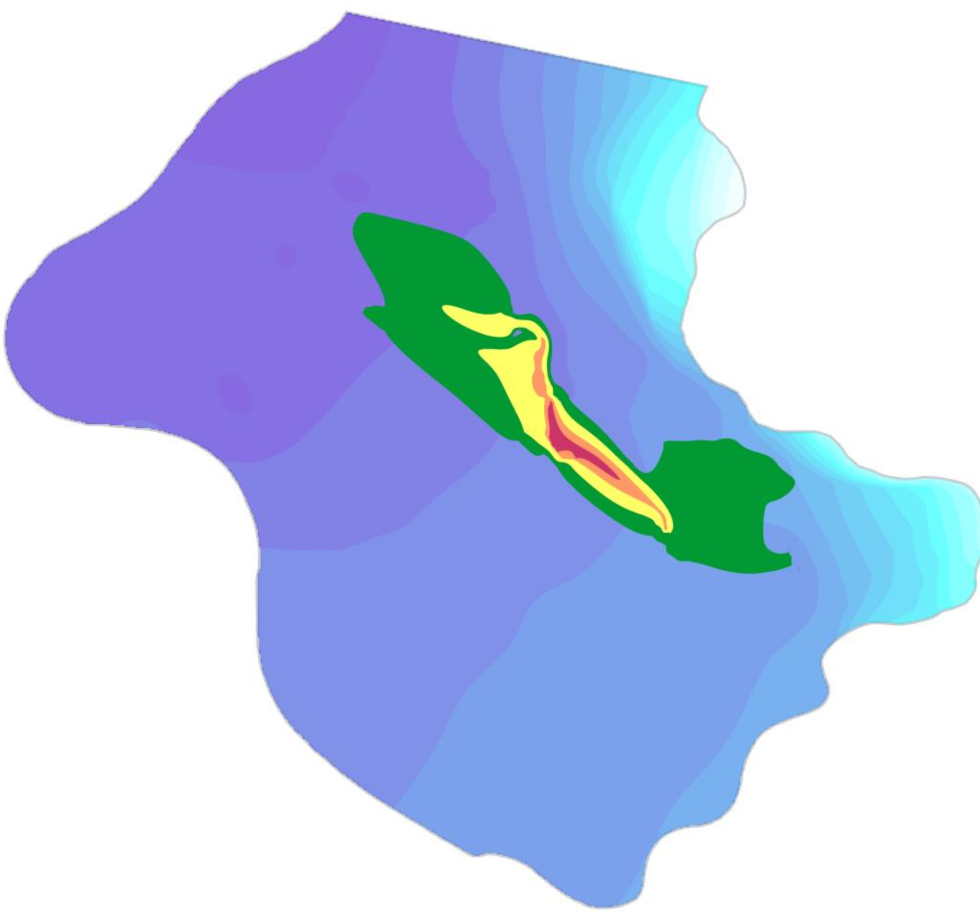
HANDS-ON GROUNDWATER MODELING

An introduction to groundwater flow and solute transport modeling with applications

Randolf Rausch & Anneli Guthke



Hochschule für Forstwirtschaft Rottenburg
Hochschule für Angewandte Wissenschaften
TECHNISCHE UNIVERSITÄT DARMSTADT
Universität Stuttgart

Cover Illustration:

The cover illustration shows an exemplary result of a 2D catchment-scale groundwater flow and solute transport simulation (Anneli Guthke, BoSS Consult GmbH).

Preface

This course on groundwater modeling is specifically designed for participants in the fields of hydrogeology and civil as well as environmental engineering. Only a basic knowledge of groundwater terms is required for participation. Hands-on modeling experience with PCs will serve to introduce the necessary concepts and theory. After intensive modeling instructions participants will have a basic knowledge of groundwater models, helping them to evaluate situations by using models, to discuss modeling needs with other professionals, to evaluate modeling efforts of others, and to understand the importance of both the data necessary for providing a viable assessment and of the appropriate choice of a model for specific situations.

This manuscript is a set of handouts and slides used in the course.

Darmstadt, Stuttgart and Rottenburg October 2018

Randolf Rausch & Anneli Guthke

Key Features

Groundwater Flow Modeling

- Application of groundwater models
- Basic concepts of groundwater flow
- Flow equation
- Analytical flow models
- Numerical flow models
- Finite difference models / finite element models
- Explicit / implicit solution of the flow equation
- A complete groundwater flow model
- 2-D- / 3-D- flow modeling

Solute Transport Modeling

- Basic concepts of transport in groundwater
- Transport phenomena
- Transport equation
- Analytical solutions of the transport equation
- Pathlines and travel times
- Numerical transport models
- Grid methods
- Stability and accuracy of solutions
- Particle tracking methods
- Random-walk method
- Method of characteristics

Process of Modeling

- Model objectives
- Collection and interpretation of data
- Development of hydrogeological (conceptual) model
- Choice of model type
- Modeling software selection / programming
- Model design
- Model calibration
- Sensitivity analysis

- Model validation
- Model application and performance of prognostic runs
- Analysis of results
- Post-auditing

All topics within the course are handled with reference to real case studies and hands on exercises.

Participants will be provided with complete versions of the groundwater models ASMWIN and PMWIN.

Contents

Introduction

What is a Groundwater Model?

- We use groundwater models for the simulation of
  - groundwater flow,
  - and transport of pollutants in groundwater.

- In case of flow models we are interested in quantities.

  Solution: h = f(x,y,z,t)

- In case of transport models we are interested in quality of groundwater.

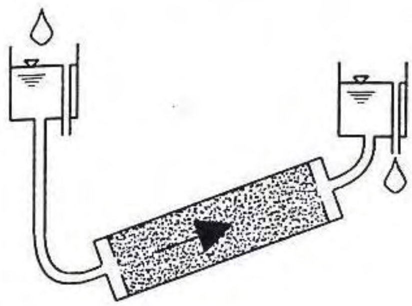
  Solution: c = f(x,y,z,t)

Why Numerical Groundwater Models?

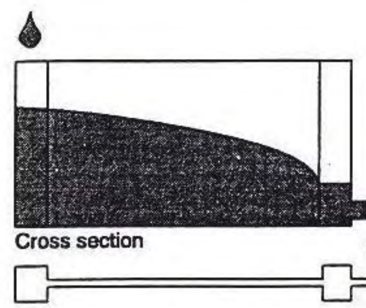
- Sparse data require concept of analysis.
- Complexity of nature requires simplification.
- Only heads can be measured, but we are also interested in flow quantities.
- Processes in groundwater are very slow. Experiments in the field take long time and are expensive. Prognostic power is required.
- Analytical solutions / models are not generally applicable.
- Big interpretation effort is justified as data are expensive.

Types of Groundwater Flow Models

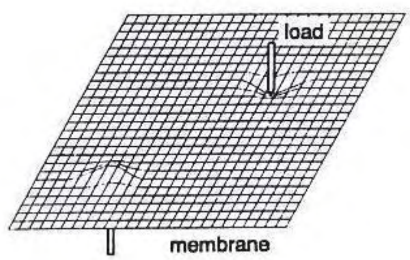
Porous Media Model



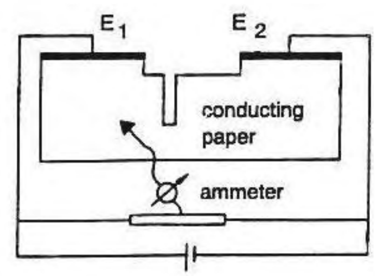
Viscous Fluid Model



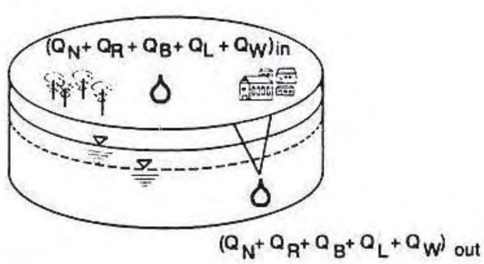
Membrane Model



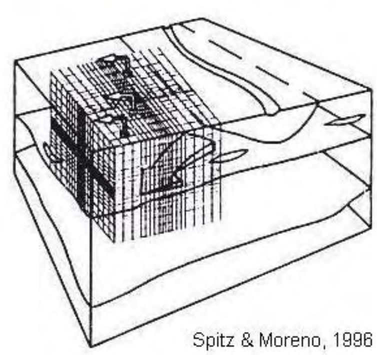
Electrical Analog Model



Mass Balance Model (Box Model)



Numerical Model



Spitz & Moreno, 1996

Applications of Flow Models

- Interpretation of observed heads
- Prediction of groundwater drawdown and build up
- Estimation of water balances or elements of water balance
- Delineation of well head protection zones and catchment areas of wells
- Preparation of transport simulation

Applications of Transport Models

- Interpretation of concentration data
- Mass balance of contaminants
- Predictions of pollutant plumes
- Design of pump and treat management
- Planning of monitoring strategy
- Risk assessment in case of waste disposals

When to use 2-D (horizontal)?

Regional flow

- aquifer thickness is much smaller than horizontal extension of the aquifer
- one layer aquifer
- fully penetrating wells
- vertical flow velocities are much smaller than horizontal flow velocities

Regional transport

- vertical mixing
- minor groundwater recharge
- no density effects

When to use 3-D?

if the above assumptions are not fulfilled, e.g.:

- small scale problems
- partially penetrating wells in aquifers of large thickness
- multi layer aquifers
- density effects
- vertical velocities in the magnitude of horizontal velocities

Classification of Groundwater Models

- ## Physical options

  confined / phreatic / leaky confined aquifer
  mixing / non mixing fluids
  flow / transport
  density effect yes / no
  chemical reactions yes / no

- ## Dimensionality

  0-D: regional balances
  1-D: column experiments
  2-D horizontal: regional flow and often transport problems
  2-D vertical: in case of negligible head and / or concentration gradients in one horizontal direction
  2 ½ – D: regional flow in layered aquifer system
  3-D: small scale problems, density effects, vertical flow, nonlinear chemistry

