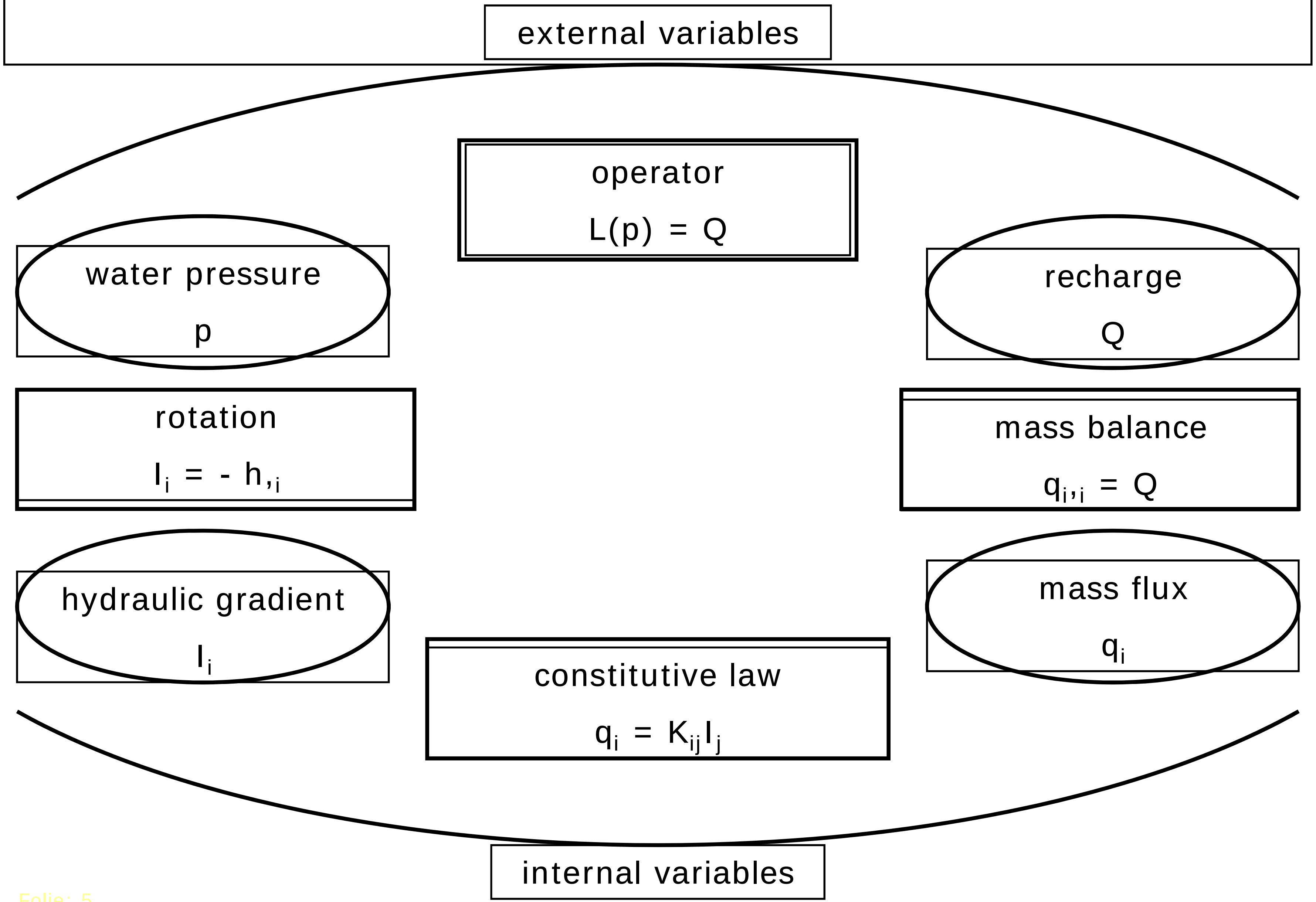
σ_{ij}

constitutive law

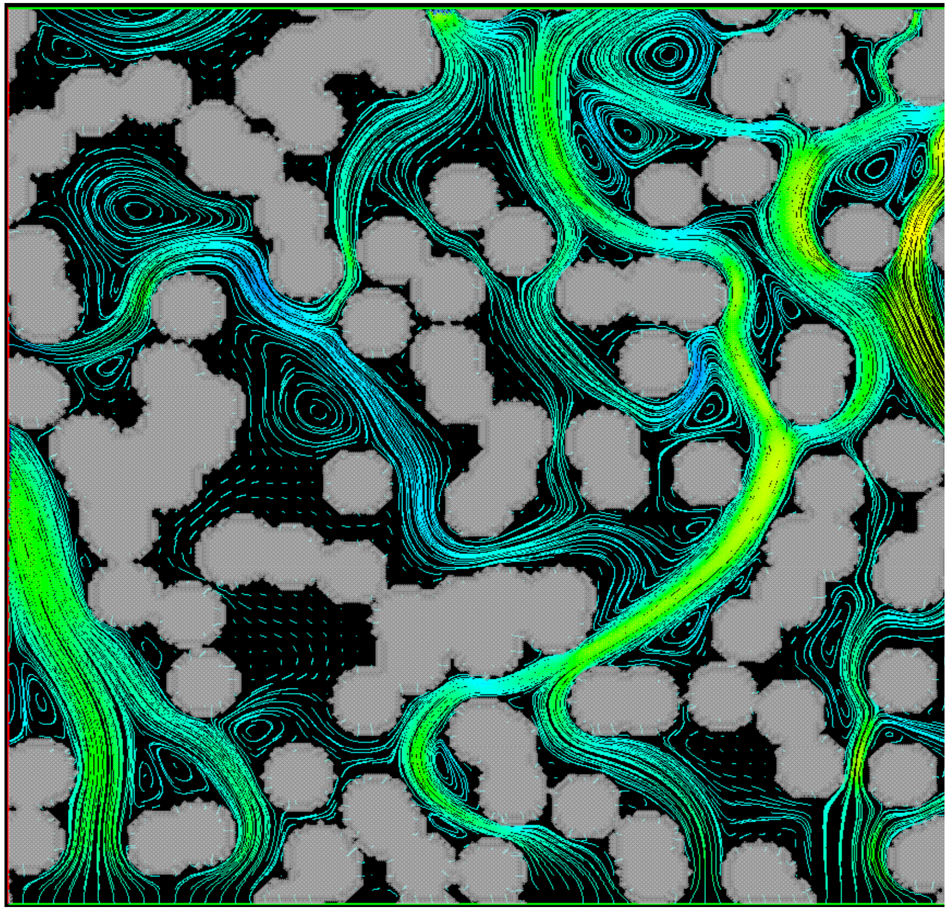
$\sigma_{ij} = E_{ijkl}\varepsilon_{kl}$

internal variables

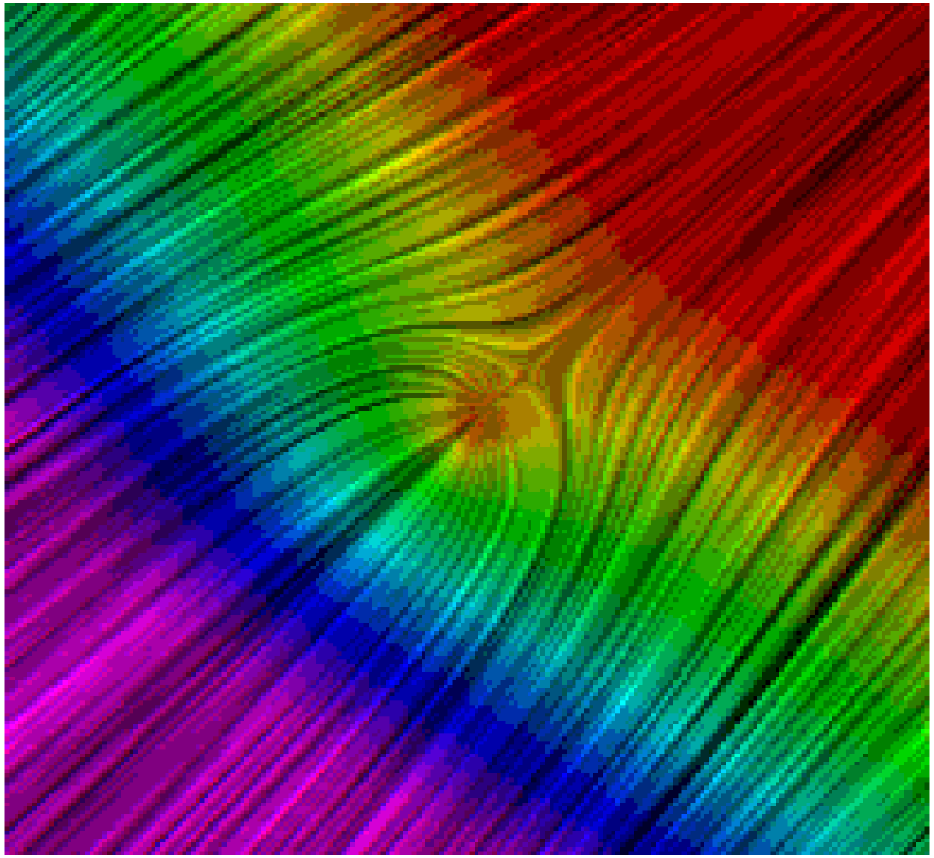
Flow Equation



local scale



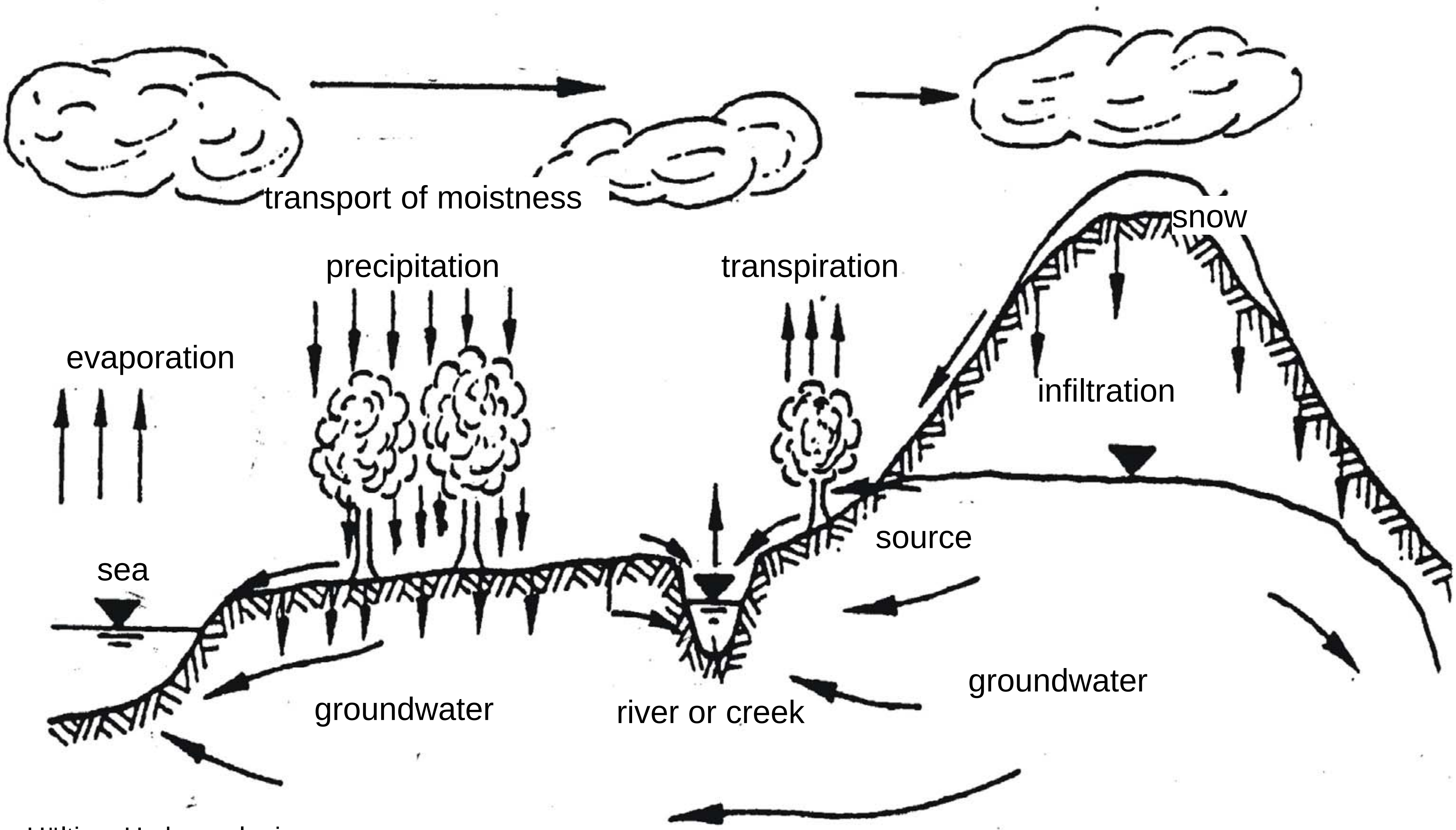
field scale



Hydrogeological Model

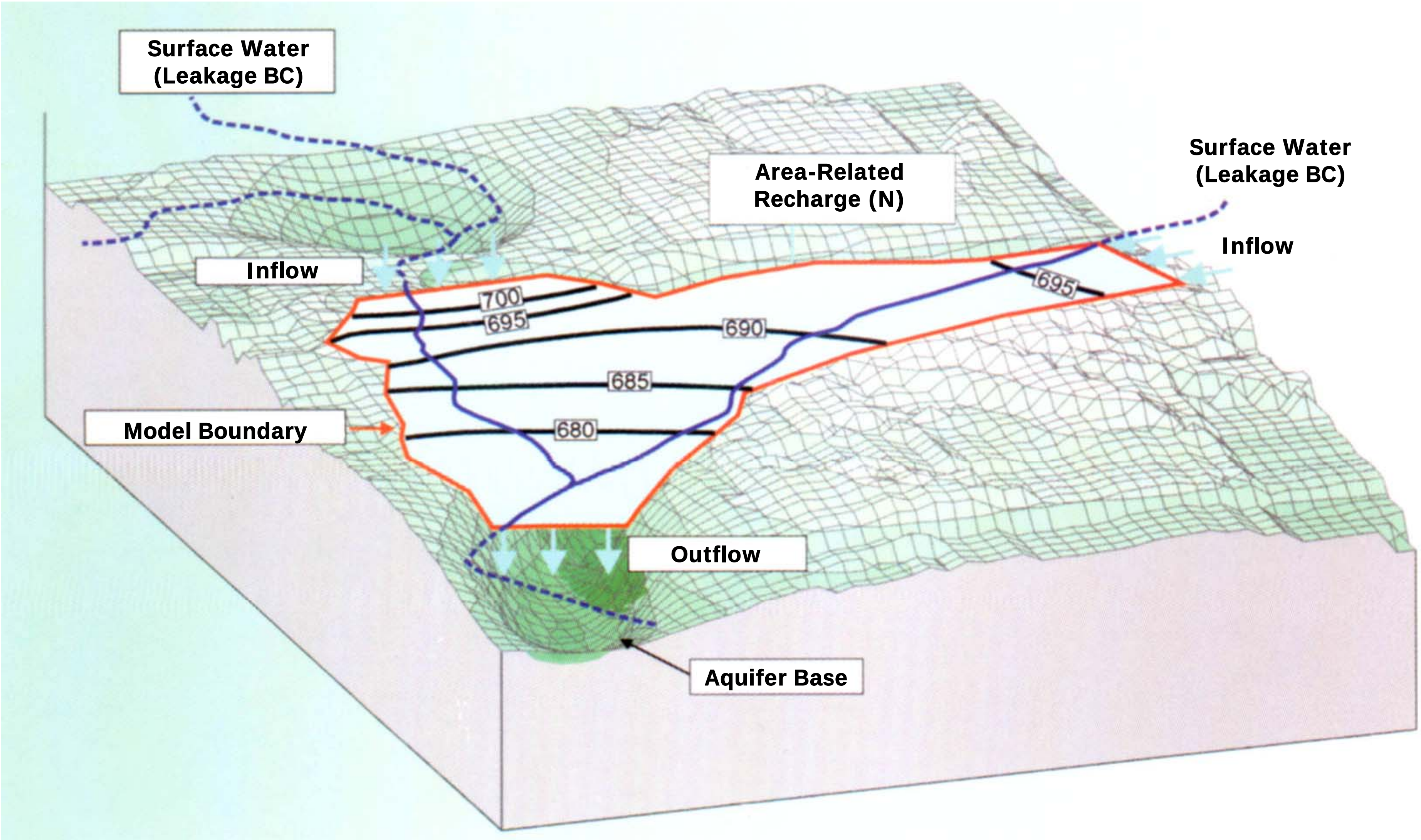
Task Scope of Investigations	Aim Scope of aim Costs
Assessment and Compilation of Data	Topography Hydrology Geology Hydraulics Hydrochemistry
Evaluation and Classification of Data	
Derivation of a Hydrogeological Concept	Work Area Balanced Area Model Area Hydrostratigraphic Units Zones of Homogenisation Aquifer Parameters Dynamics Boundary Conditions Balance
Review of the Hydrogeological Concept	Field Data Mathematical Models