- ## Solution method

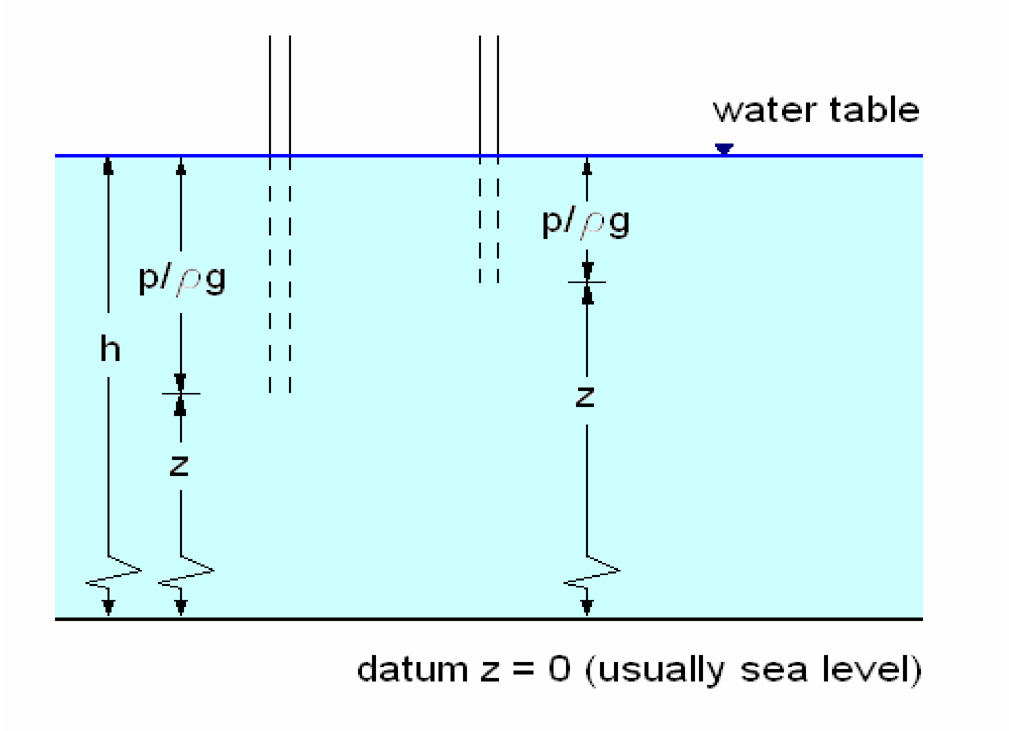
  analytical solutions
  finite differences / finite volumes
  finite elements
  for transport: Random Walk, MOC

- ## Time

  steady flow
  transient flow

Groundwater Flow Modeling

Hydraulic Head



$$h = z + \frac{p}{\rho g} + \left(\frac{v^2}{2g}\right)$$

h: hydraulic head or simply "head"
z: elevation head
p/ρg: pressure head
g: acceleration due to gravity
v: velocity

Assumption for definition: ρ = constant

Hydraulic Properties

The hydraulic properties of an aquifer are characterized by

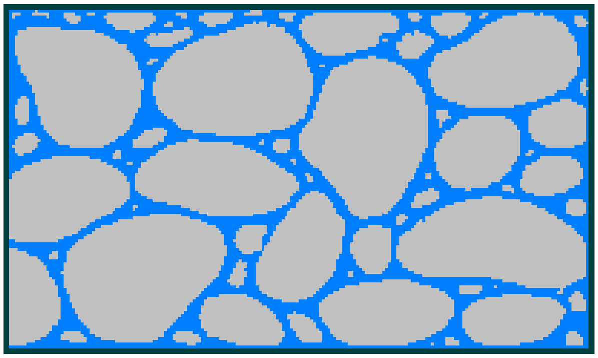
- **permeability** (which is a measure of the amount of flow of fluid through a rock), and

- **storativity** (which is a measure of the ability of an aquifer to store water).

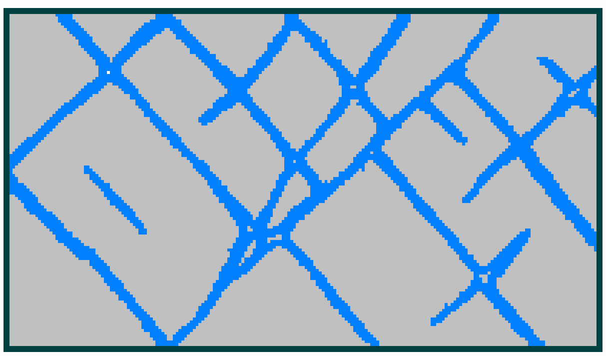
Permeability and storativity are functions of the voids within the aquifer and the connectivity of the voids.

Note: A rock may be porous, but if the pores or voids are not connected, it will have no permeability.

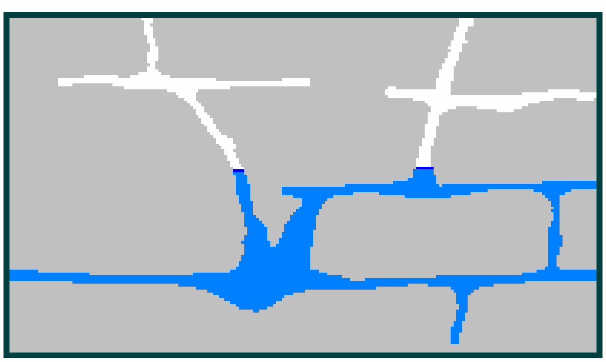
Aquifer Types



Porous media aquifer

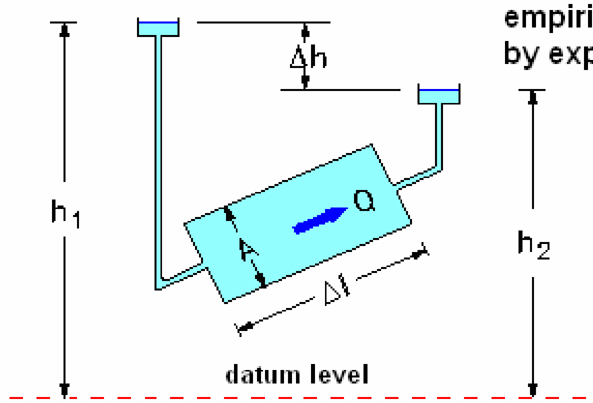


Fractured media aquifer



Karst aquifer

DARCY'S LAW



empirical law found by experiments

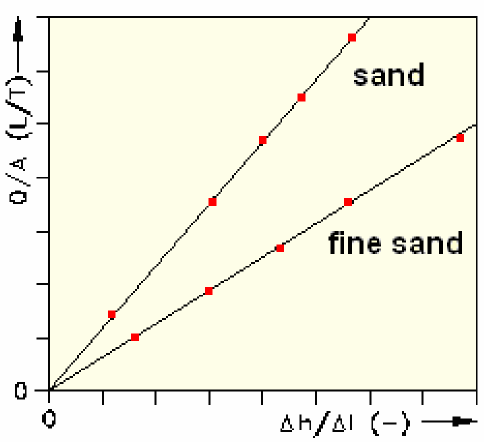
$$Q \propto A, \qquad Q \propto h_1 - h_2 = \Delta h, \qquad Q \propto \frac{1}{\Delta l}$$

$$Q = -K\,A\,\frac{\Delta h}{\Delta l}$$

where K: constant of proportionality
hydraulic conductivity

respectively

$$\frac{Q}{A} = v_f = -K\,\frac{\Delta h}{\Delta l} = -K\,\frac{dh}{dl}$$



DARCY, H. (1856):
Les Fontaines publiques de la Ville de Dijon. - Victor Dalmon, Paris

(The public water supply of Dijon)

LES

FONTAINES PUBLIQUES

DE LA VILLE DE DIJON

EXPOSITION ET APPLICATION

DES PRINCIPES A SUIVRE ET DES FORMULES A EMPLOYER

DANS LES QUESTIONS

DE

DISTRIBUTION D'EAU

OUVRAGE TERMINÉ

PAR UN APPENDICE RELATIF AUX FOURNITURES D'EAU DE PLUSIEURS VILLES

AU FILTRAGE DES EAUX

ET

A LA FABRICATION DES TUYAUX DE FONTE, DE PLOMB, DE TOLE ET DE BITUME

PAR

HENRY DARCY

INSPECTEUR GÉNÉRAL DES PONTS ET CHAUSSÉES.

ATLAS

PARIS

VICTOR DALMONT, ÉDITEUR,

Successeur de Carilian-Gœury et V[ve] Dalmont,

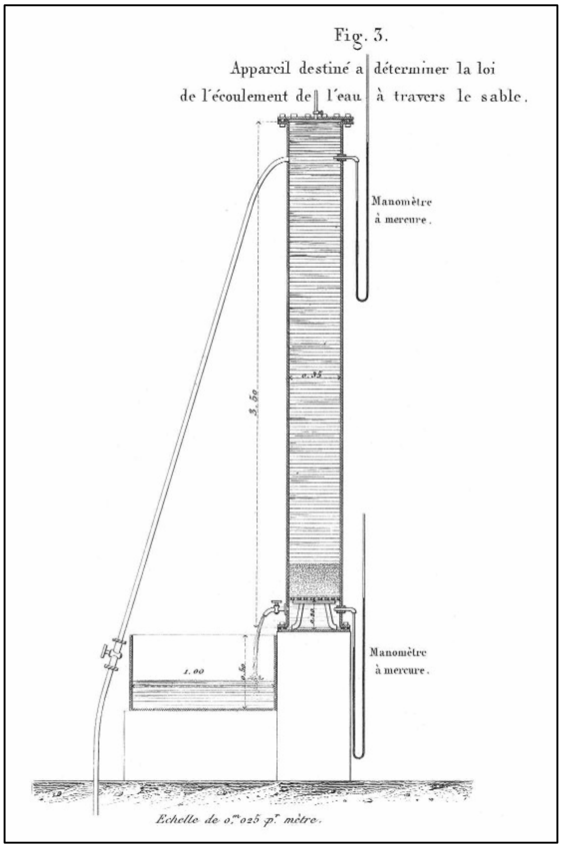
LIBRAIRE DES CORPS IMPÉRIAUX DES PONTS ET CHAUSSÉES ET DES MINES,

Quai des Augustins, 49.