Natural water cycle



Hölting, Hydrogeologie

Definition


Surface Water
(Leakage BC)
Area-Related
Recharge (N)
Surface Water
(Leakage BC)
Inflow
Inflow
700
695
690
695
685
Model Boundary
680
Outflow
Aquifer Base

Nature

Verification

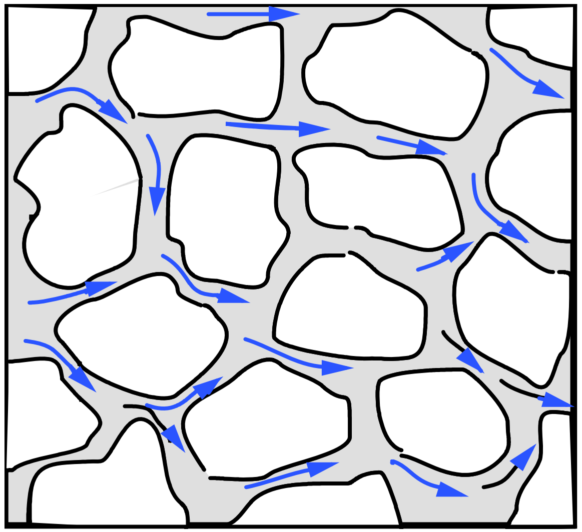
Physical model
Homogenisation

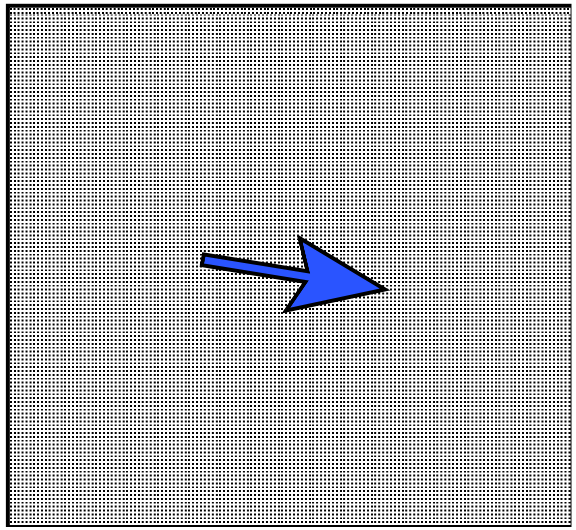
Calibration

Mathematical model
Darcy-
Fourier-
Fick-
Hook-law
with constitutiv laws

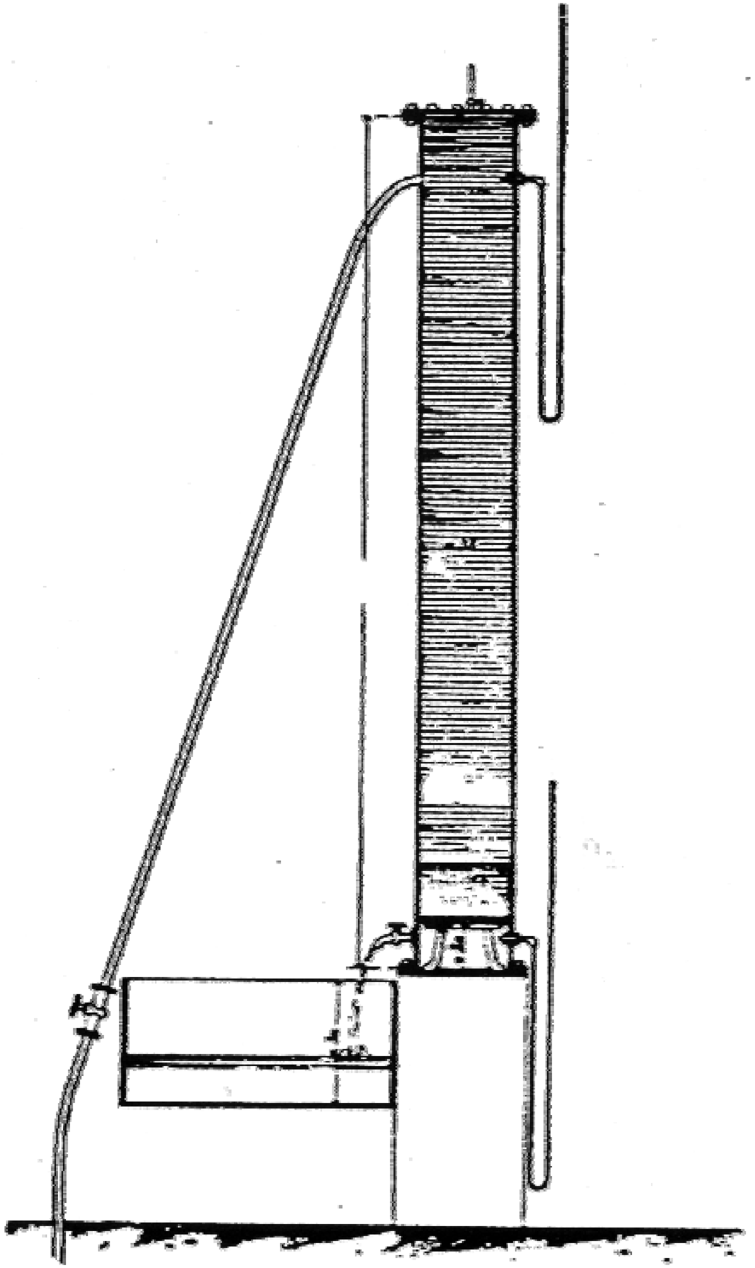
Numerical Model
FEM, FVM, FDM, BEM, LBT

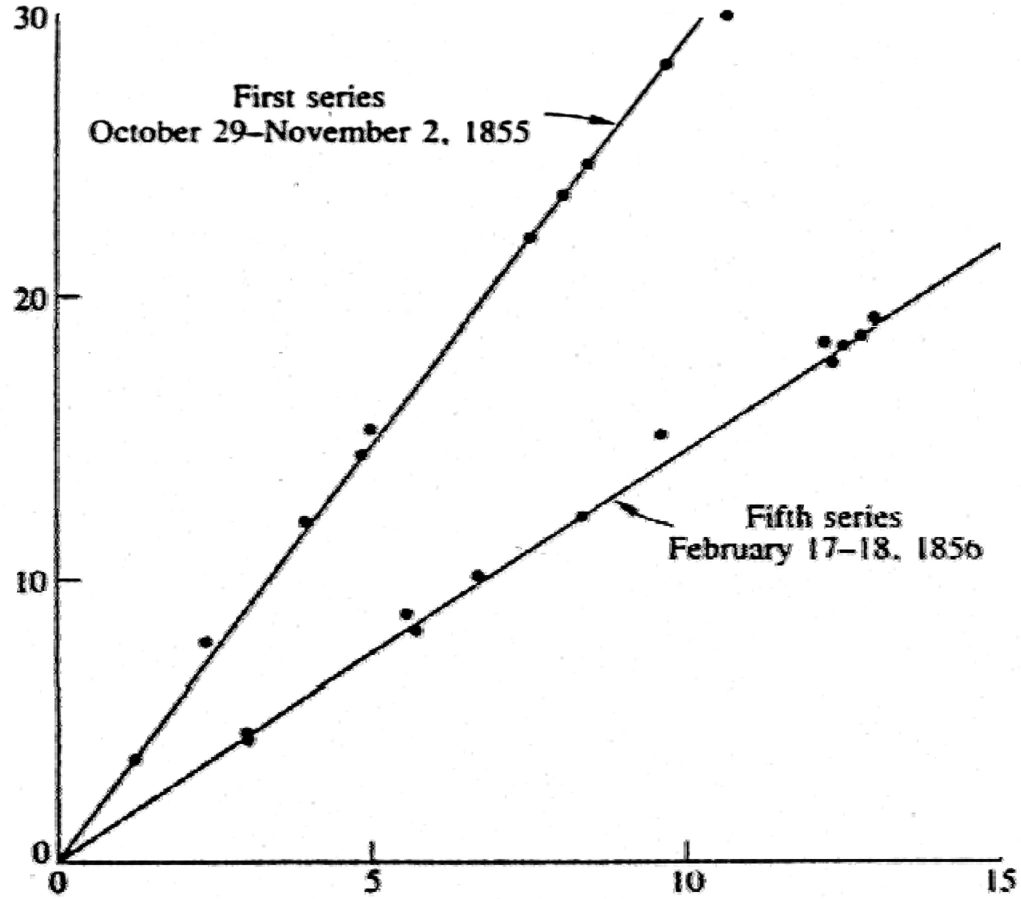
Homogenisation





Darcy´s law (1856)





Water Supply and Distribution

- Assessment of catchment areas
- Optimisation of site distribution for water suppliers
- Determination of drinking water protection areas
- Evaluation of measures for groundwater withdrawal and artificial groundwater recharge
- Assessment of recharge and bank filtration

Water Supply and Distribution

- Groundwater balances, assessment of groundwater supply
- Prognosis and evaluation of measures that result in lowering / raising the groundwater table
- Conception and monitoring of drainage systems
- Assessment of the impact of mining or exploration measures on the groundwater
- Assessment of the impact of hydraulic engineering measures on the groundwater

Groundwater Composition and Quality

- Classification of groundwater
- Determination of the origin and genesis
- Age determination
- Surveying alterations in the groundwater composition
- Assessment of salinisations / acidifications
- Assessment of furnishes (i.e. nitrate due to agricultural activities)
- Prognoses on the spreading of contaminants
- Conception and optimisation of protection and remediation actions

Models

- Simplified abstractions of reality, designed to predict the effects of certain actions in the natural System
- Types of groundwater models
  - Physical analogs
  - Mathematical Models
    - analytical models
    - numerical models

- Typical applications of groundwater models
- Optimization studies in groundwater management and remedial design
- Design in waterworks
- Parameter studies and sensitivity analysis

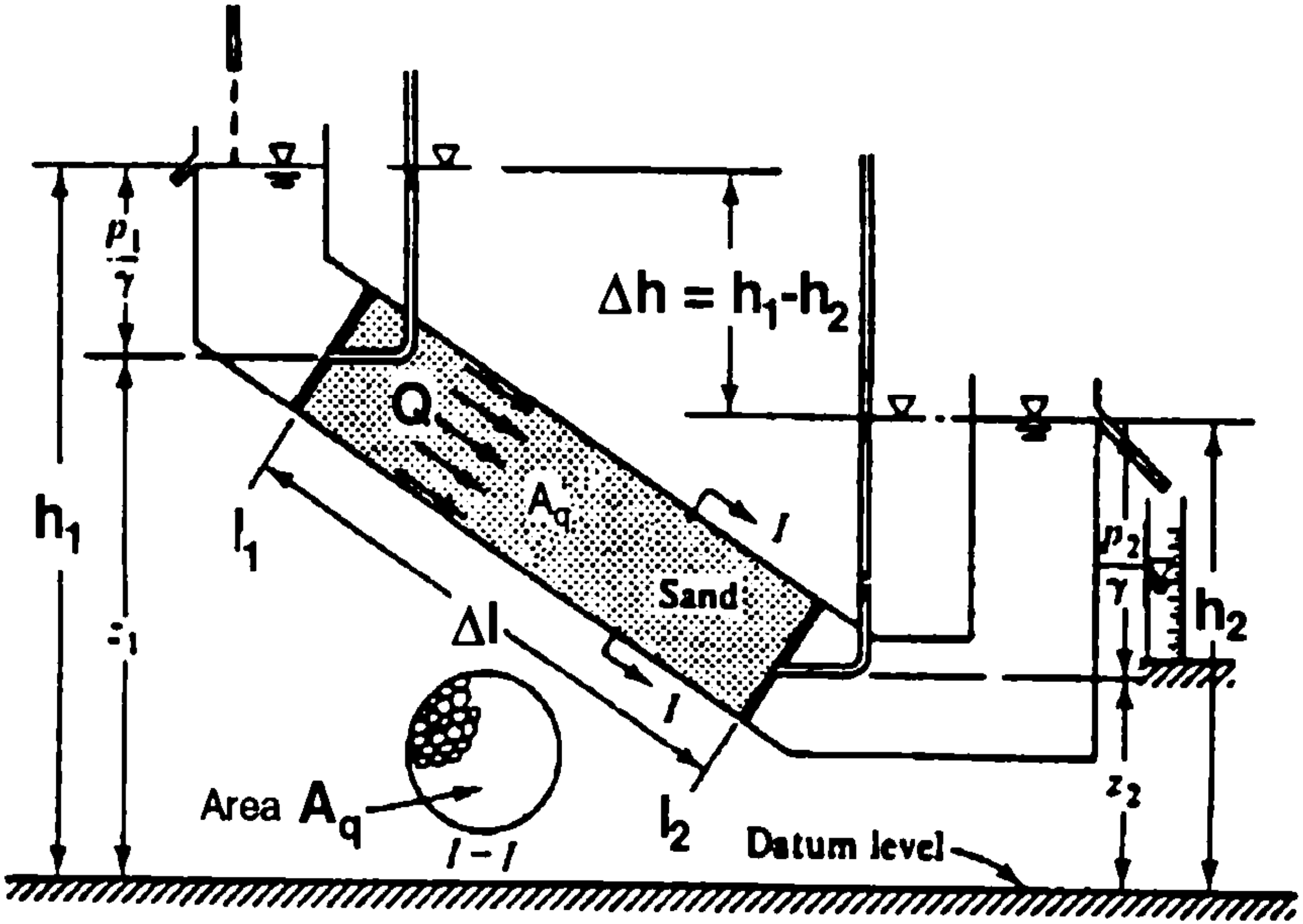
Darcy's Law

$$Q \sim A_q \frac{\Delta h}{\Delta l}$$

$$Q = -k_f \cdot A_q \frac{\Delta h}{\Delta l}$$

or

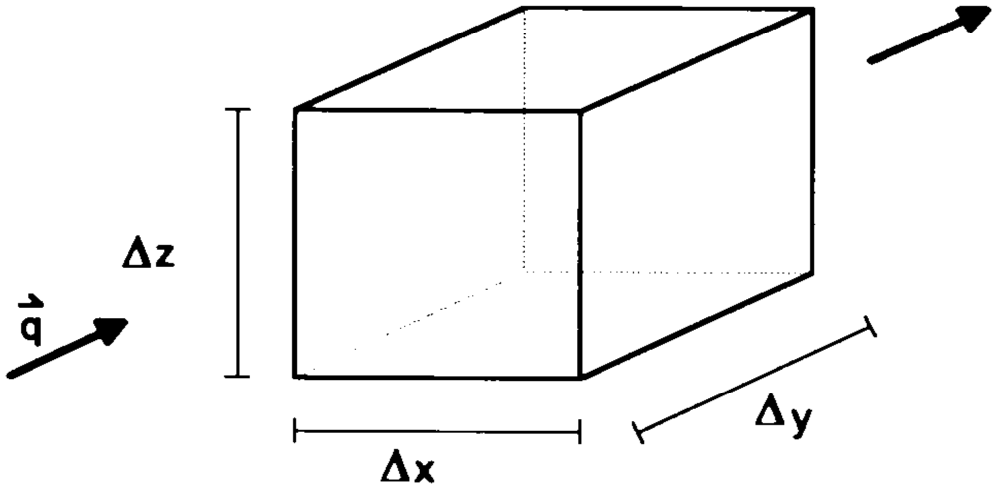
$$\frac{Q}{A_q} = v_f = \boxed{\vec{q} = -k_f \frac{\Delta h}{\Delta l}}$$