1856

DARCY'S LAW

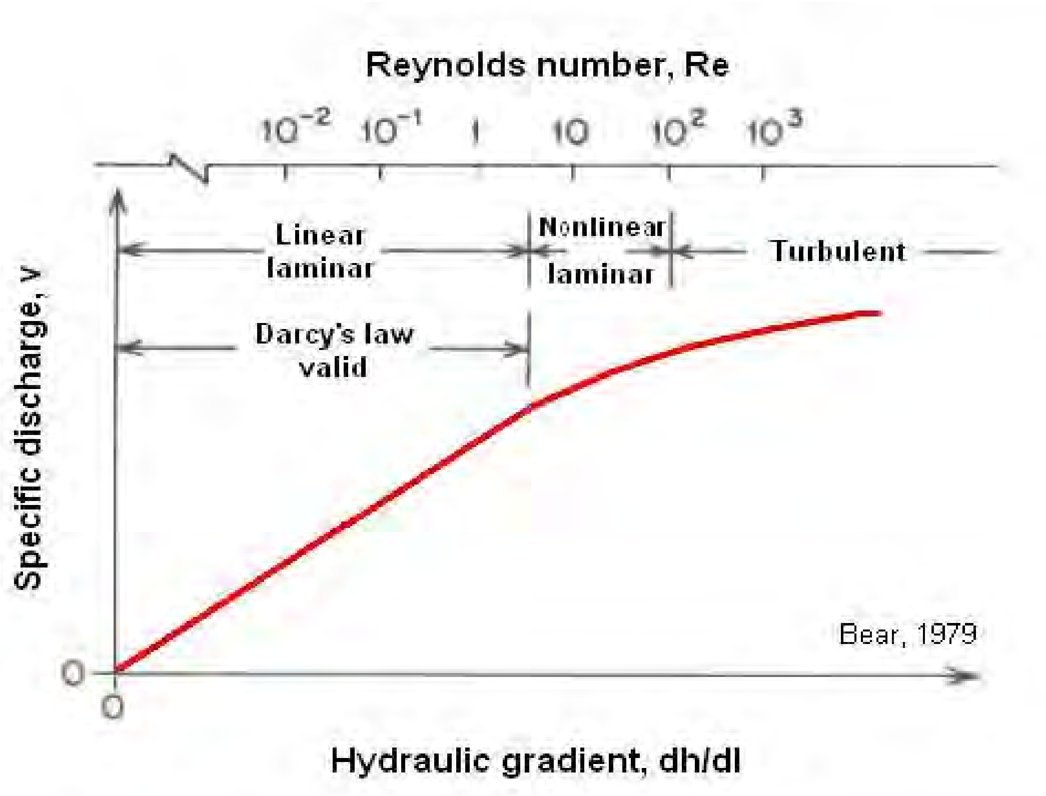
DARCY, H. (1856) : Les fontaines publiques de la ville de Dijon - Exposition et application des principes a suivre et des formules a employer dans les question de distribution d'eau – Ouvrage termine par un appendice relatif aux fourniture d'eau de plusieurs villes au filtrage des eaux a la fabrication des tuyaux de forte, de plomb de tôle de bitume. – 647 p. & Atlas ; Victor Dalmont, Paris.



The apparatus used by DARCY and RITTER in the development of DARCY's law, 1855 – 1856.

HENRY DARCY 1803 – 1858.

Range of Validity of DARCY´s Law

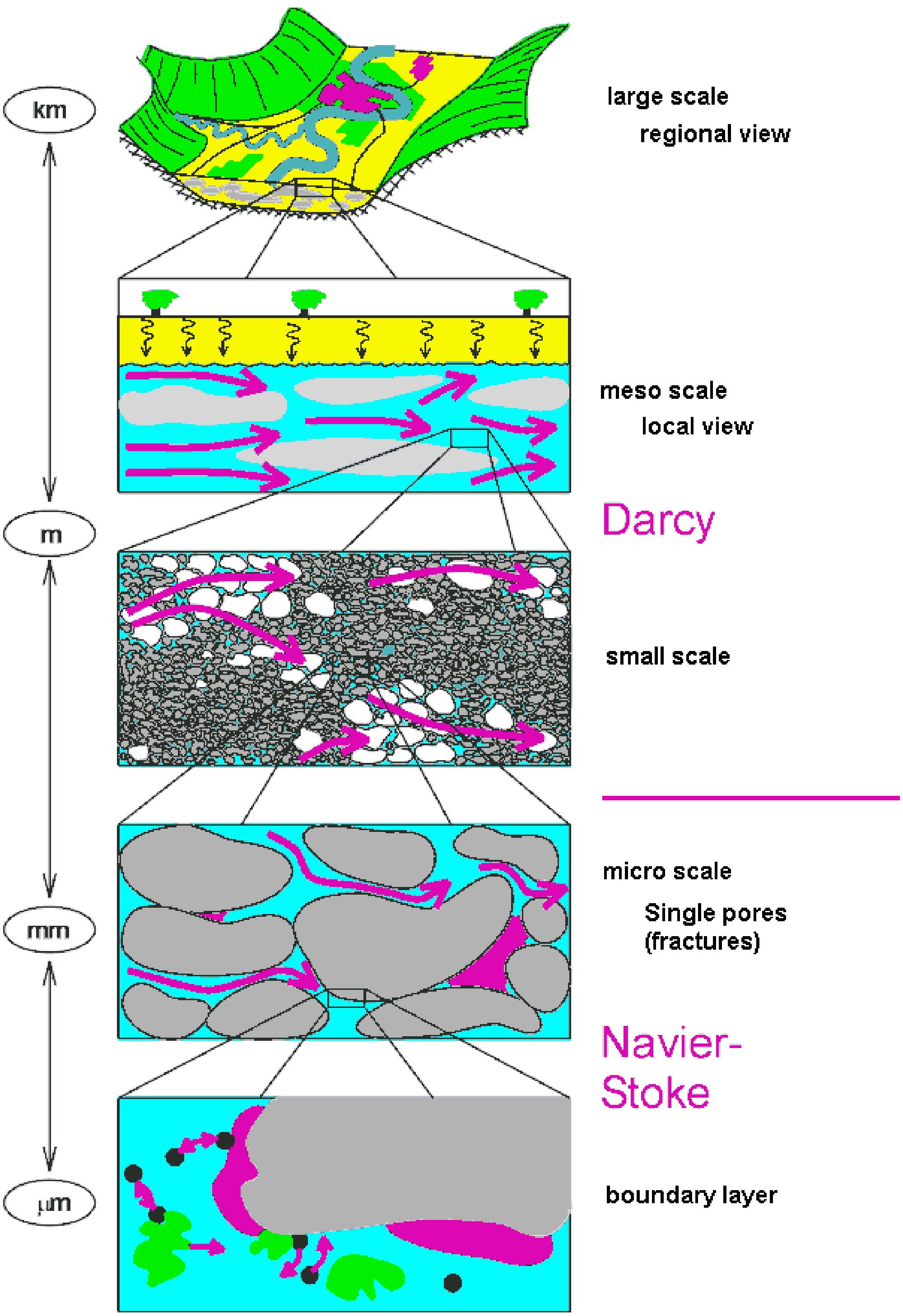


$dh/dl \propto v$ linear relation $\Rightarrow$ linear flow

$dh/dl \propto v^2$ nonlinear relation $\Rightarrow$ turbulent flow

$(v = \sqrt{dh/dl}\,)$

Scale Dependence of Flow Laws



Hydraulic Conductivity - Intrinsic Permeability

- **Hydraulic conductivity (K)**

- **Intrinsic permeability (k)**

  (k charcterizes the medium through which the fluid flows. k is independent of the properties of fluid)