Mass balance

Conservation of mass

$$\frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} + \frac{\partial q_z}{\partial z} = 0$$



Basic equation of groundwater flow

$$\frac{\partial^2 h}{\partial x^2}(-k_x) + \frac{\partial^2 h}{\partial y^2}(-k_y) + \frac{\partial^2 h}{\partial z^2}(-k_z) = 0$$

considering sources and sinks

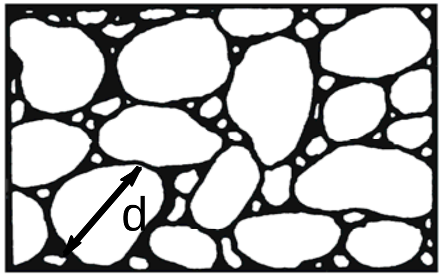
$$\frac{\partial^2 h}{\partial x^2}(-k_x) + \frac{\partial^2 h}{\partial y^2}(-k_y) + \frac{\partial^2 h}{\partial z^2}(-k_z) = R$$

and transient flow

$$\frac{\partial^2 h}{\partial x^2}(-k_x) + \frac{\partial^2 h}{\partial y^2}(-k_y) + \frac{\partial^2 h}{\partial z^2}(-k_z) = R - S\frac{\partial h}{\partial t}$$

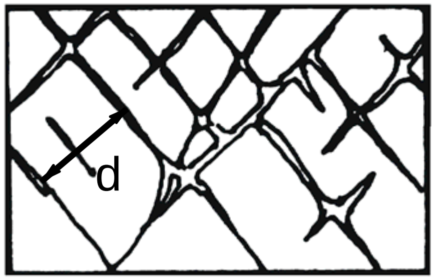
Aquifer

porous aquifer



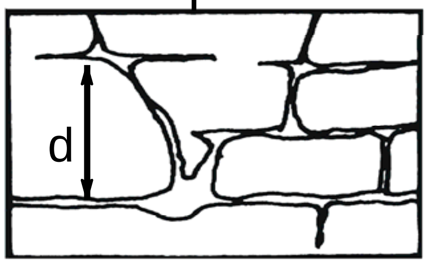
d = 10^{-5} - 10^{-3} m

fractured aquifer



d = 10^{-1} - 10^{1} m

karst aquifer



d = 10^{0} - 10^{2} m

d: size of Hohlräume

- Most soils have a higher permeability than rock
- soils are porous aquifers

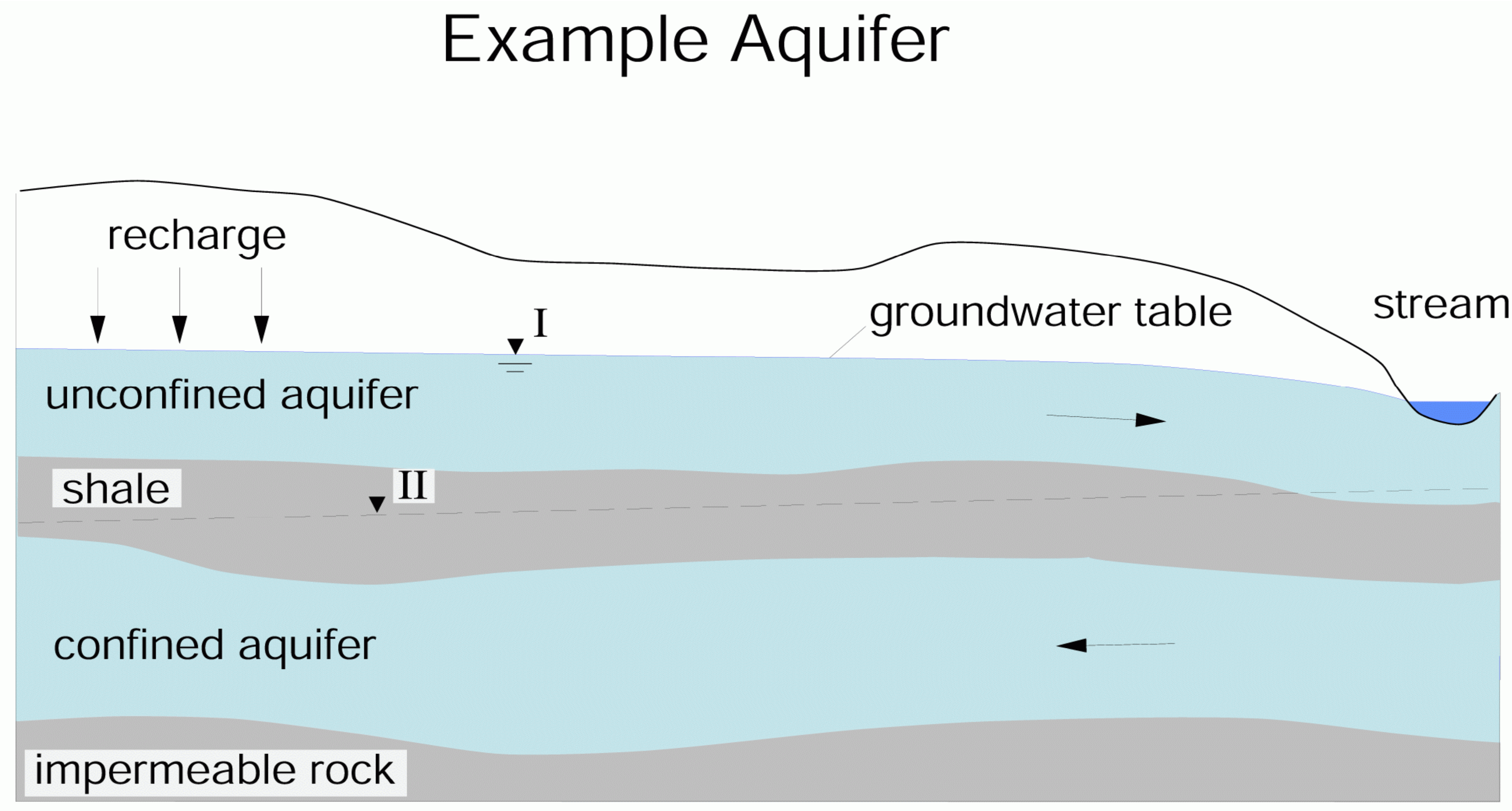
- Rock is often fractured. Fractures are the flowproducing voids (e.g. marl, sandstone, granite)

- The porosity of some rock is so high, that also pores are flowproducing (sedimentary rocks, e.g. sandstone)
- => fractured porous aquifer

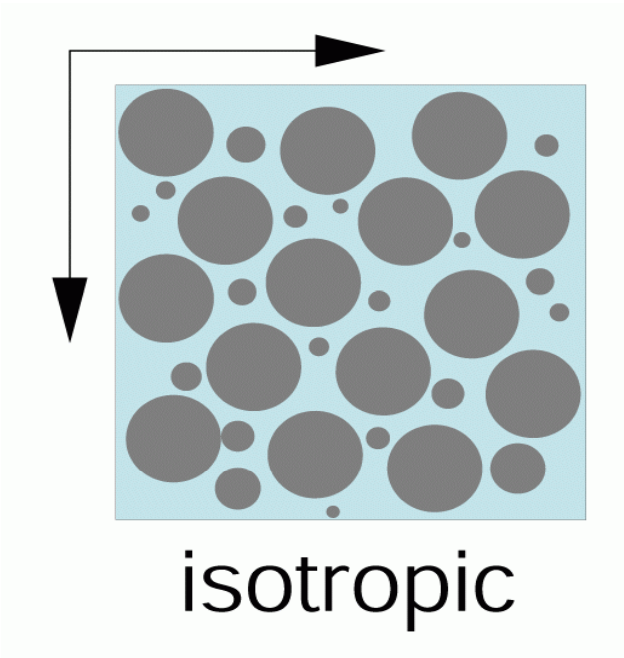
Rocks have a lower permeability

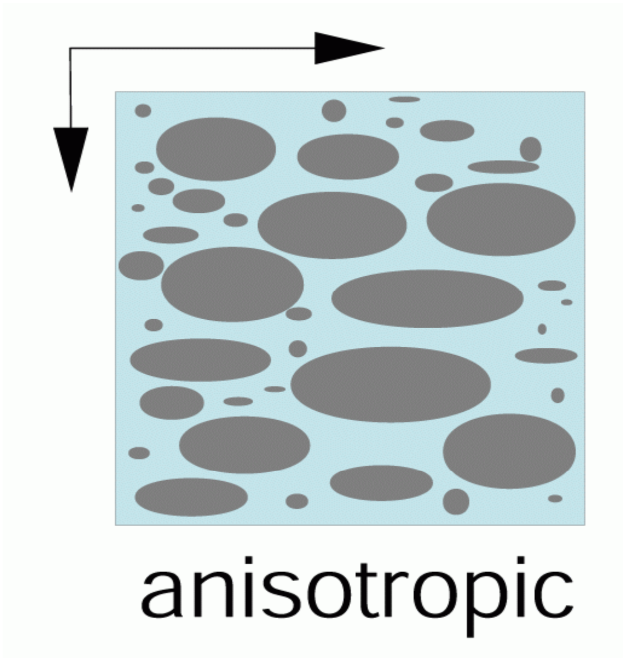
- karst aquifer is characterized by cavities, which even can create a subsurface river system

Aquifer Properties

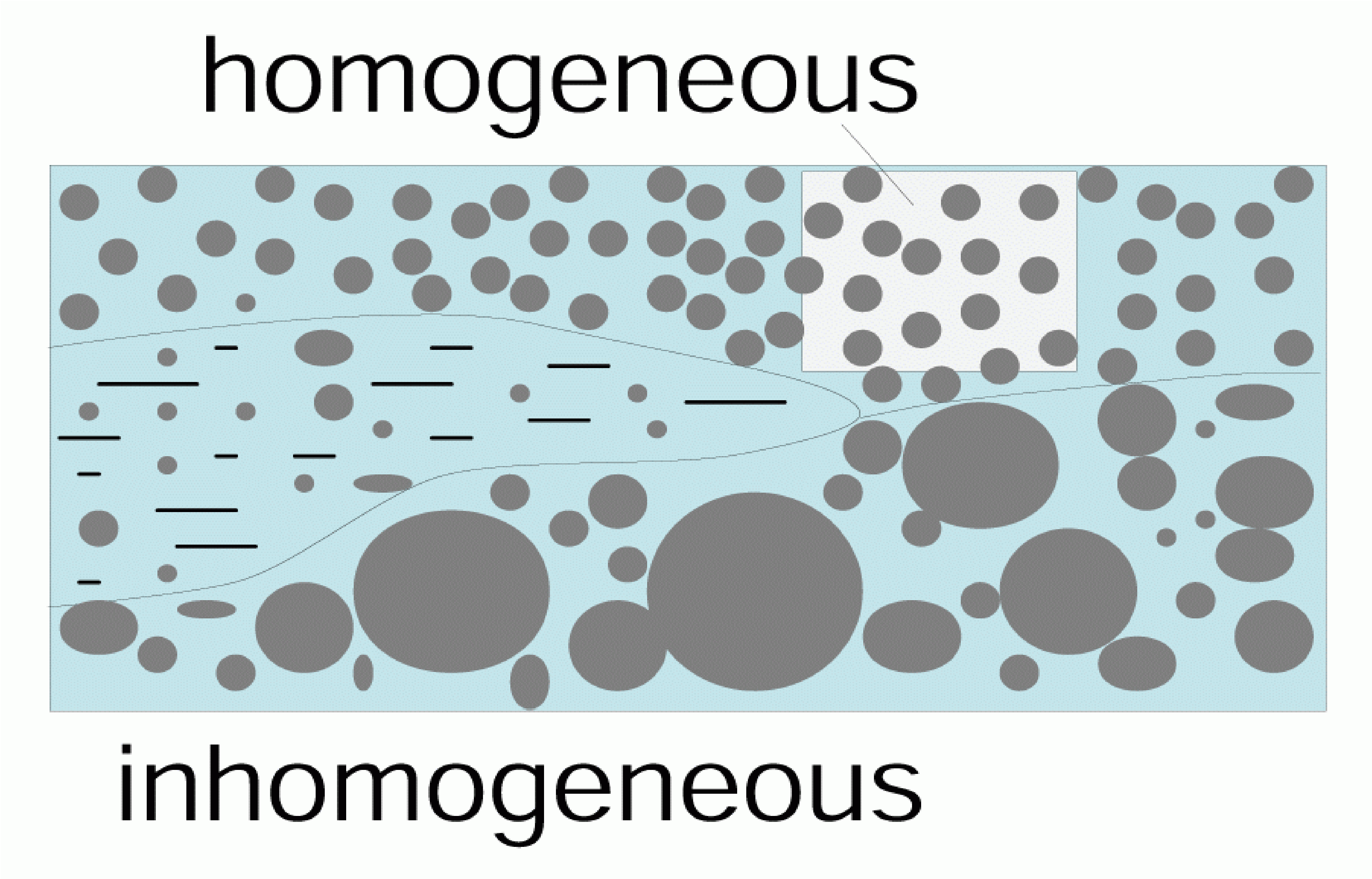


Aquifer Properties

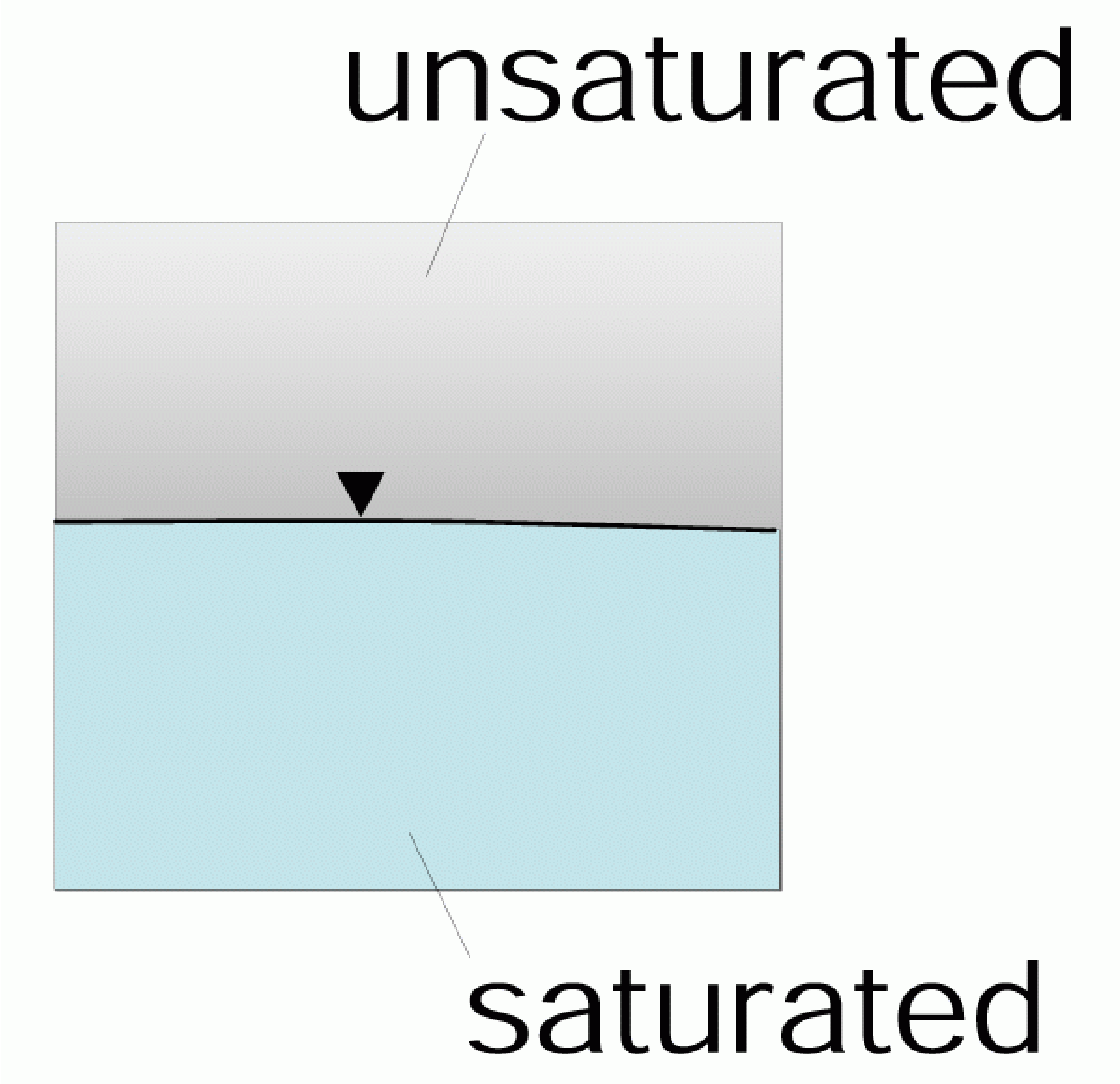




Aquifer Properties



Aquifer Properties



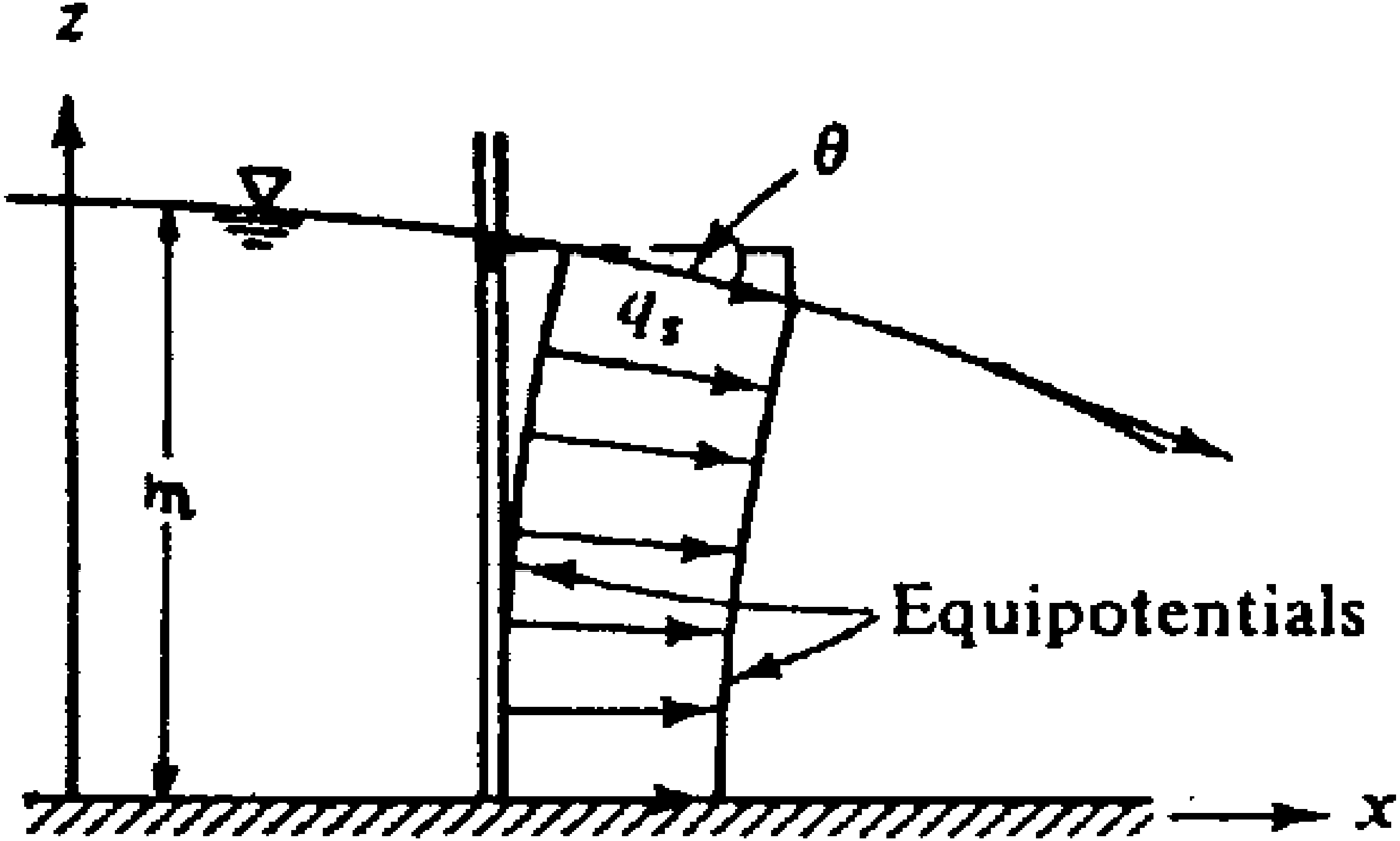
Time dependency of groundwater flow and transport processes

- Steady state
  - equilibrium situation
  - no change in time
- Transient
  - changes in flow and/or contaminant transport process in time

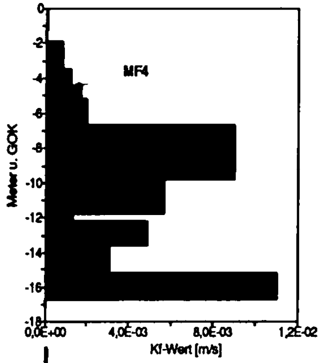
Dimension of models

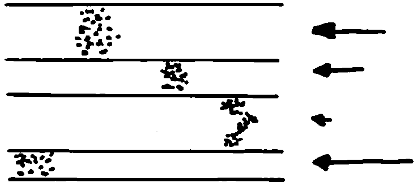
- 1-dimensional
  - in unsaturated zone
  - mixing cell geo-hydrochemical transport models
- 2-dimensional
  - horizontal (neglecting z-component of flow vectors)
  - vertical (along a representative transection)
- 3-dimensional
  - most general
  - most expensive in computing time and storage
- Coupled 2-d and 3-d
  - combination of efficiency and needed precision

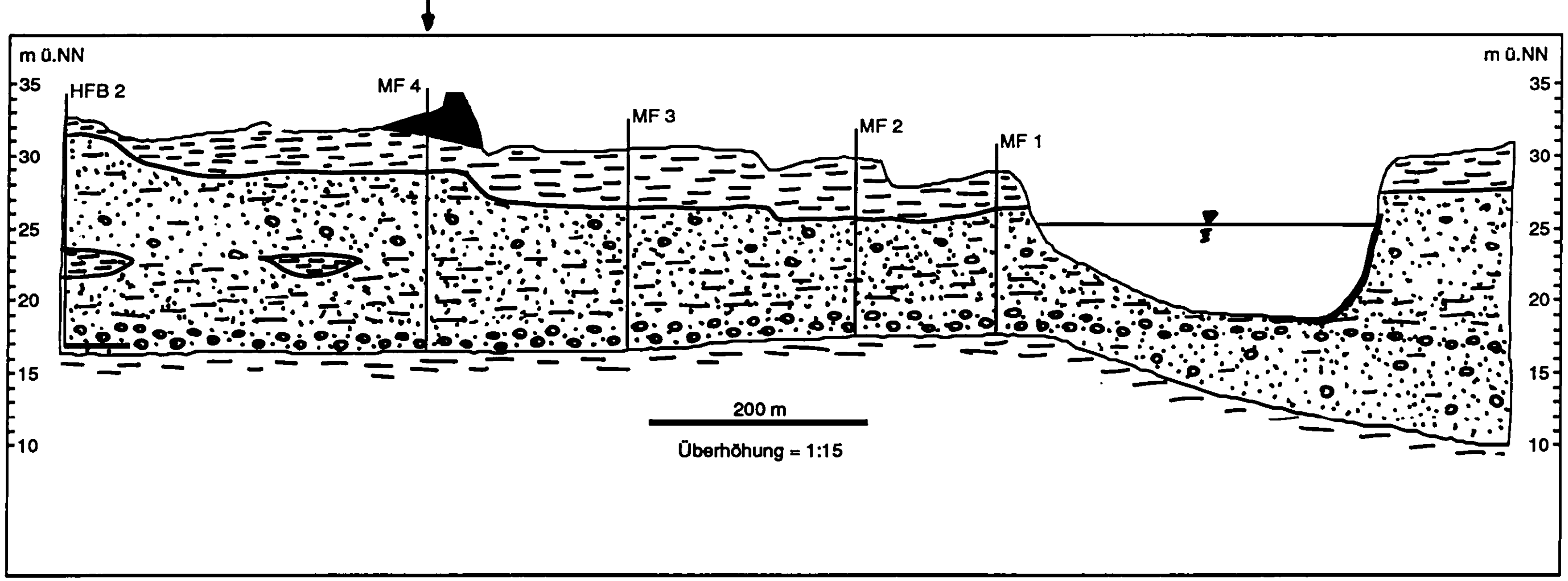
Equipotentials



vertical Permeability







Solution of mathematical models

- Analytical solutions

- Numeric solutions

  - Finite Difference (FD) or Finite Element (FE) method

    spatial and time discretisation

    FD: regular and irregular grids

    FE: mesh of irregular distributed nodes

Boundary conditions

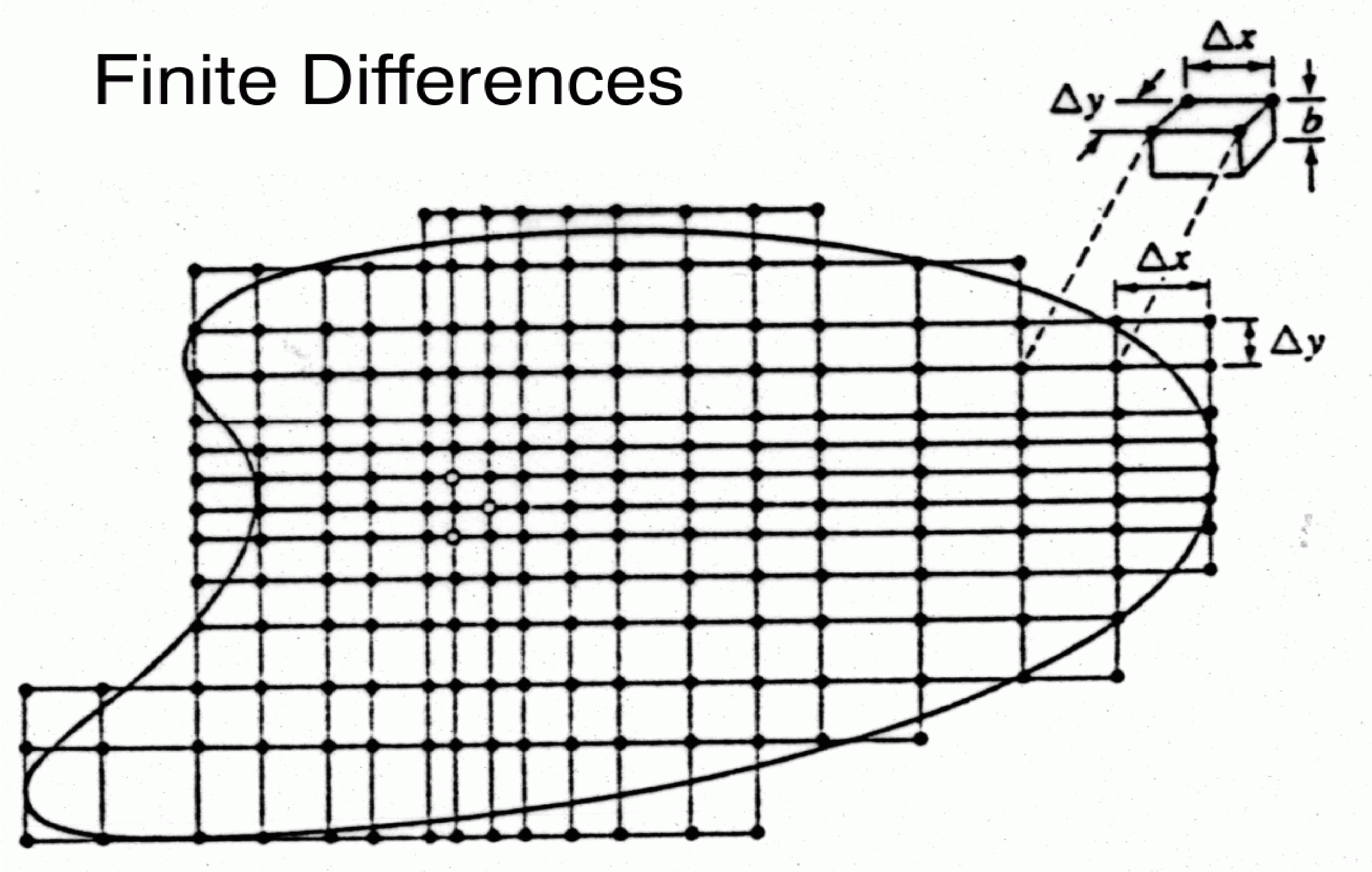
- Dirichlet conditions
  - Hydraulic head known

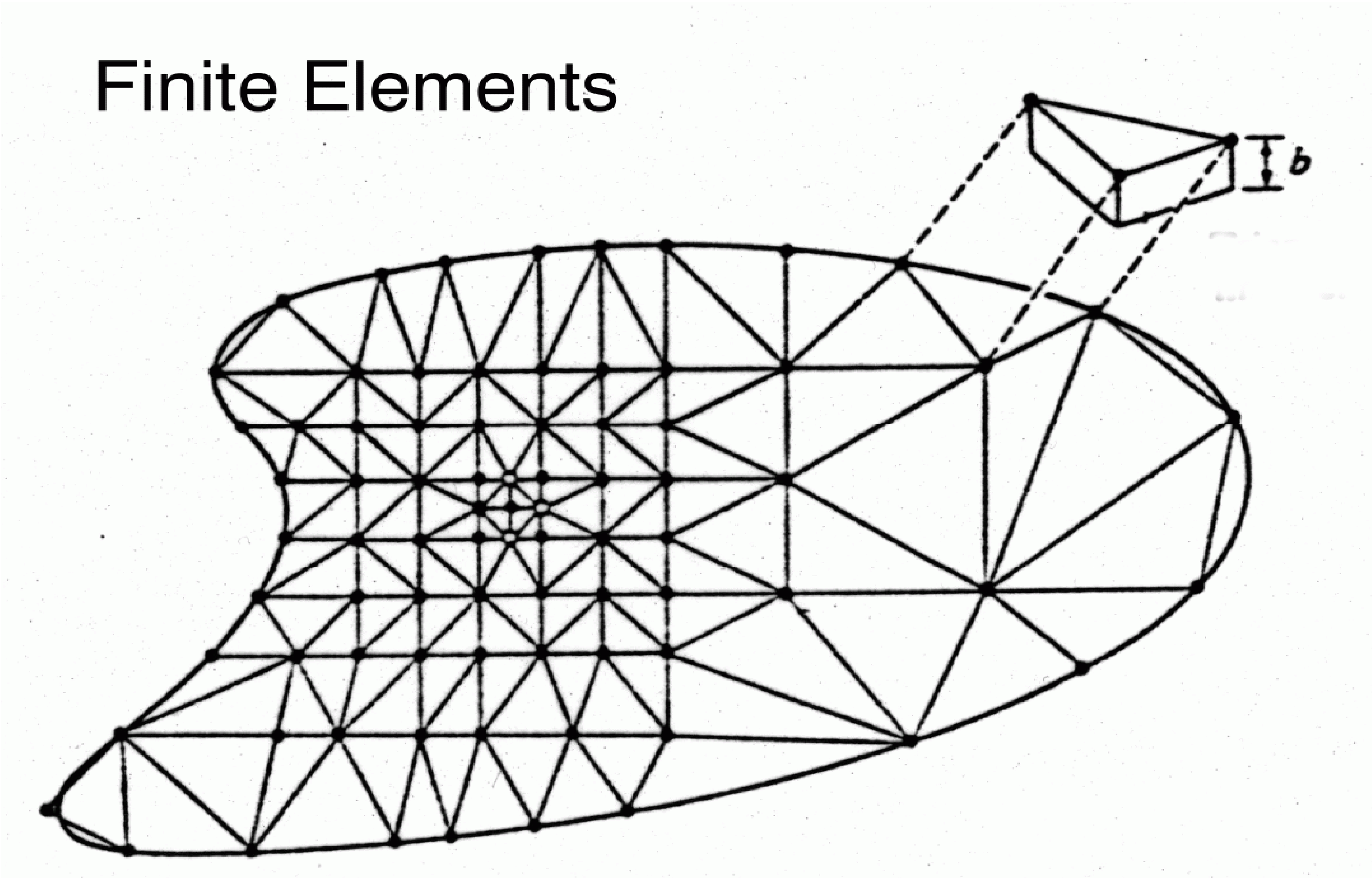
- Neumann conditions
  - Flow rate across boundary known