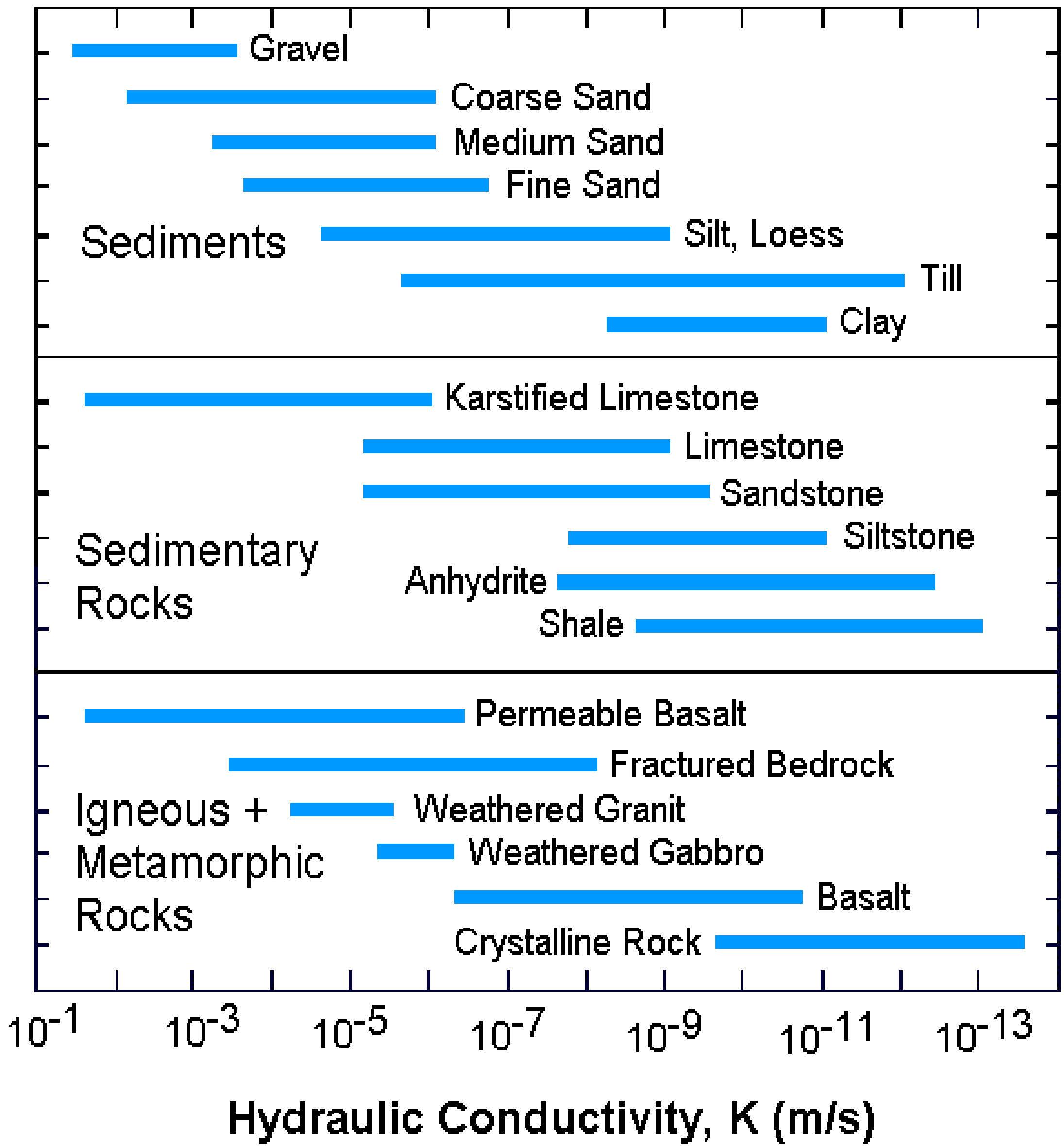
Relation K $\rightarrow$ k

$$K = \frac{k \rho g}{\mu}$$

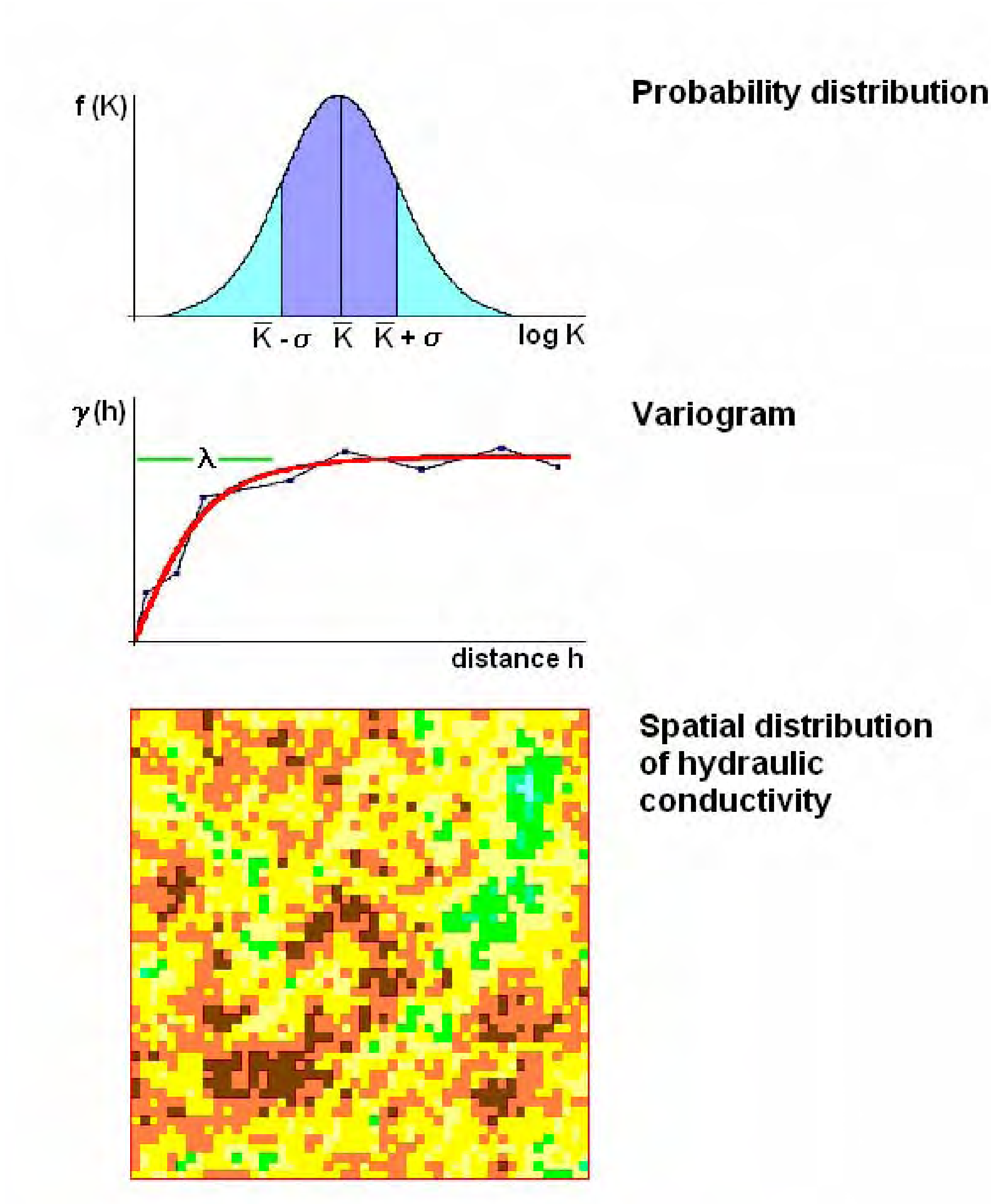
K: hydraulic conductivity (LT^{-1} or $m\ s^{-1}$)
k: intrinsic permeability (L^2 or m^2)
ρ: fluid density (ML^{-3} or $kg\ m^{-3}$)
μ: dynamic viscosity ($ML^{-1}T^{-1}$ or $kg\ m^{-1}s^{-1}$)
g: gravitational acceleration (LT^{-2} or $m\ s^{-2}$)

Note: 1 darcy = 1x 10^{-12} m^2

Hydraulic Conductivity of Different Geological Materials



Spatial Distribution of Hydraulic Conductivity

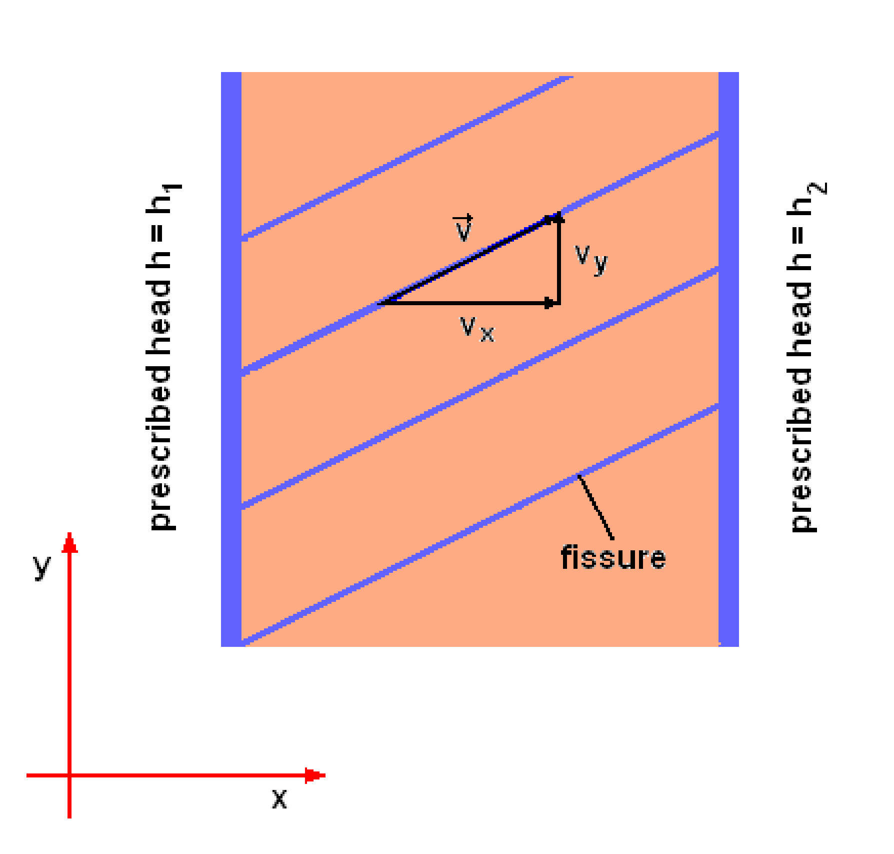


General Form of DARCY'S Law

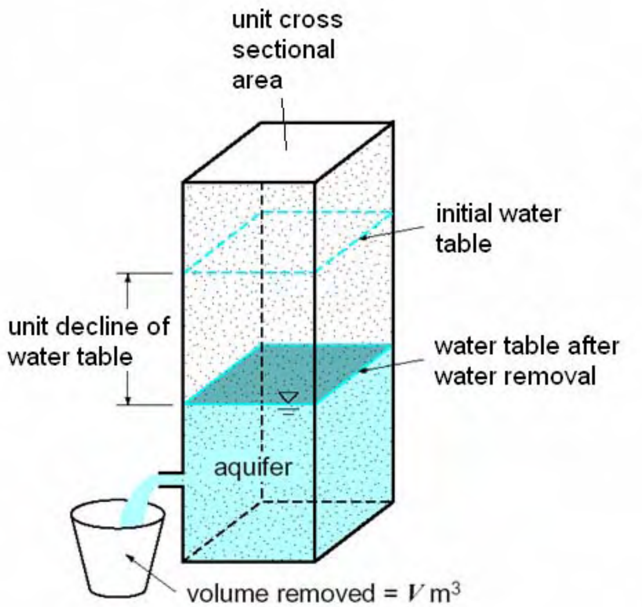
$$\vec{v}_f = \mathbb{K}\,\nabla h, \qquad \vec{v}_f \ \text{ not} \parallel \text{to } \nabla h$$

Anisotropy 2-D

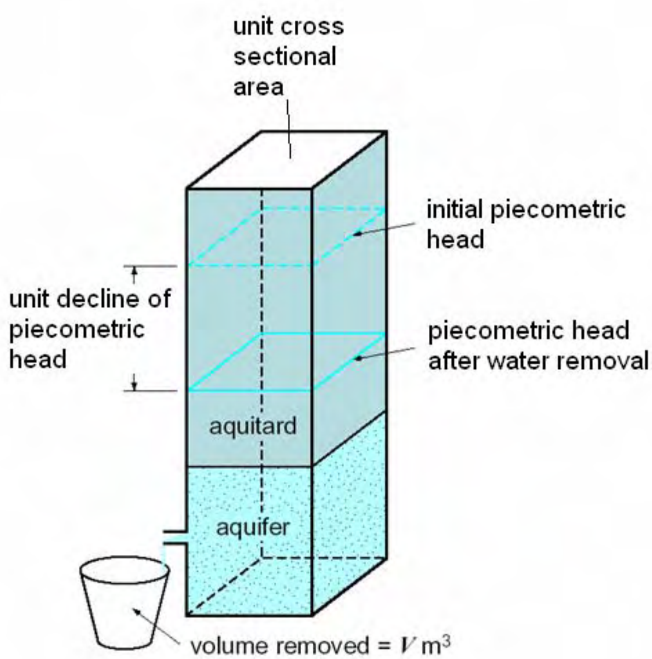
$$T \Rightarrow \ \mathrm{T} = \begin{pmatrix} T_{xx} & T_{xy} \\ T_{yx} & T_{yy} \end{pmatrix} \quad \text{resp } \mathbb{K} \Rightarrow \ \mathbb{K} = \begin{pmatrix} K_{xx} & K_{xy} \\ K_{yx} & K_{yy} \end{pmatrix}$$



Schematic Representation of Aquifer Storativity



Unconfined ("phreatic) Aquifer



Confined Aquifer

Water Storage in an Aquifer

Confined Aquifer

Elastic storage due to compressibility of matrix and water. If water is removed from a confined aquifer, the pressure declines and more weight must be taken by the aquifer framework, causing it to compress slightly and causing a slight expansion of the water. If water is put into the aquifer the pressure increases, the aquifer framework expands and the water is compressed slightly.