- Cauchy (mixed) conditions

Initial conditions

- Transient modeling
  - hydraulic head (contaminant concentration) at all nodes known


Finite Differences
Δx
Δy
b
Δx
Δy


Finite Elements
b

Contaminant transport modeling

- Transport processes
  - Advection
  - Diffusion
  - Dispersion
  - Retardation:
    - Sorption/Desorption
    - Decay
    - Loss by chemical / biological reactions

Contaminant transport modeling

- Numerical problems

- Peclet Number

$$P_e = \frac{|v_a| L}{D_L} < 2$$

Courant criterion

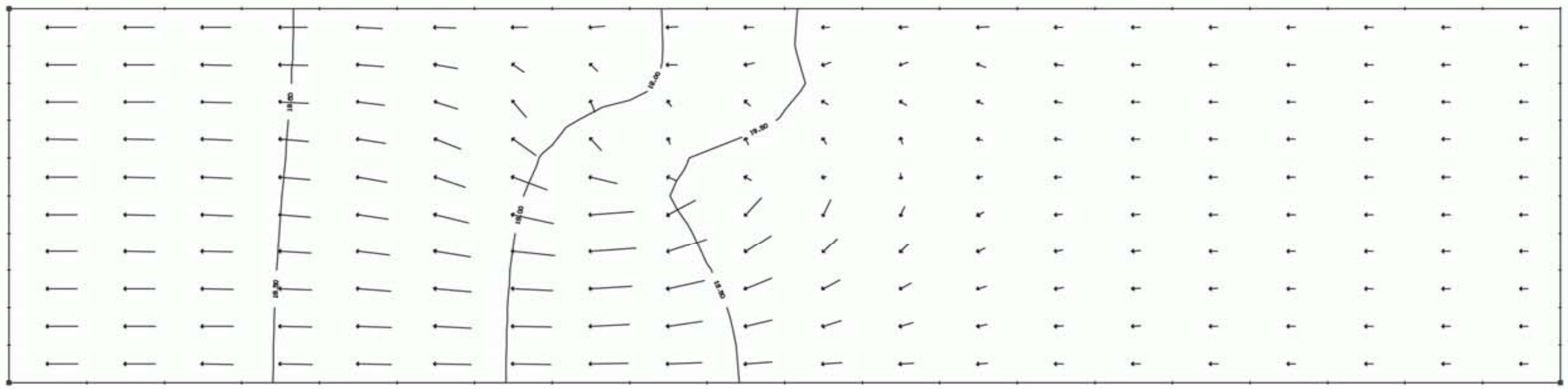
$$C_o = \left| \frac{\Delta t \cdot v_a}{L} \right| \leq 1$$

Model design process

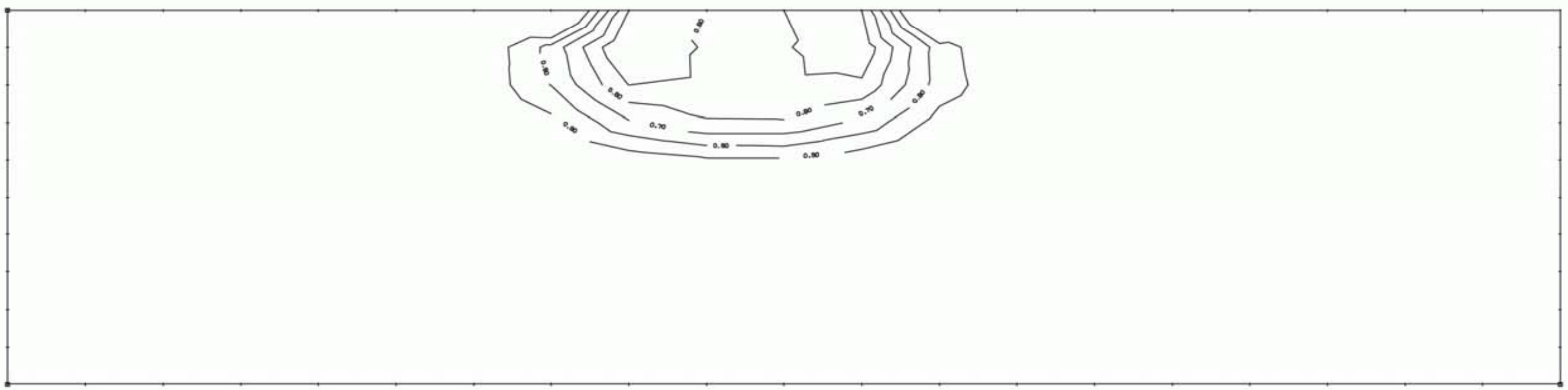
- Parameter evaluation (field studies)
- Mesh design
- Model calibration
- Model validation
- Simulation (Prediction)
- Interpretation of results (with respect to the quality of input data)

- Fractured rock models
- Multiphase flow and transport
- Multicomponent reactive modeling coupled with transport modeling

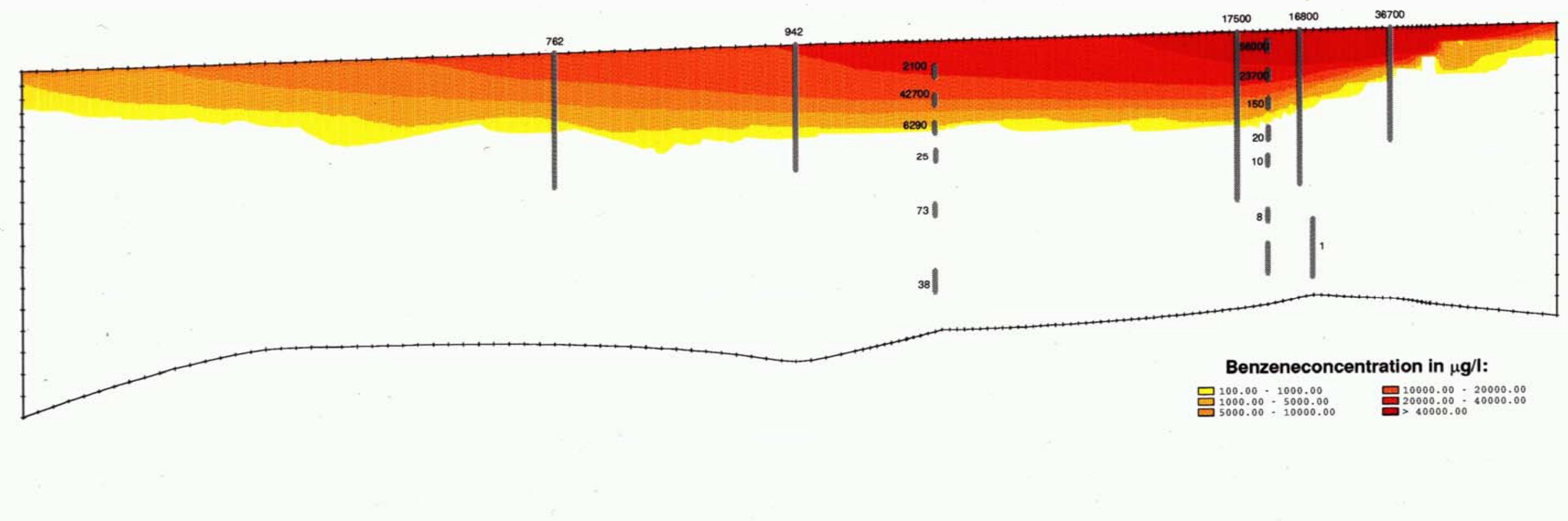
Equipotentials and flow field



Non aqueous phase (NAPL) saturation

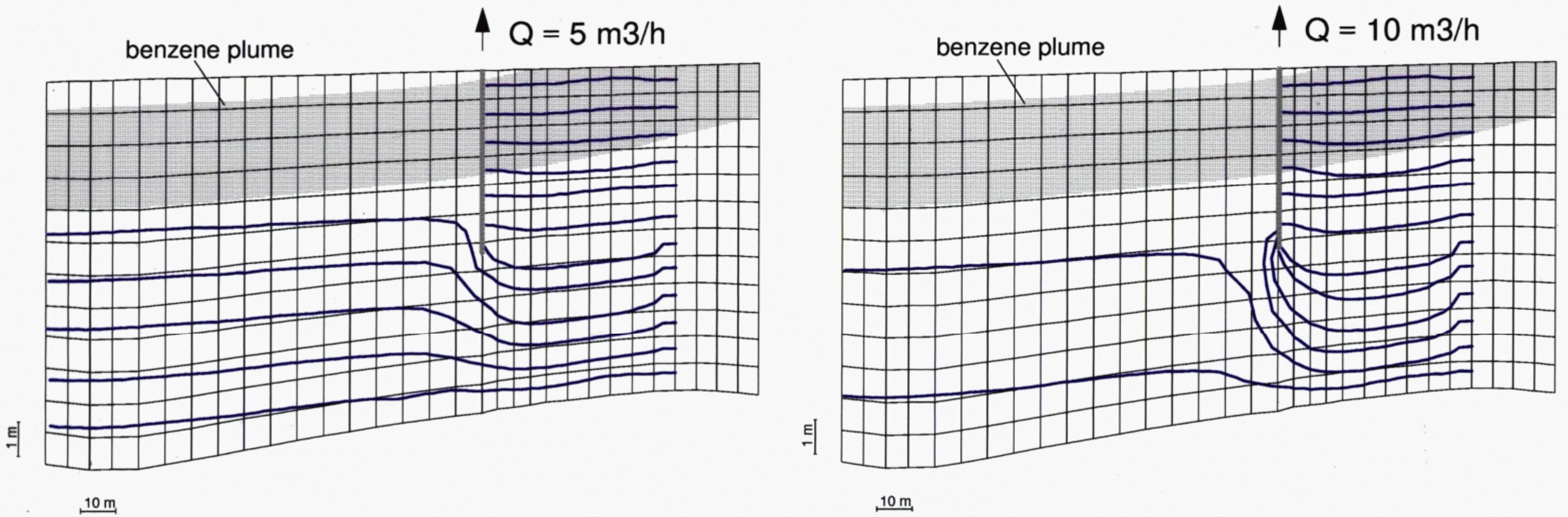


Calculated bencene plume ... (Grafik)

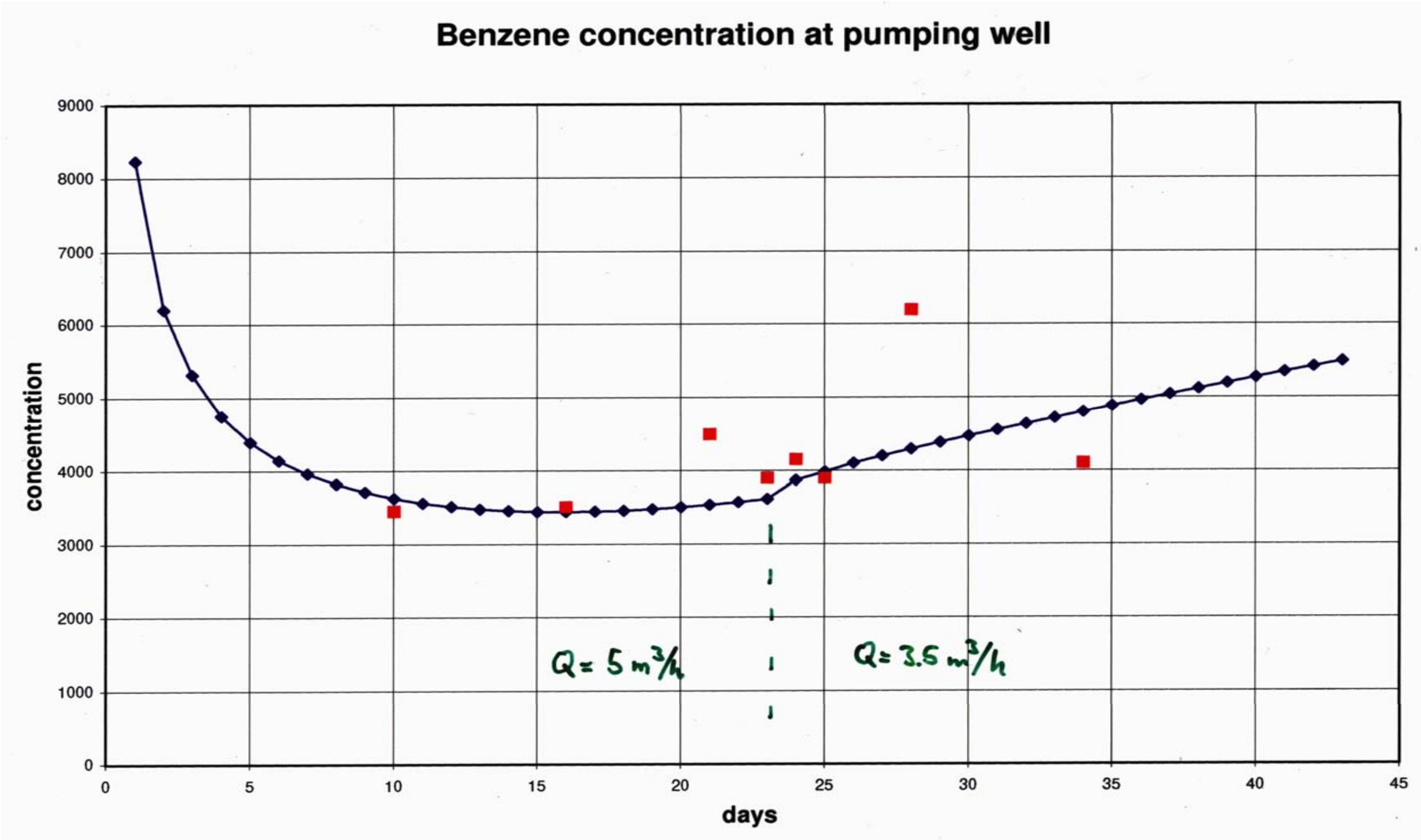


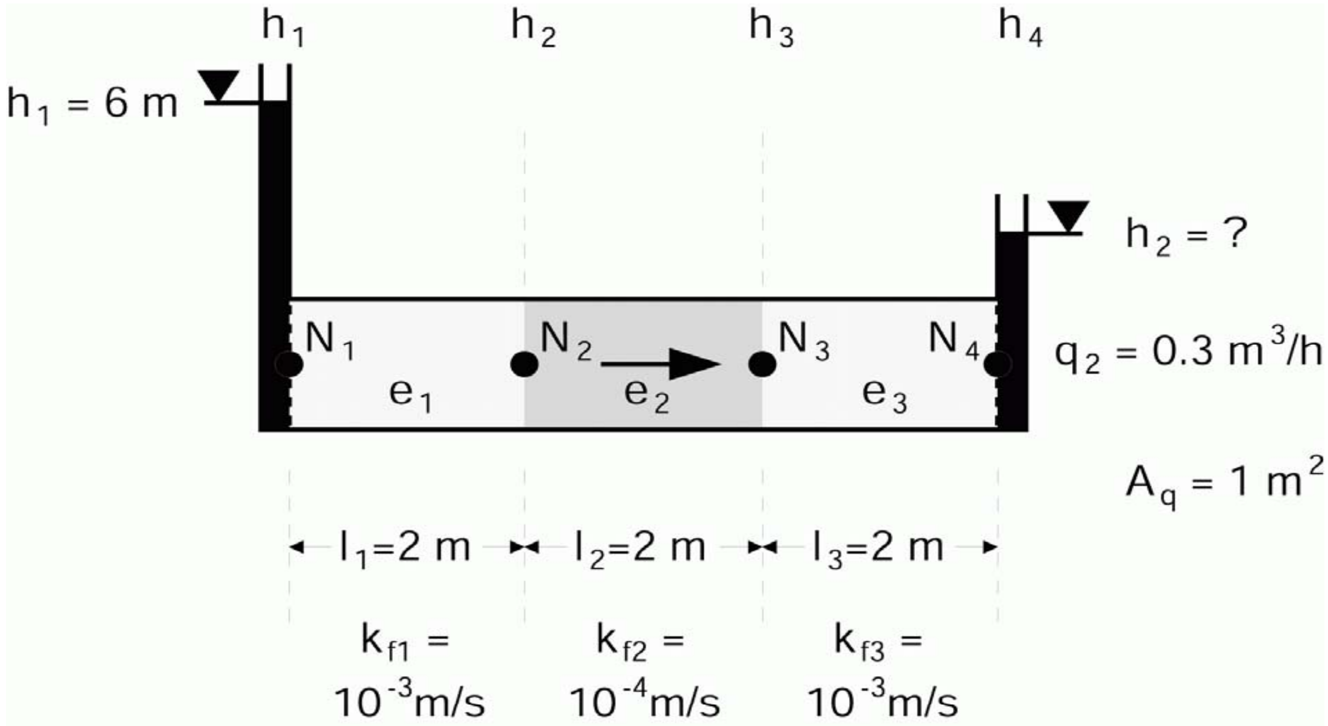
Calculated bencene plume and measured concentrations

Vertical catchment area of a partialy penetrating well with... (Grafik)



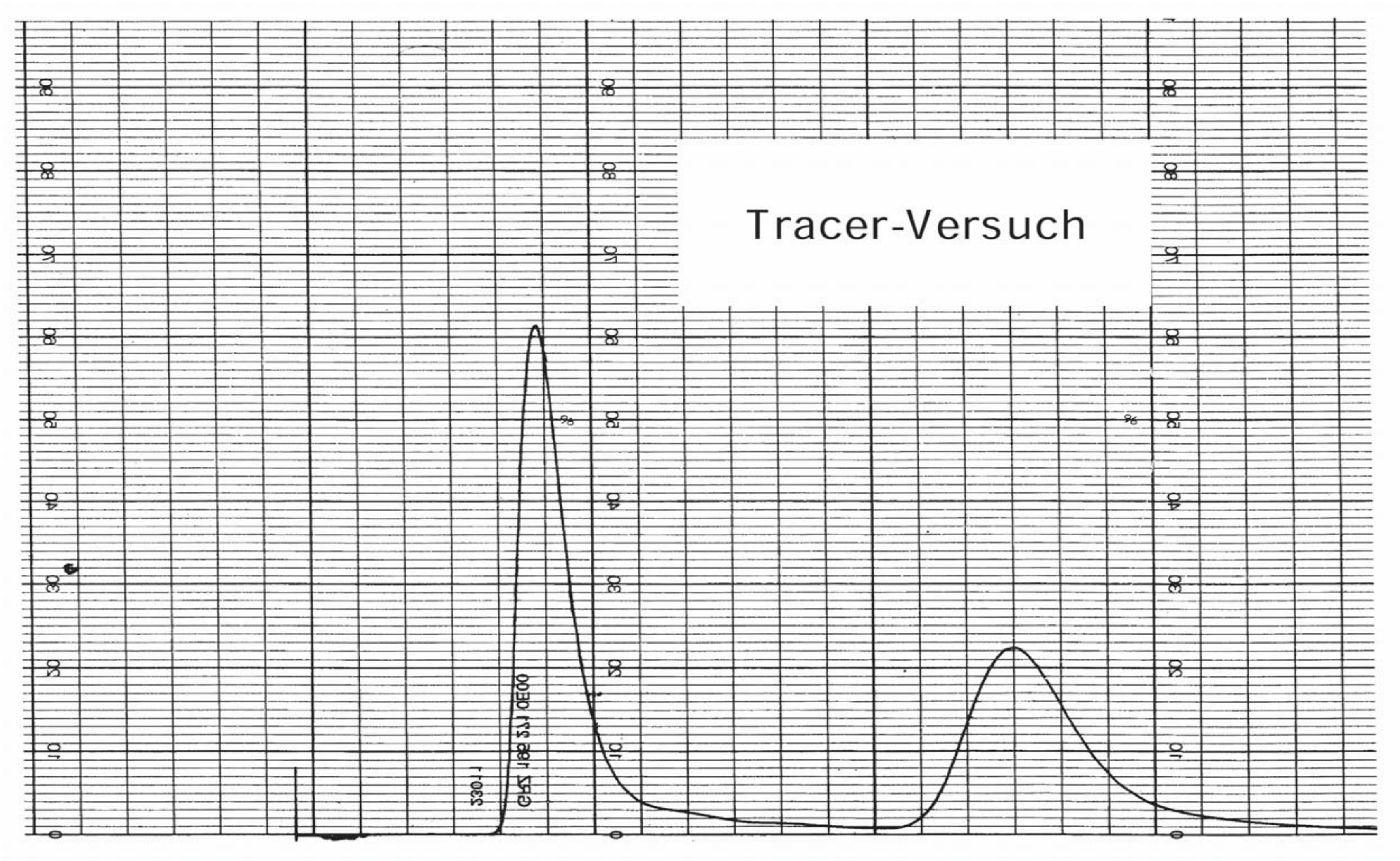
Vertical catchment area of a partialy penetrating well with pathlines


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



1-dimensional Example

Tracer Experiment

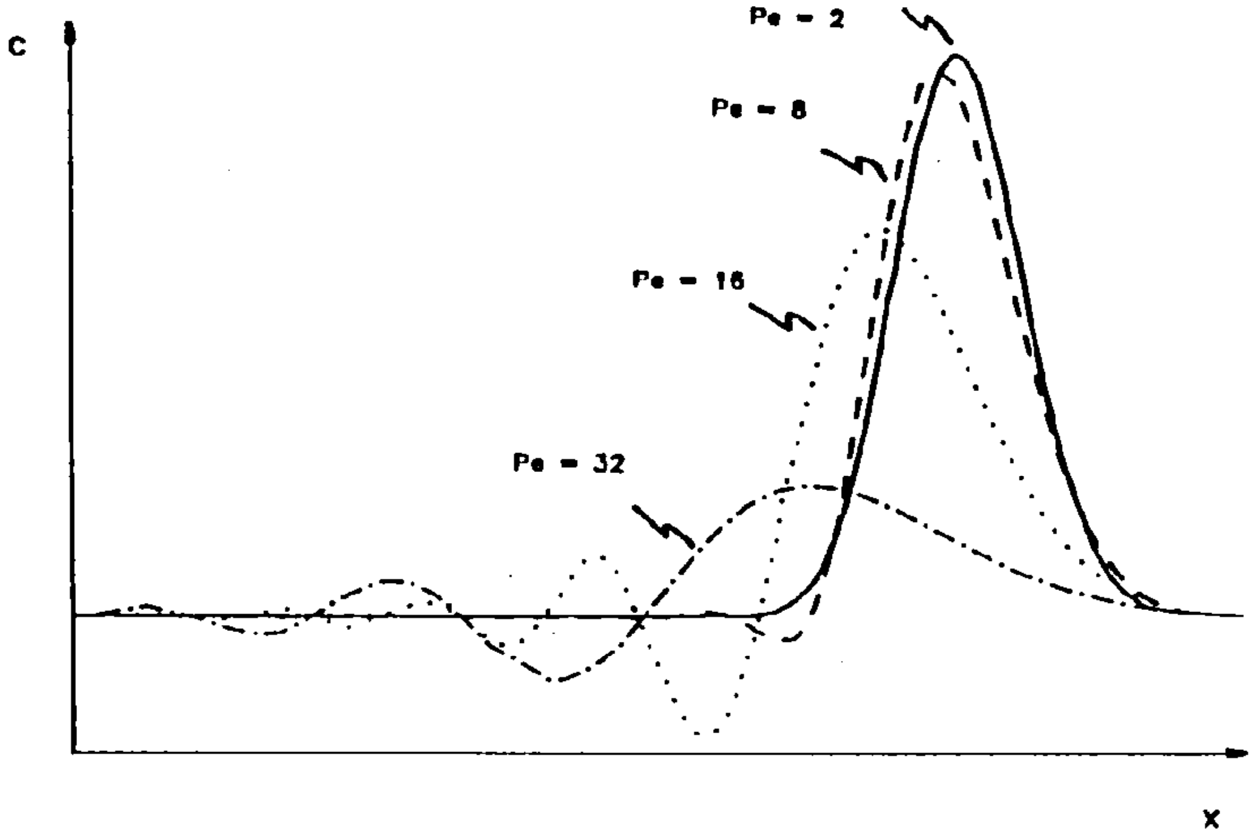


Equation solving algorithms

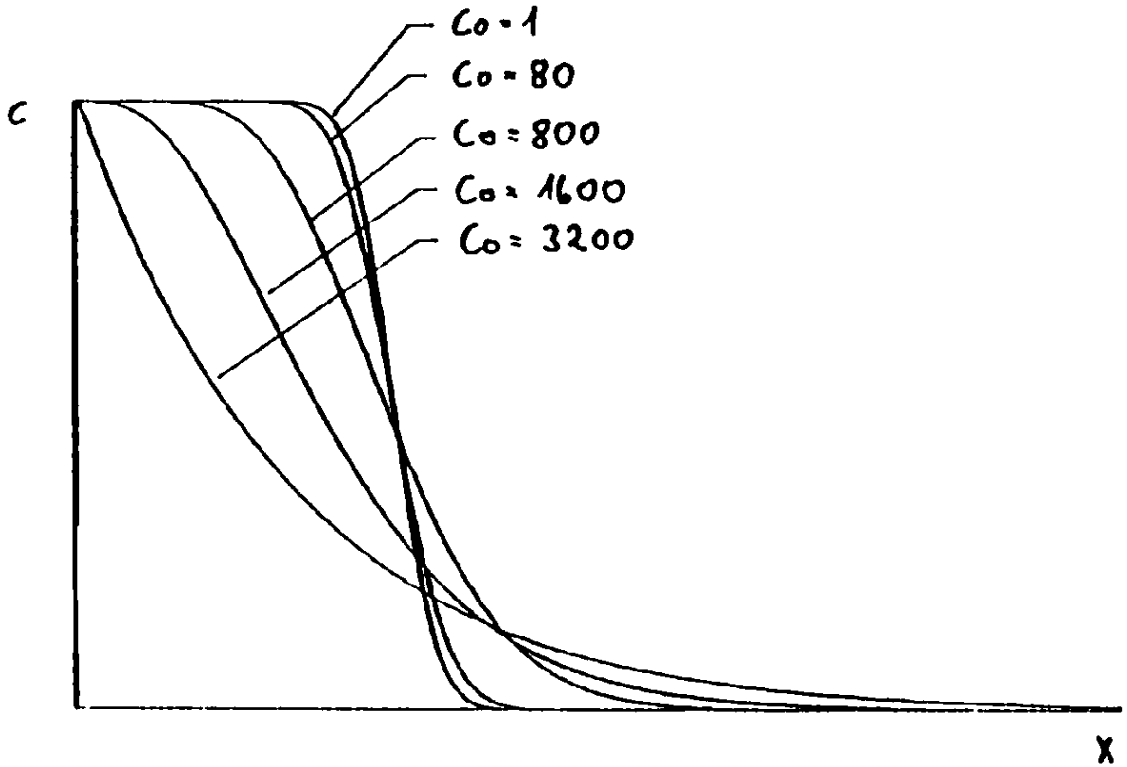
Given is an equation system with n unknown n equations (n = number of nodes)