Pressure increase Δh in volume element V leads to an increase of stored water volume ΔV:

$$\frac{\Delta V}{V} \propto \Delta h \Rightarrow \frac{\Delta V}{V} = S_0 \Delta h$$

S_0: constant of proportionality => specific storage coefficient (1/m)

Magnitude of S_0: 10^{-2} 1/m clay …, 10^{-7} 1/m hard rocks.

Pressure change related to time Δt:

$$\frac{\Delta V}{V\,\Delta t} = S_0 \frac{\Delta h}{\Delta t} \quad \Rightarrow \quad \frac{Q}{V} = S_0 \frac{dh}{dt}$$

Unconfined Aquifer

Storage due to moving water table

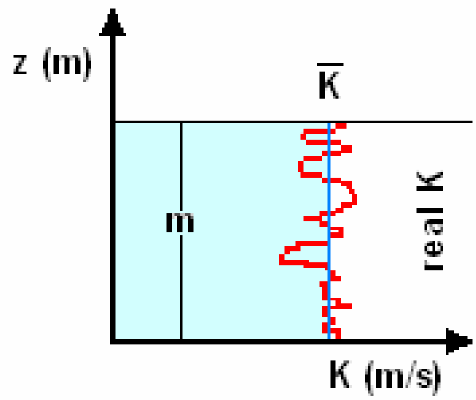
$S_0 = S_y/m$, where S_y: specific yield, m: aquifer thickness
In addition: elastic storage << specific yield

Range of Values of Compressibility

	Compressibility (m^2/N or Pa^{-1})
Clay	$10^{-6} – 10^{-8}$
Sand	$10^{-7} – 10^{-9}$
Gravel	$10^{-8} – 10^{-10}$
Jointed rock	$10^{-8} – 10^{-10}$
Sound rock	$10^{-9} – 10^{-11}$
Water	4.4×10^{-10}

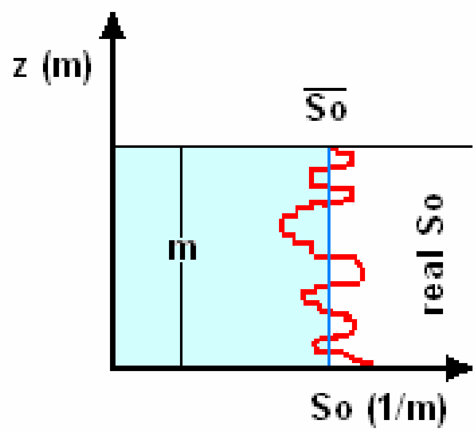
Transmissivity - Storage Coefficient

(Derived terms)



Transmissivity

$$T = \int_0^m K \, dz = \overline{K} \, m \quad (m^2/s)$$

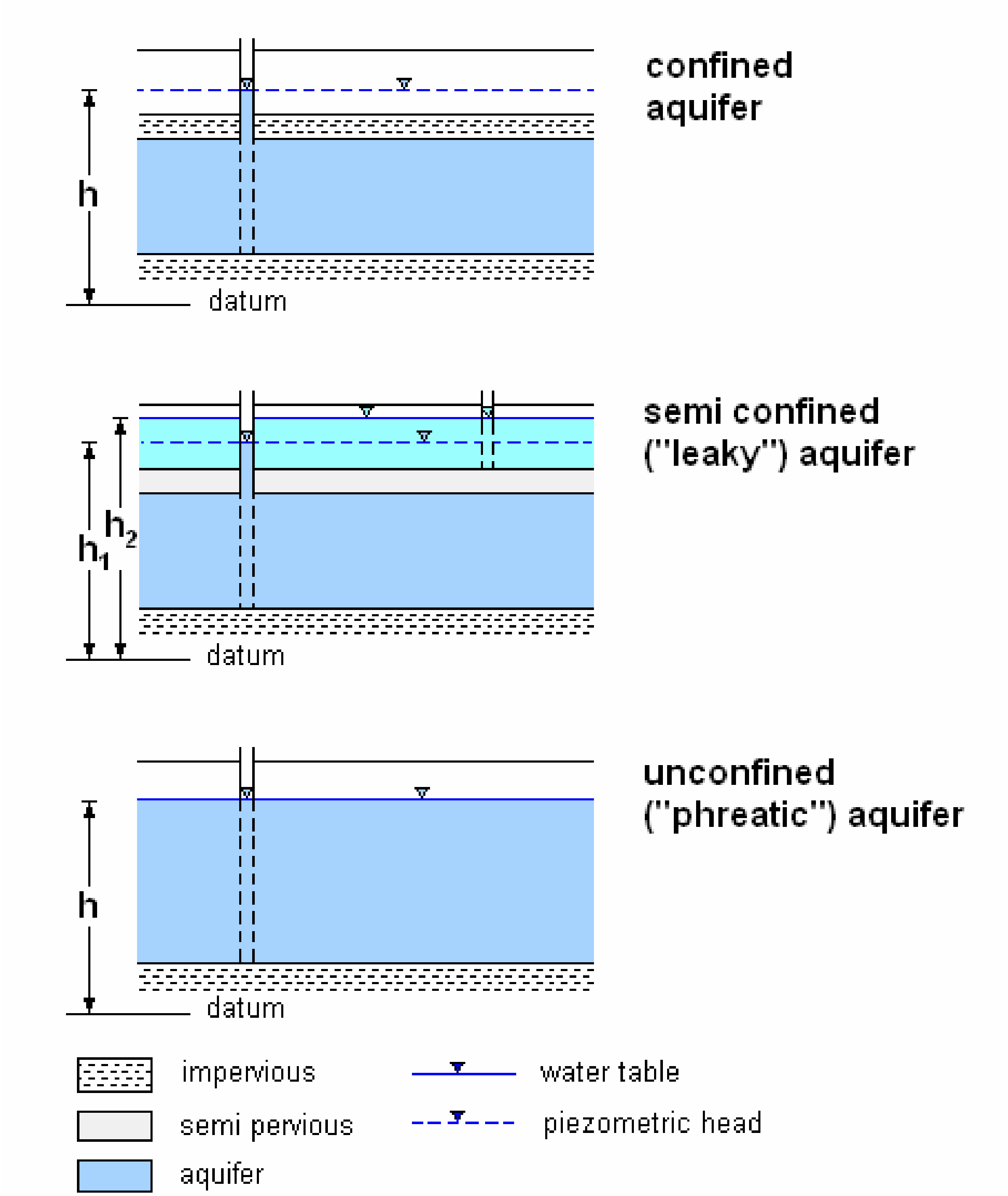


Storage coefficient

$$S = \int_0^m S_0 \, dz = \overline{S}_0 \, m \quad (-)$$

K:	hydraulic conductivity	(L/T)
T:	transmissivity	(L^2/T)
S_0:	specific storage coefficient	(1/L)
S:	storage coefficient	(-)
m:	thickness of aquifer	(L)

Aquifer Types



Basic Flow Equation

(2-D, confined aquifer)

1. Continuity

$$-\frac{\partial}{\partial x}(m\,v_{fx})-\frac{\partial}{\partial y}(m\,v_{fy})+q=S\frac{\partial h}{\partial t}$$

2. DARCY's-law (isotropic)

$$v_{fx}=-K\frac{\partial h}{\partial x}$$

$$v_{fy}=-K\frac{\partial h}{\partial y}$$

$$\text{where } T=K\,m$$

$$\frac{\partial}{\partial x}\left(T\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(T\frac{\partial h}{\partial y}\right)+q=S\frac{\partial h}{\partial t}$$

Partial differential equation of 2nd order

Required for solution: boundary conditions and initial conditions

Solution: h = f (x, y, t)

2-D Flow Equations

Confined aquifer:

$$\nabla(T\nabla h)+q=S\frac{\partial h}{\partial t}$$

Unconfined ("phreatic“) aquifer:

$$\nabla((h-b)K\,\nabla h)+q=S_y\,\frac{\partial h}{\partial t}$$

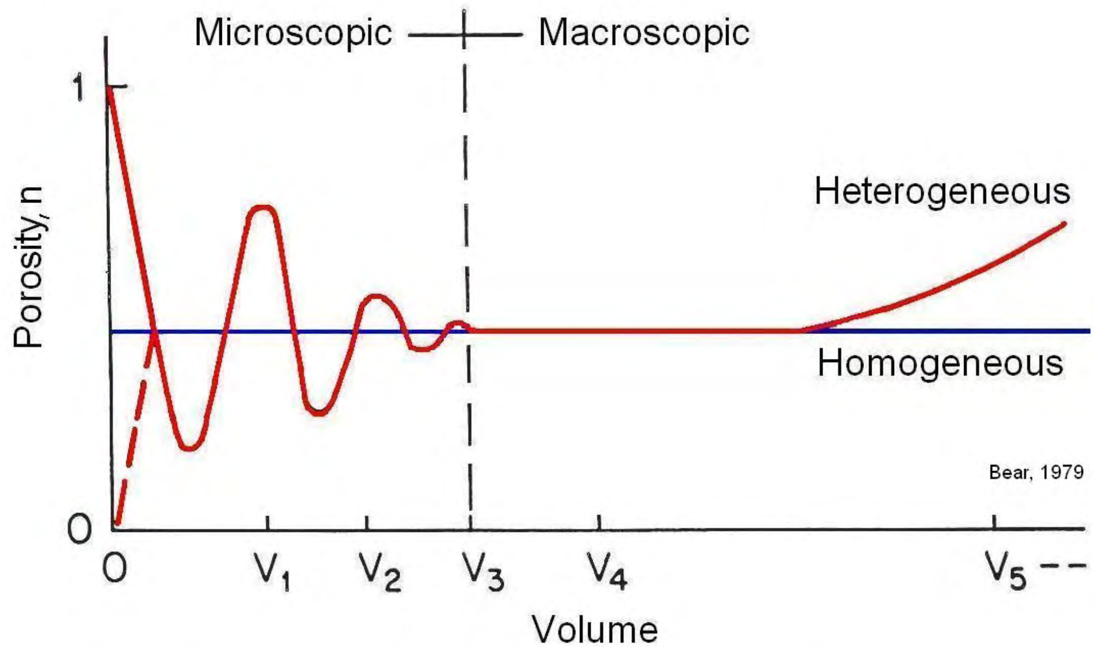
Semiconfined („leaky“) aquifer:

$$\nabla(T\nabla h)+q+l_i(h_i-h)=S\frac{\partial h}{\partial t}$$

where $\nabla=(\partial/\partial x,\ \partial/\partial y)$

Applicability of Flow Equation

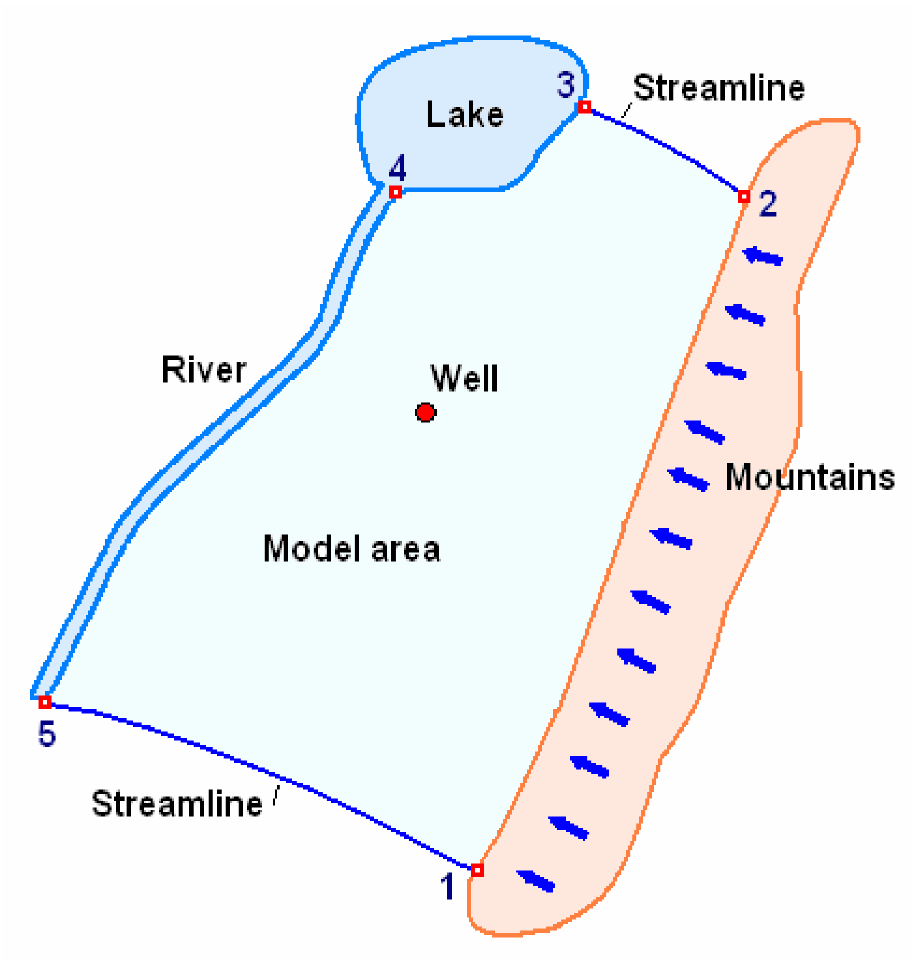
Strictly speaking the groundwater flow equation based on DARCY's law is only valid for porous aquifers.



Microscopic and macroscopic domains and the representative elementary volume V_3

The application for other aquifer types is possible if the Representative Elementary Volume (REV) is smaller than the model domain and the ground-water velocity is within the range of DARCY's law.

Example of Boundary Conditions in a Flow Model



Boundary 1-2: prescribed flux (non zero)
Boundary 2-3: zero flux
Boundary 3-4: prescribed head
Boundary 4-5: semi pervious
Boundary 5-1: zero flux

Boundary Conditions

- **Boundary condition of the first type (DIRICHLET-type)**

  Prescribes the head value $h = f(t)$. Special case $h = \text{const.}$ (fixed head).

- **Boundary condition of the second type (NEUMANN-type)**

  Specifies the boundary flux , i.e. the head gradient normal to the boundary $\partial h/\partial n = f(t)$. A special case is the impervious boundary where the flux is zero.

- **Boundary condition of the third type (CAUCHY-type)**

  Specifies semi pervious boundaries, e.g. leakage from a surface water body. $\alpha h + \beta\, \partial h/\partial n = f(t)$.

- **Boundary condition: Pressure = 0**

  Water table, seepage face.

- **Moving boundaries**

  Falling dry or wetting of parts of the aquifer in case of varying water table.

Note: To guarantee the uniqueness of the solution in case of steady state conditions, it is necessary that in a modeled domain there should be at least one point that constitutes a first or third type boundary.

Initial conditions

- **known head distribution at time t_0**

Solutions of Flow Equation

Analytical solutions

e.g. THEIS-, HANTUSH-, NEUMANN-formula etc.

Assumptions for applicableness:

- Trivial initial and boundary conditions
- Homogeneity
- Isotropy
- Infinite extension etc.

Numerical solutions

Finite-Difference method
Finite-Volume method
Finite-Element method

Assumptions for applicableness:

No restriction in applicableness

Coordinate Transformation: Cartesian to Cylindrical Coordinates

2-D Flow equation in Cartesian coordinates

$$\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2} = \frac{S}{T}\frac{\partial h}{\partial t}$$

Flow equation in cylindrical coordinates

$$\frac{\partial^2 h}{\partial r^2} + \frac{1}{r}\frac{\partial h}{\partial r} = \frac{S}{T}\frac{\partial h}{\partial t}$$

where $r = \sqrt{x^2 + y^2}$

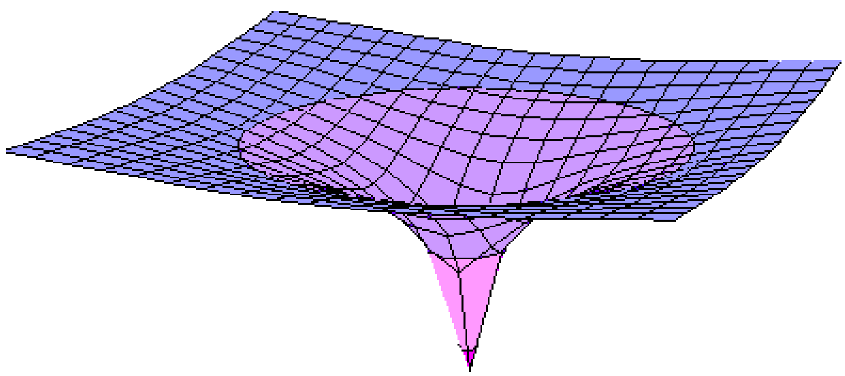
Replace head h by drawdown s.

Inserting s = H- h $\rightarrow$

$$\frac{\partial^2 s}{\partial r^2} + \frac{1}{r}\frac{\partial s}{\partial r} = \frac{S}{T}\frac{\partial s}{\partial t}$$

THEIS – Equation

$$h_0 - h = s = \frac{Q}{4\pi T}\int_u^\infty \frac{e^{-u}}{u}\,du$$



where $u = \dfrac{r^2 S}{4Tt}$

and $\displaystyle\int_u^\infty \frac{e^{-u}}{u}\,du$ is the well function, $W(u)$

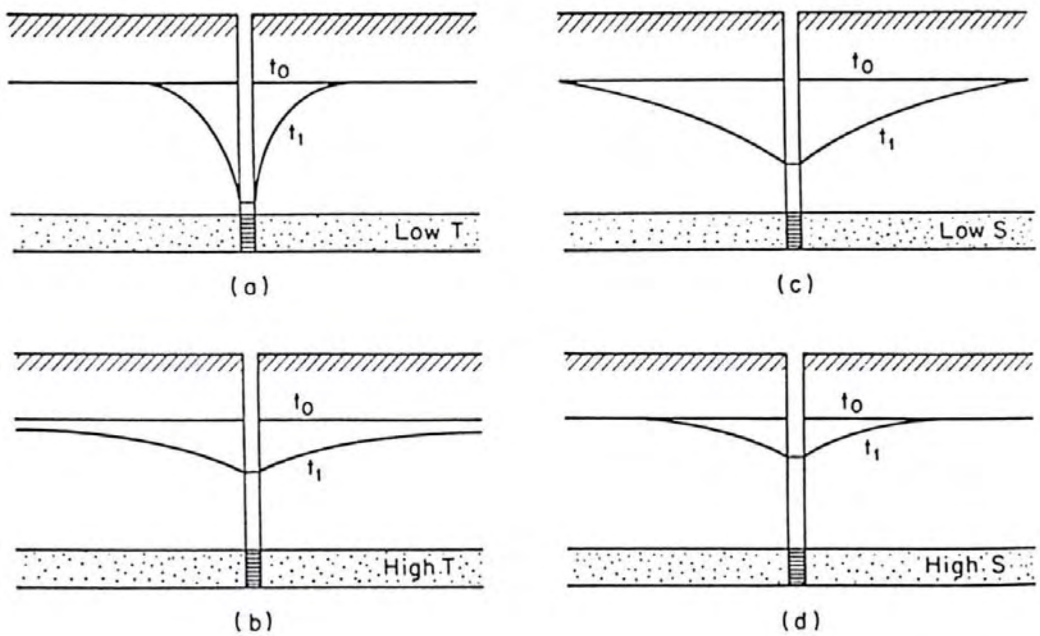
h_0: initial head
h: head
s: drawdown
Q: pumping rate
T: transmissivity
S: storage coefficient
r: radial distance from pumping well

Note: Superposition of solutions is possible!