- Direct algorithms
- Iterative algorithms

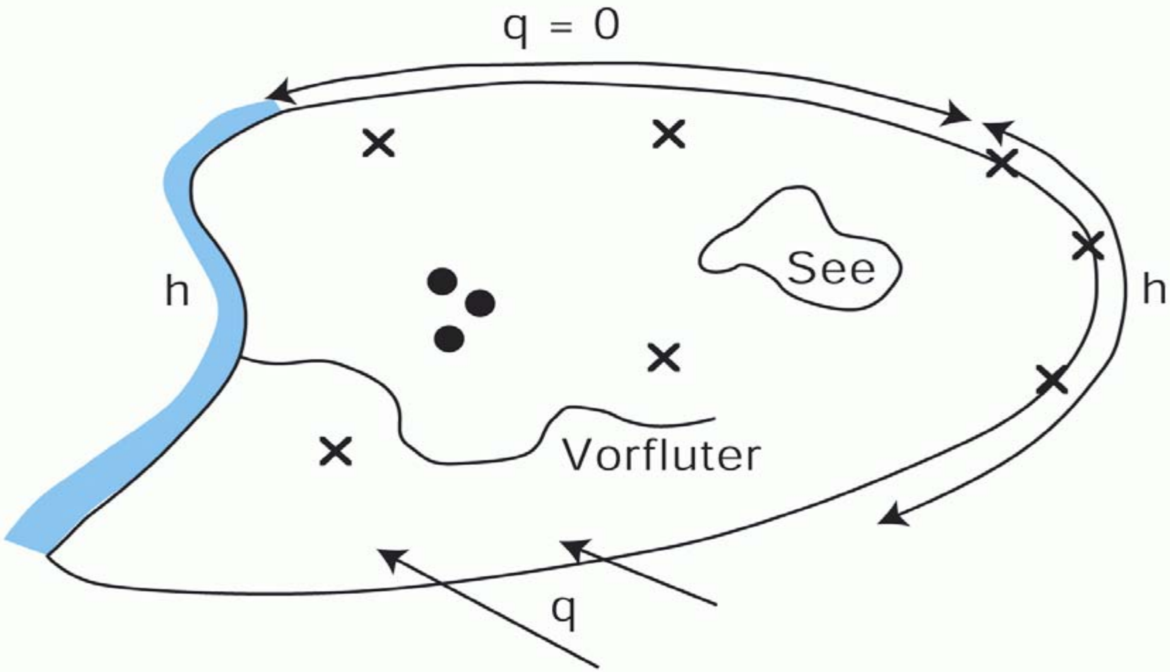
Influence of peclet number



Influence of courant criterion

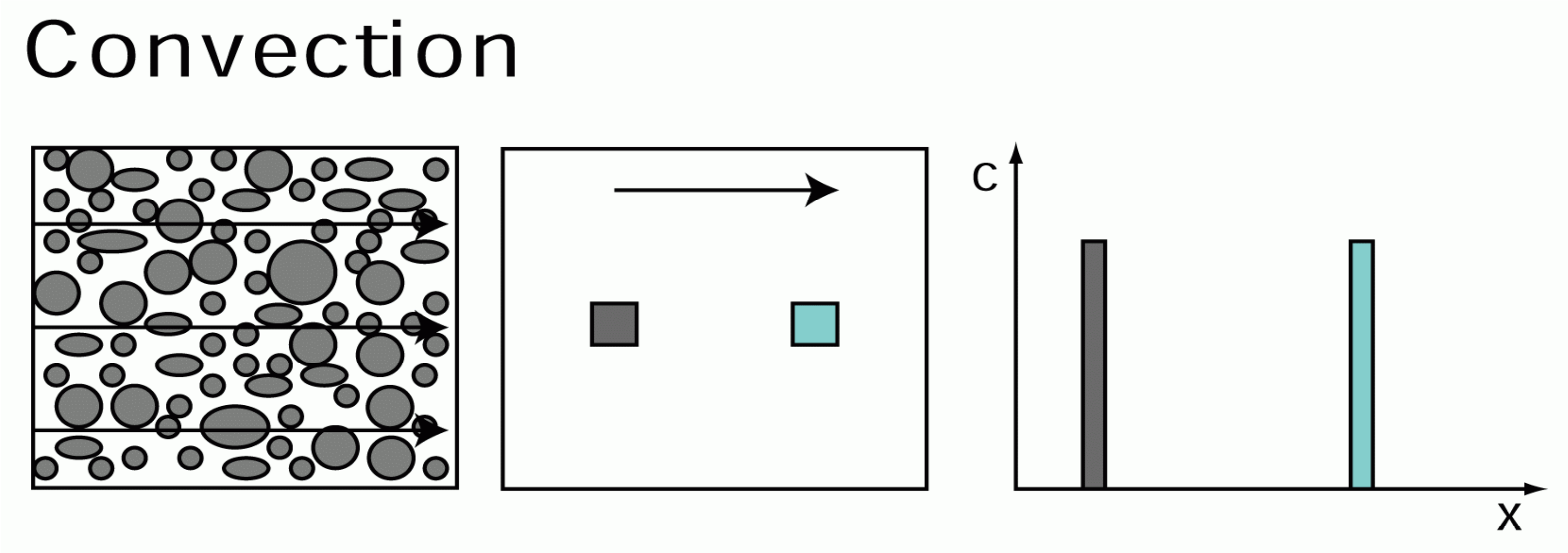


Boundary conditions and parameters



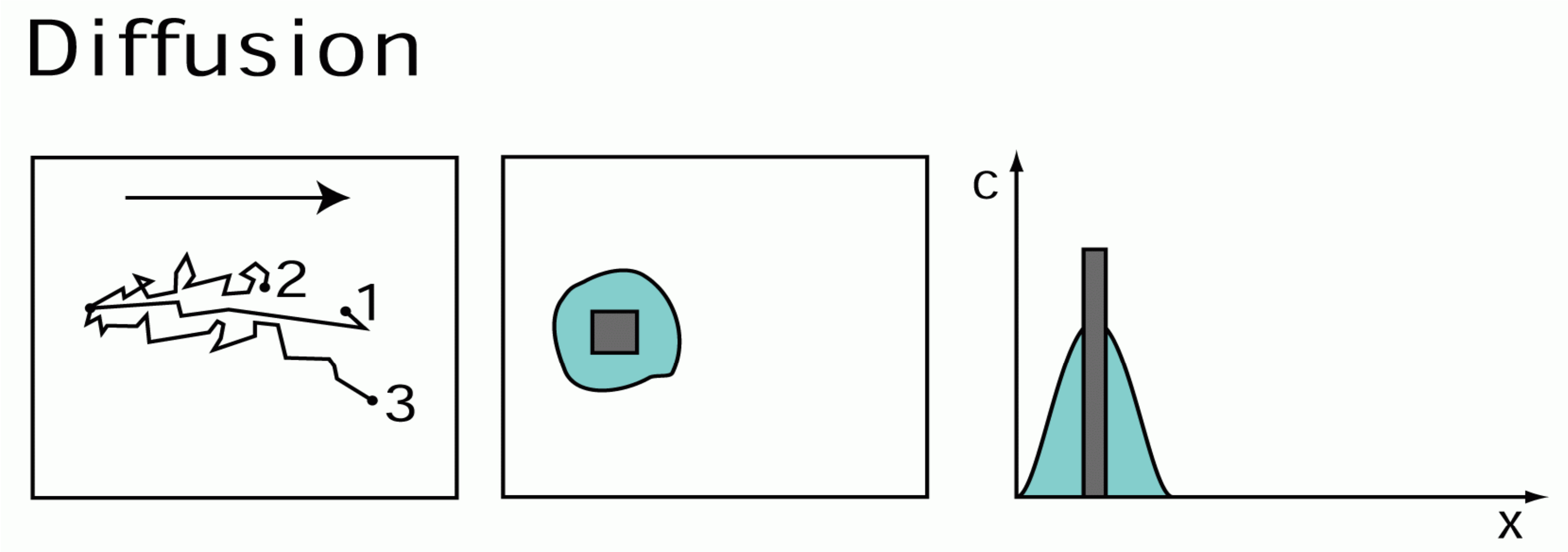
Transport processes 1

(Grafik)



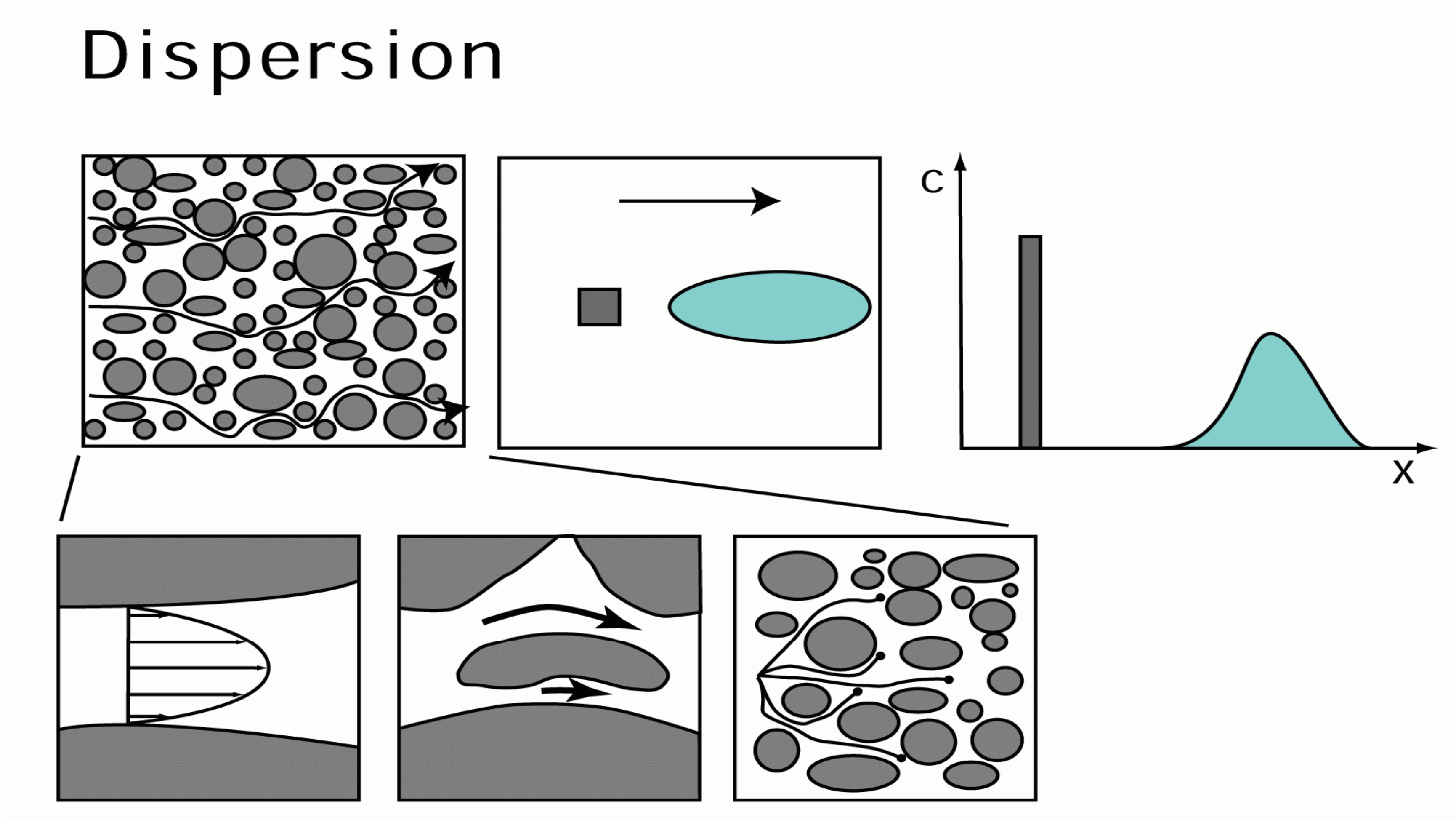
Transport processes 2

(Grafik)



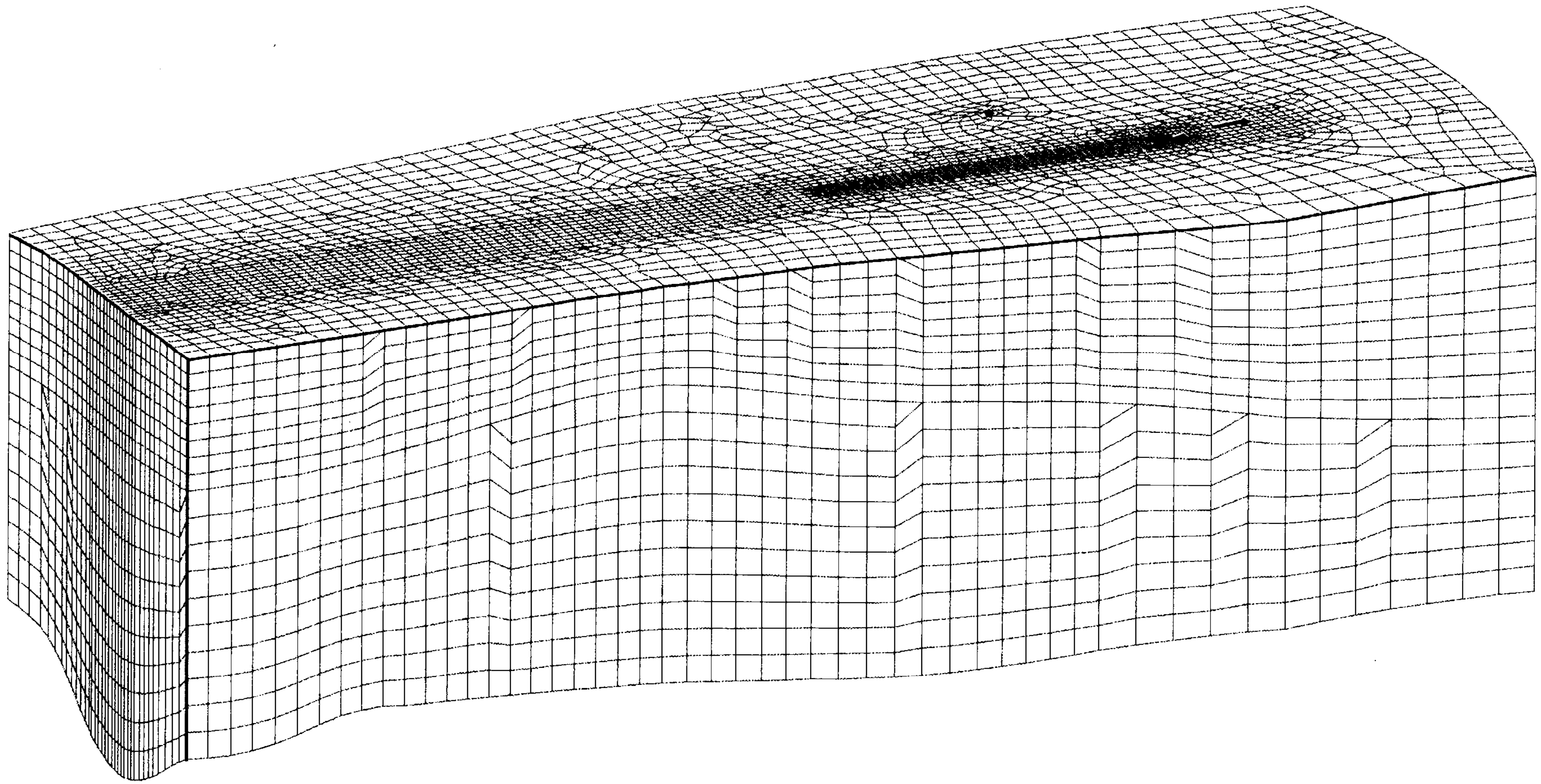
Transport processes 3

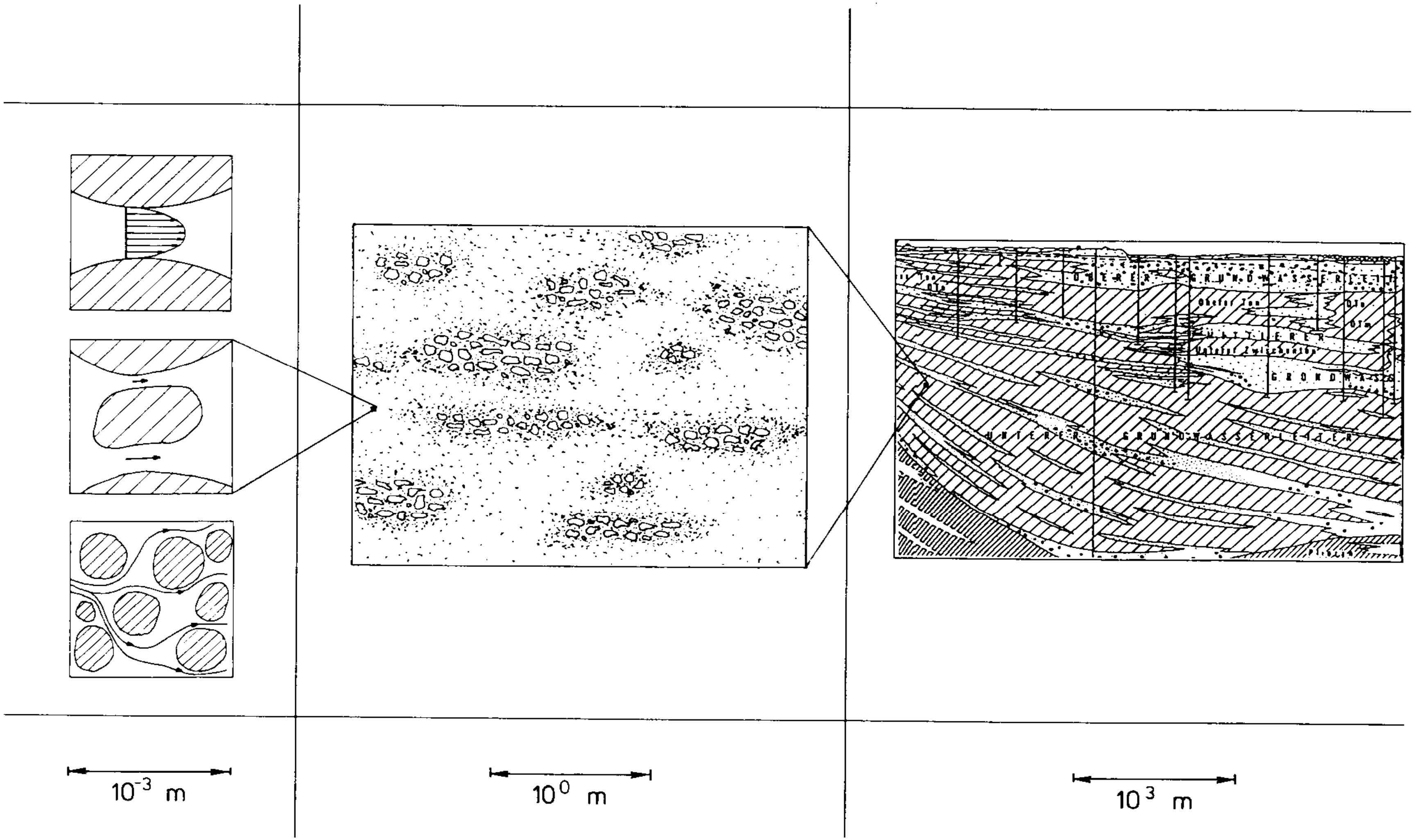
(Grafik)