Comparison of Drawdown Cones at a given Time for different Aquifers

a) low transmissivity **b) high transmissivity**

c) low storativity **d) high storativity**



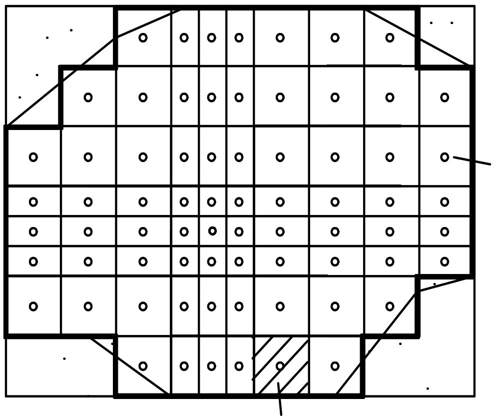
Freeze & Cherry, 1979

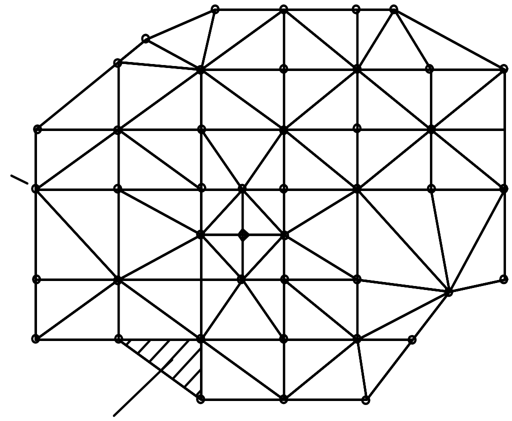
Program-Listing: THEIS.BAS

```
'==========================================================================
'
'                    PROGRAM: THEISE.BAS
'            Analytical computation of drawdown after Theis
'
'==========================================================================

    DECLARE FUNCTION W! (U!)

' input of data and parameters

' aquifer parameters: Transmissivity (m2/s), storage coefficient (-)

    READ TR, SK
    TR = TR * 86400   ' transformation m2/s => m2/d

' maximum pumping time (d), time increment (d)

    READ TM, Dt

' number of wells

    READ NW

' dynamic dimensioning of arrays

    DIM X(NW), Y(NW), Q(NW)

' position, discharge/recharge of wells

    FOR I = 1 TO NW
     READ X(I), Y(I), Q(I)
     Q(I) = Q(I) * 86400          ' transformation m3/s => m3/d
    NEXT I

' observation window: XMin, XMax, Dx, YMin, YMax, Dy

    READ XMin, XMax, Dx, YMin, YMax, Dy

' computation of drawdown

    PI = 4 * ATN(1)               ' PI

' time loop

    FOR TI = Dt TO TM STEP Dt
     CLS
     PRINT "DRAWDOWN (M) AT TIME T ="; TI; " D"
     PRINT

'     loop over Y and X

     FOR Y = YMax TO YMin STEP -Dy
         FOR X = XMin TO XMax STEP Dx

'      loop over wells

          SG = 0
          FOR I = 1 TO NW

'        Theis-function
  R = SQR((X(I) - X) ^ 2 + (Y(I) - Y) ^ 2)
           IF R = 0 THEN R = .01
           U = R * R * SK / (4 * TR * TI)
```

```
            S = Q(I) * W(U) / (4 * PI * TR)
            SG = SG + S
           NEXT I
           PRINT USING "###.## "; SG;
          NEXT X
          PRINT
     NEXT Y
     PRINT
     PRINT "PRESS ANY KEY TO CONTINUE ..."
     A$ = INPUT$(1)
    NEXT TI

END

' ------------------------------ input data ------------------------------

' aquifer parameters: Transmissivity (m2/s), storage coefficient (-)

    DATA 0.01, 0.001

' maximum pumping time (d), time increment (d)

    DATA .01, .0005

' number of wells

    DATA 2

' x-, y-coordinate (m), discharge/recharge wells (m3/s) discharges have a minus sign, recharges a positiv sign

    DATA 30, 50, -.01
    DATA 60, 50,  .01

' observation window: XMin, XMax, Dx, YMin, YMax, Dy (m)

    DATA 0, 90, 10, 0, 100, 10

'===========================================================================
'
FUNCTION W (U)

' computation of W(u)-function by polynomial approximation after Abramowitz & Stegun (1970)

    IF U < 1 THEN
     A0 = -.57721566#
     A1 = .99999193#
     A2 = -.24991055#
     A3 = .05519968#
     A4 = -.00976004#
     A5 = .00107857#
     W = -LOG(U) + A0 + A1 * U + A2 * U * U + A3 * U * U * U + A4 * U * U * U * U + A5 * U * U * U * U * U
    ELSEIF U >= 1 THEN
     A1 = 8.5733287401#
     A2 = 18.059016973#
     A3 = 8.6347608925#
     A4 = .2677737343#
     B1 = 9.5733223454#
     B2 = 25.0329561486#
     B3 = 21.0996530827#
     B4 = 3.9584969228#
     WU = U * U * U * U + A1 * U * U * U + A2 * U * U + A3 * U + A4
     WU = WU / (U * U * U * U + B1 * U * U * U + B2 * U * U + B3 * U + B4)
     W = WU / (U * EXP(U))
    END IF
END FUNCTION
```