3D-Model Mesh

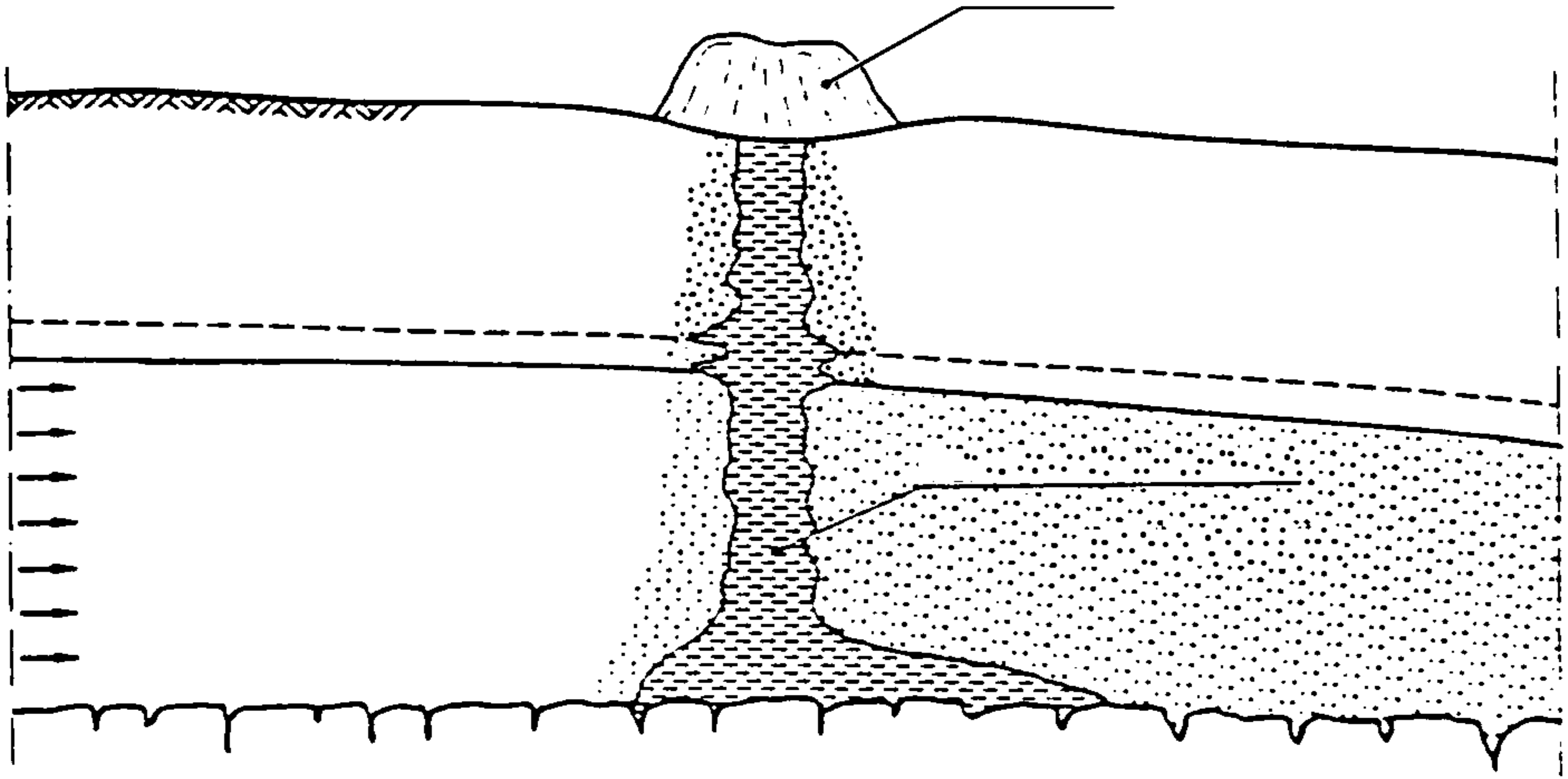
Flingern Transportmodell (Grafik)



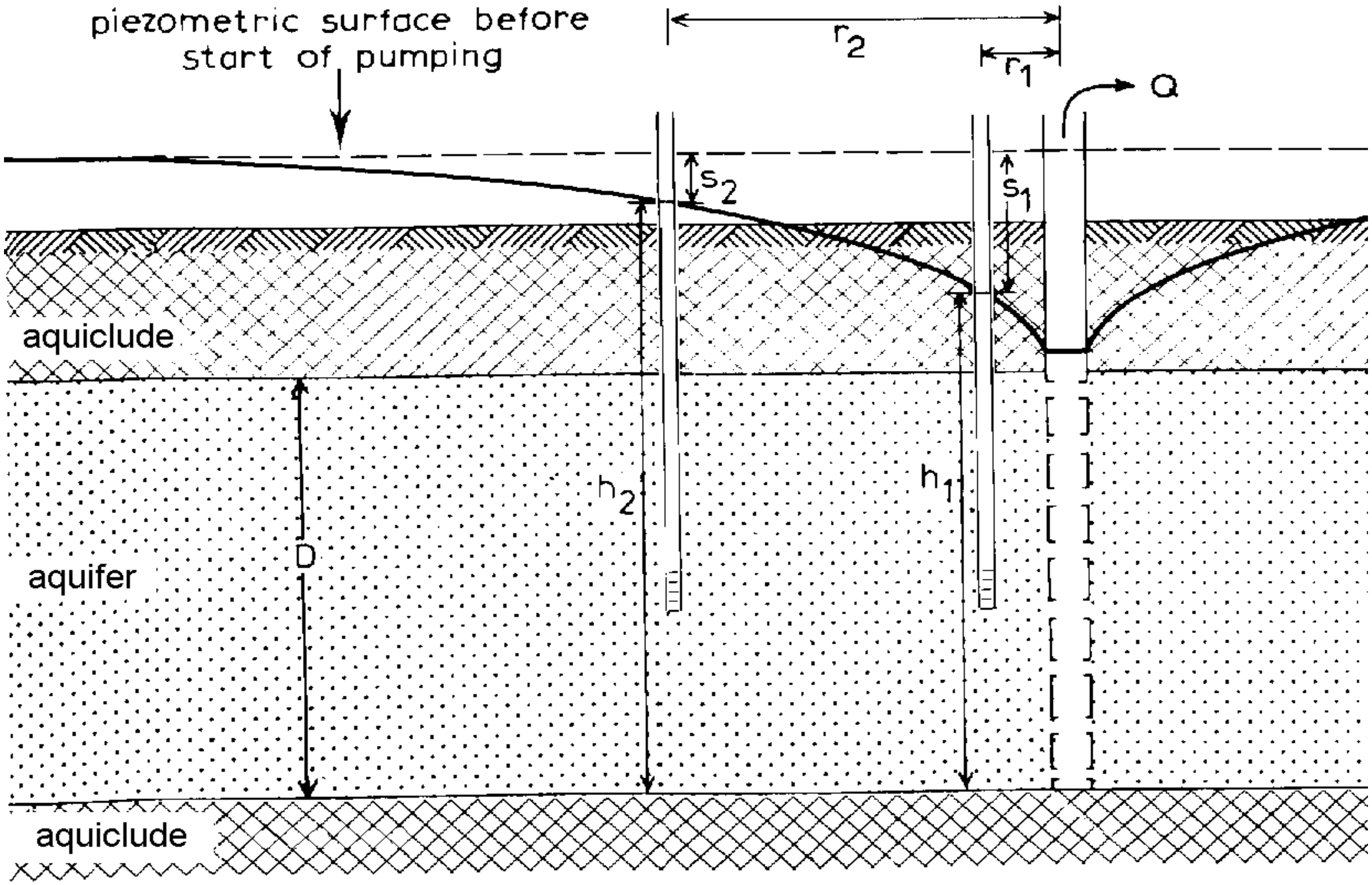


10^{-3} m
10^{0} m
10^{3} m

Phase 1

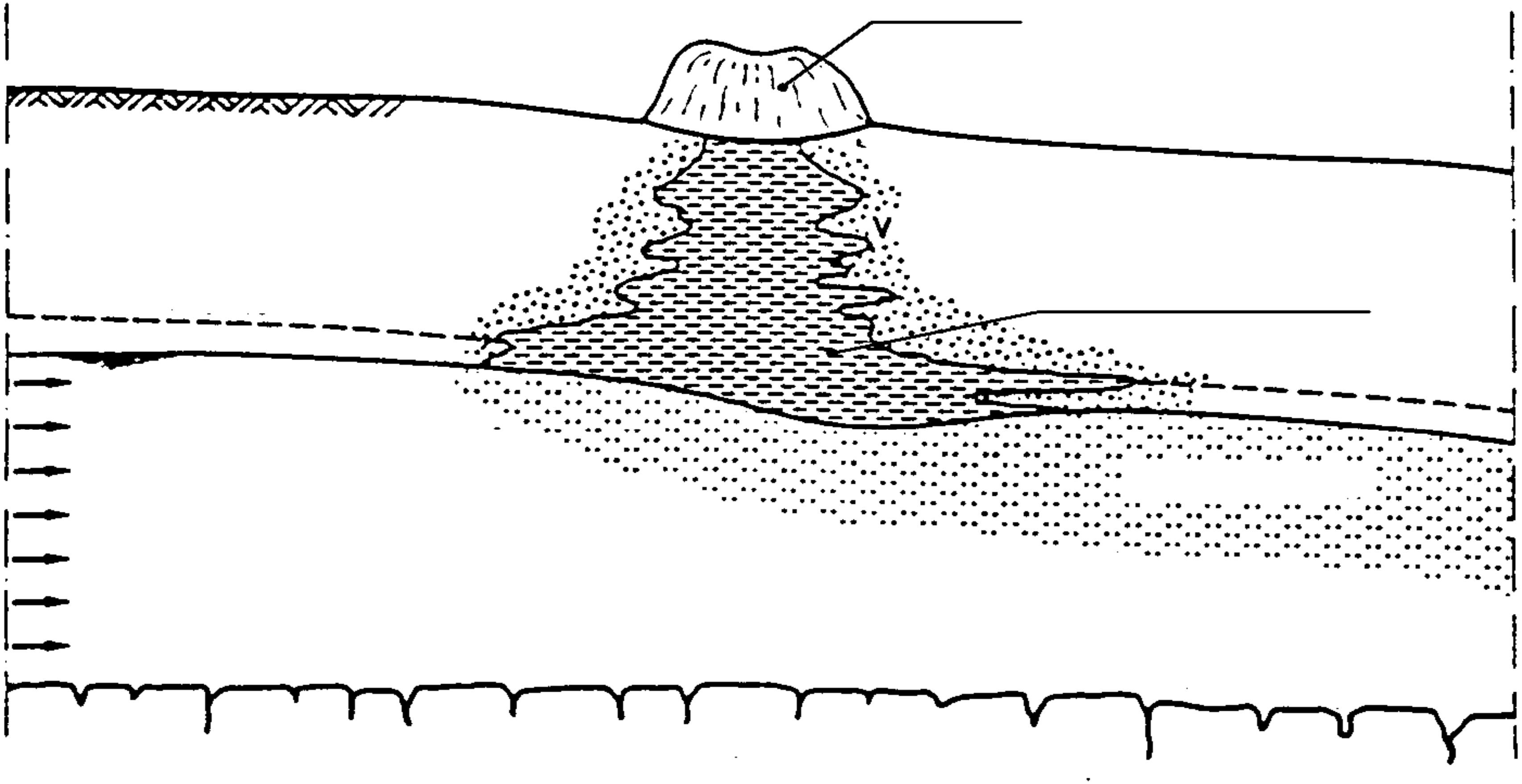


Well



Cross-section of a pumped confined aquifer

Phase 2



Rock as a barrier

- Hydraulic barrier
  - Matrix permeability
  - Fracture aperture
  - Fracture conductivity
  - Initial saturation
- Diffusion from fracture into the rock matrix
  - tailing

Rock as a barrier

- Adsorption
  - Henry
  - Freundlich
  - Langmuir
- Chemical reactions

Discontinuities in rock

- Mega scale
  - Faults and shear zones
  - Length: $10^2 – 10^4$ m
  - Geographic position is known
- Meso scale
  - Fractures
  - Length: $10^{-1} – 10^1$ m
  - Main direction of fracture cluster and statical data are known
  - Aperture: $10^{-5} – 10^{-3}$ m

Discontinuities in rock (2)

- Micro scale
  - Micro fracture and pores
  - Length: $<10^{-1}$ m
  - Direction is known

Automatic mesh generation

- Mesh creation without any user intervention
- Consideration of defined nodes, edges and faces
- Fulfillment of quality criteria
- Fast node and mesh generation

Physical processes in fracture flow

- Diffusion into rock mass
  - Mass transport in fracture is advection dominated
  - Mass transport in rock matrix is diffusion dominated
  - Tailing
- Sorption
  - Sorption to the grains
  - In rock matrix larger than in fracture

Physical processes in fracture flow (2)

- Permeability
  - High permeability in fracture
    => High velocity
  - Low permeability in rock matrix
    => Low velocity
- Storage capacity
  - Pore volume of rock mass: 2 – 6% (sand stone)
    => high storage capacity
  - Volume of fractures: 0,2 – 0,6% (sand stone)
    => limited storage capacity

Physical processes in fracture flow

- Saturation
  - Pore diameter 10-6 – 10-5 m

    =>large capillary pressure
  - Fracture aperture 10-4 – 10-3 m

    => Low capillary pressure

Fluid Parameters

- Compressibility of water:
  $\beta = 4{,}47\ 10^{-10}\ m^2/N$
- Dynamic viskosity of water:
  $\mu = 8{,}5\ 10^{-2}\ kg/ms$
- Density of RAG water:
  RAG = 1105 kg/m^3
- Tempreture of formation water:
  t = 40 °C

Rock Parameters (1)

- Compressibility of matrix:
  α=2,13 10^{-8} m^2/N
- Residual initial saturation of matrix:
  Swres=0,9
- Initial pressure:
  $P < 0 \, N/m^2$
- Van Genuchten parameters of saturation:
  aa=1,25 10^{-4} / ss=1,30

Rock Parameters (2)

- Dispersivity:

  $\alpha_1 = 1$ m
- Diffusion coefficiant:

  $D = 2{,}0\ 10^{-11}$ m²/s
- Density of host rock:

  $\rho_G = 2500$ kg/m³

Facture Parameters

cluster	azimuth	dipangle	Concentration para-meter	Cone of confi-dence	Sperical aperture
1	274	88	181	0.95	8.2
2	71	6	98	0.95	8.2
3	309	4	44	2.35	12.3

- average fracture aperture: a= 200 μm
- dispersivity α_1 =0.2m

Generation of fracture planes

- Fracture plane is defined by:
  - Origin of fracture
  - Normal direction
  - Length of the edges
  - aperture

1. Origin of fracture

- Uniform distributed:
- Model size (x,y,z) is multiplied by a uniform distributed random number in the range of (0,1).

2. Normal direction

- Fisher-Distribution (sperical Normal distribution)
- Circular symmetrical arrangement of data around a vector
- Density function:

$$f(\phi,\kappa) = \frac{\kappa \exp^{\kappa \cos\phi}}{4\pi \sinh \kappa}$$

- ϕ angle between mean value and observed value

- Orientation in space
- Orientation (α, φ):
  - Down dip α=deviation to North direction
  - Angle of fall ϕ=angle to the horizontal

3. Lengths of fracture

- Lognormal, exponentional or Gaussian distribution random generator

Aperture

- Lognormal or Gaussian distribution random generator

!!! Generation Finished !!!