Finite Differences   Finite Elements

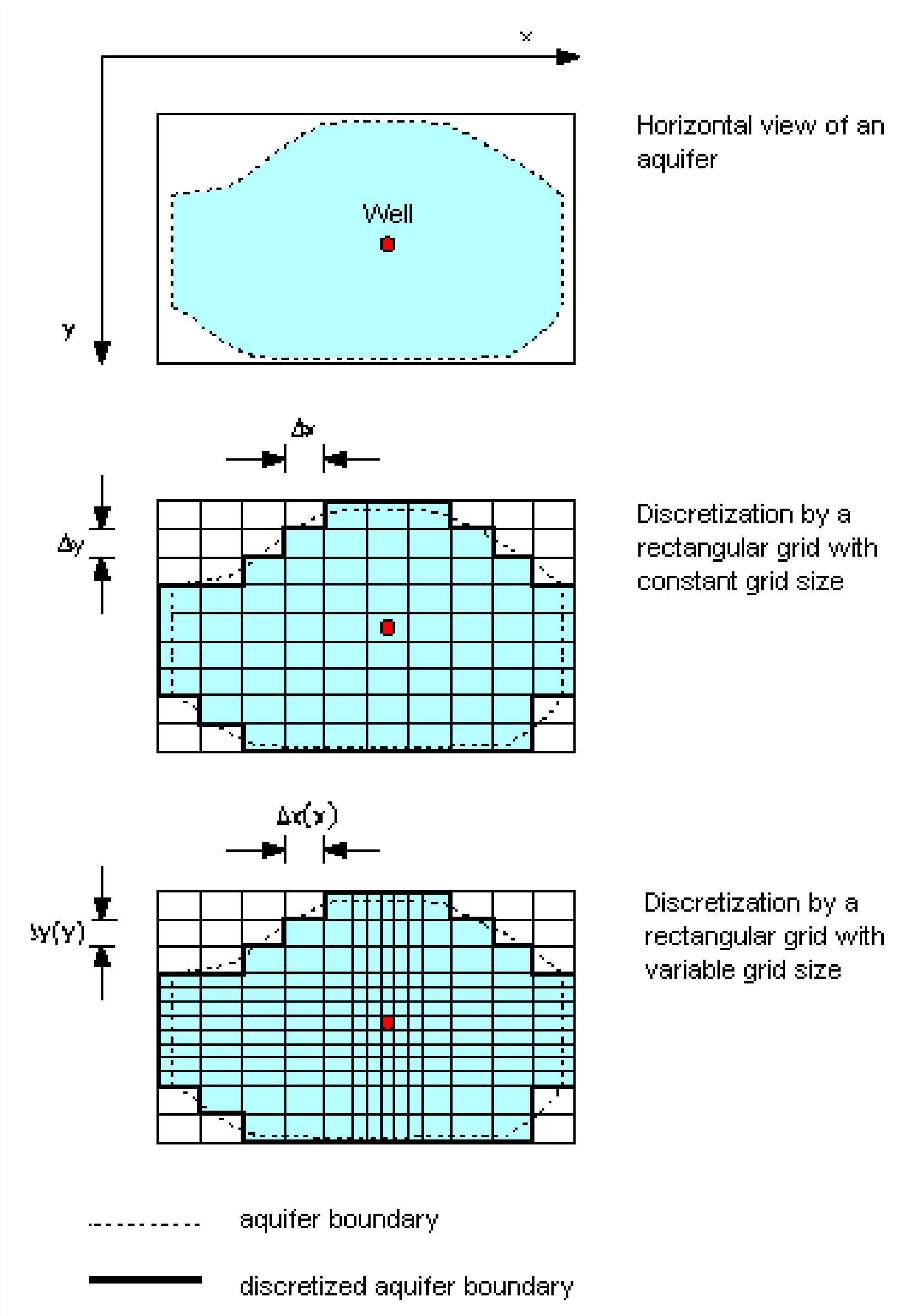




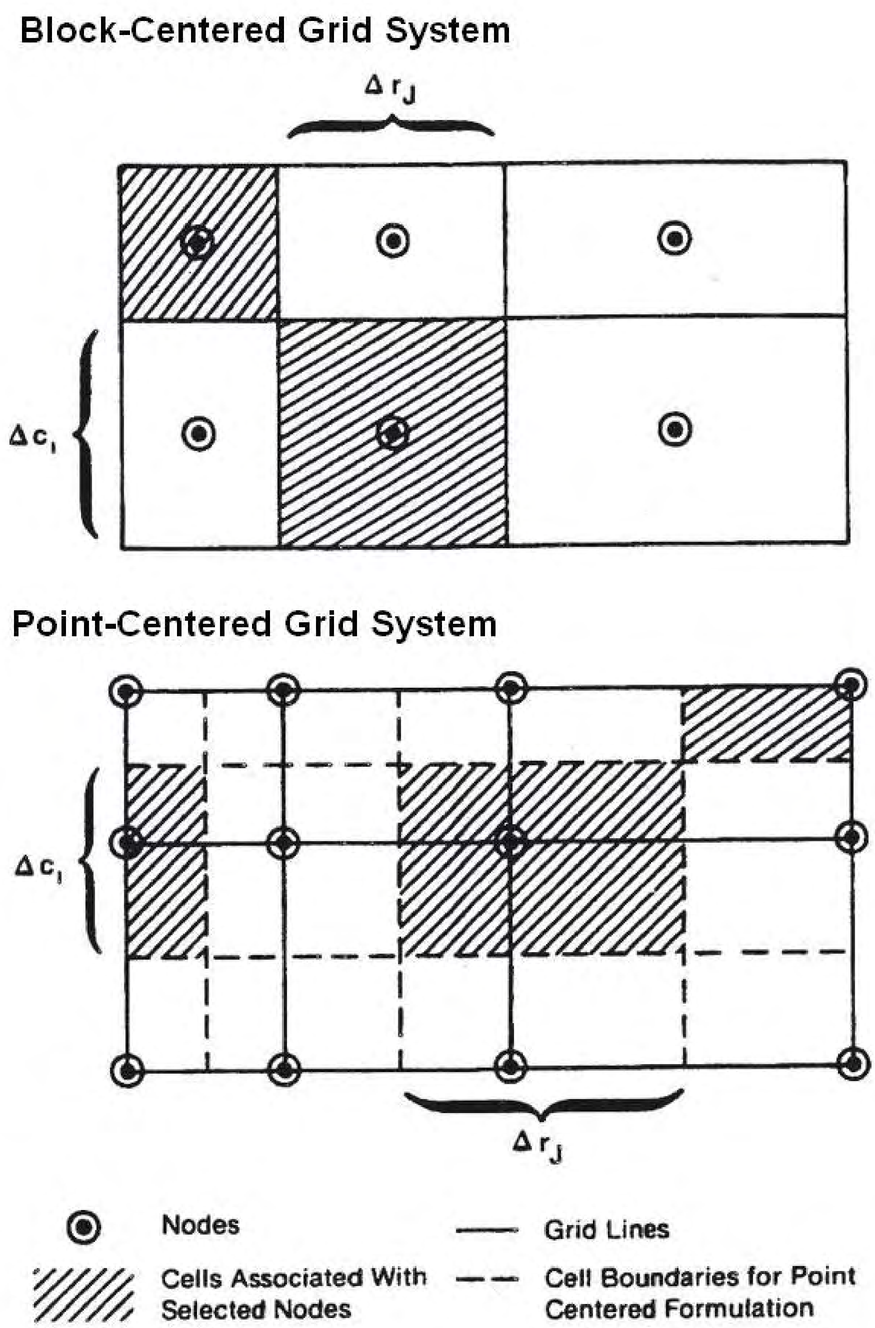
Comparison of Methods

Finite Differences	Finite Elements
Heads are only defined at cell nodes	Heads are defined at any point within an element by an approximate interpolation function
Material properties (conductivity, storage coefficient) are defined cell by cell	Material properties (conductivity, storage coefficient) are defined element by element
Continuity is fulfilled at every node	Continuity is fulfilled for every patch of elements
Velocities are determined from fluxes between adjacent cells	Velocities are determined from derivations of the head distribution and element properties

Discretization: FD-Method



Difference between Block-Centered and Point-Centered Grids



Basic Idea of FD-Method

Step 1:

Calculate the water budget for every cell (node) within the model area. Express the budget as a function of the head (h). h is unknown!

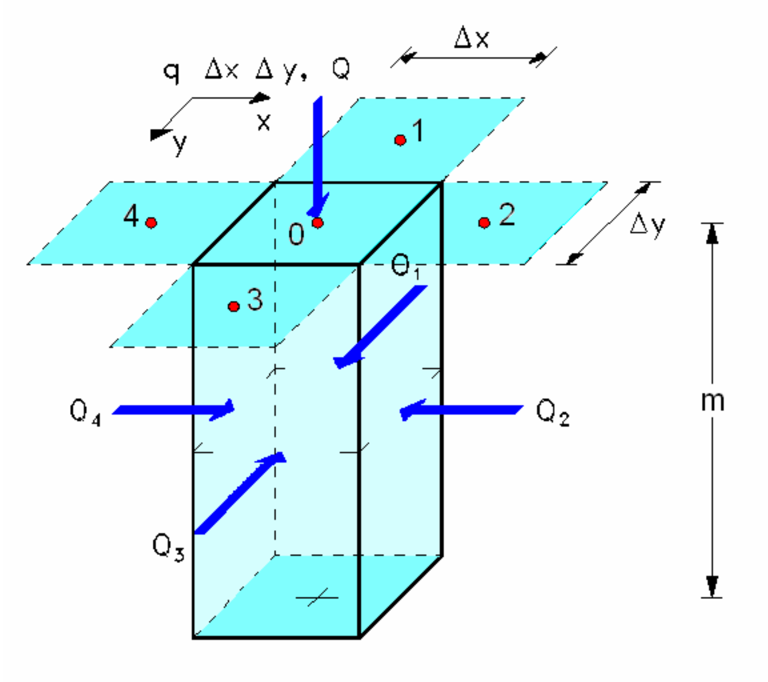
Step 2:

This yields to N = Nx x Ny equations for the estimation of h.

Step 3:

Solve the set of equations for h. The results are the heads as a function of space and time (h = f(x,y,z,t).

Water Balance around one Cell over Time Interval (t, t + Δt)



$$\text{horizontal in}-/\text{ outflows}+\text{vertical in}-/\text{ outflows}=\text{storage}$$

$$\Delta t\,(Q_1+Q_2+Q_3+Q_4+Q+q\,\Delta x\,\Delta y)=(h_0\,(t+\Delta t)-h_0\,(t))\,\Delta x\,\Delta y\,S \qquad (1)$$

using Darcy's law we obtain:

$$Q_1=\Delta x\,T_{10}\,\frac{h_1(t')-h_0\,(t')}{\Delta y},\qquad Q_2=\Delta y\,T_{20}\,\frac{h_2(t')-h_0\,(t')}{\Delta x} \qquad (2)$$

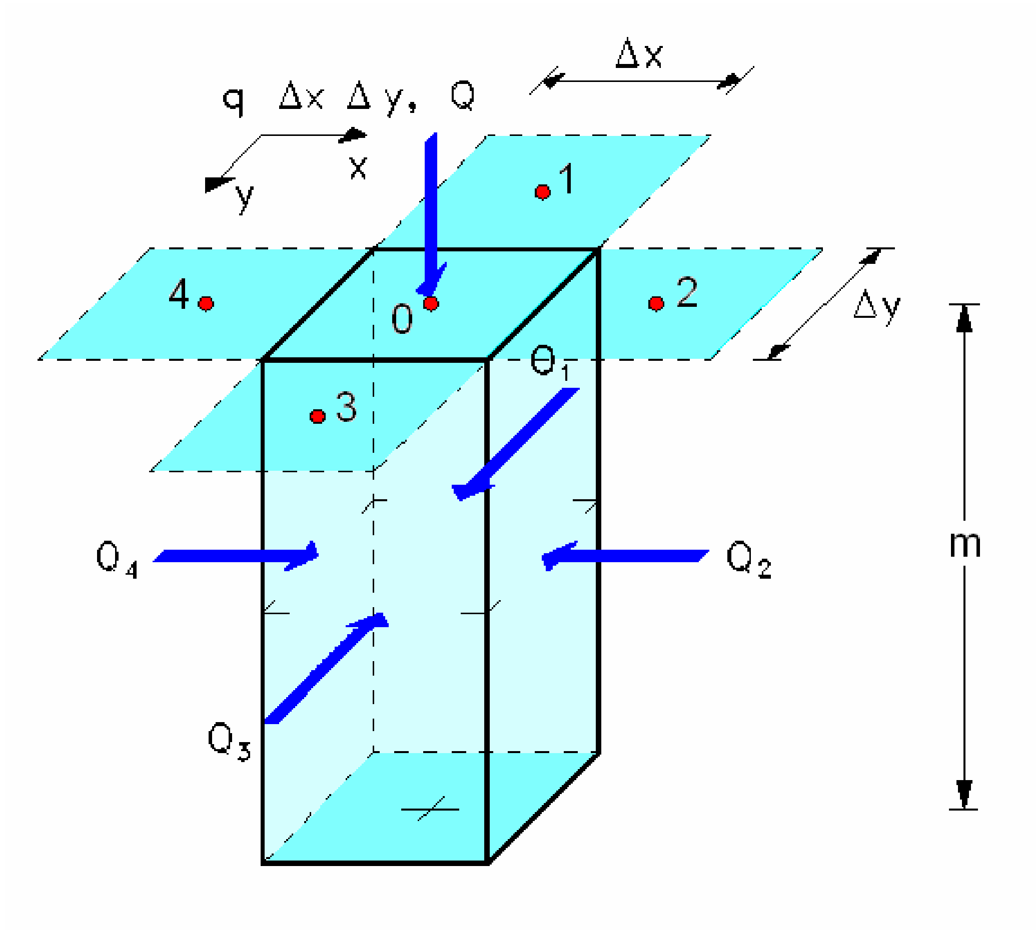
$$Q_3=\Delta x\,T_{30}\,\frac{h_3(t')-h_0\,(t')}{\Delta y},\qquad Q_4=\Delta y\,T_{40}\,\frac{h_4(t')-h_0\,(t')}{\Delta x}$$

inserting (2) in (1) yields:

$$S\,\Delta x\,\Delta y\,(h_0(t+\Delta t)-h_0(t))=T_{10}\Delta x\frac{h_1(t')-h_0\,(t')}{\Delta y}\Delta t+T_{20}\Delta y\frac{h_2(t')-h_0\,(t')}{\Delta x}$$

$$+T_{30}\Delta x\frac{h_3(t')-h_0\,(t')}{\Delta y}\Delta t+T_{40}\Delta y\frac{h_4(t')-h_0\,(t')}{\Delta x}\Delta t+Q\,\Delta t+q\,\Delta x\,\Delta y\,\Delta t$$

Flow from Node 1 to Node 0



$$Q_1 = v_f\ A \quad \text{where } v_f = K\, I \text{ and } A = \Delta x\, m$$

$$I = \frac{h_1(t') - h_0\ (t')}{\Delta y}, \quad T_{10} = K\, m$$

$$Q_1 = T_{10} \Delta x \frac{h_1(t') - h_0(t')}{\Delta y}$$

Hydraulic Conductance

The notation can be simplified by combining grid dimensions and hydraulic conductivity into a single constant, the “hydraulic conductance (CR)” or, more simply the “conductance”.

$$Q_1 = K_{10}\ m\ \Delta x\ \frac{h_1(t') - h_0(t')}{\Delta y}$$

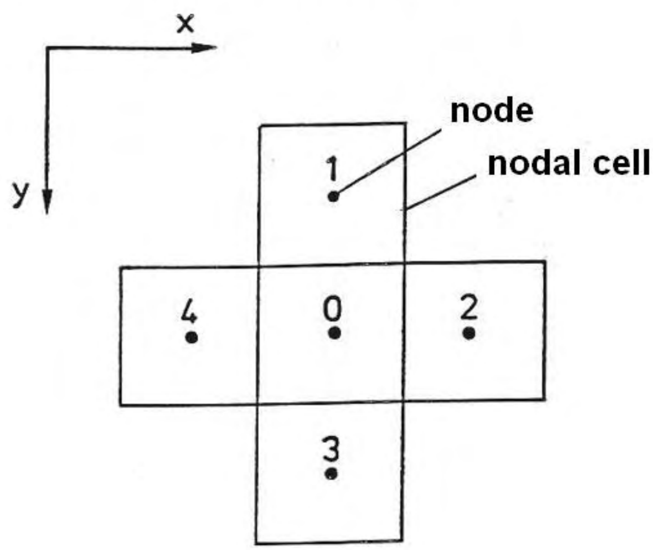
$$CR = \frac{K_{10}\ m\ \Delta x}{\Delta y}$$

$$Q_1 = CR\,(h_1(t') - h_0\ (t'))$$

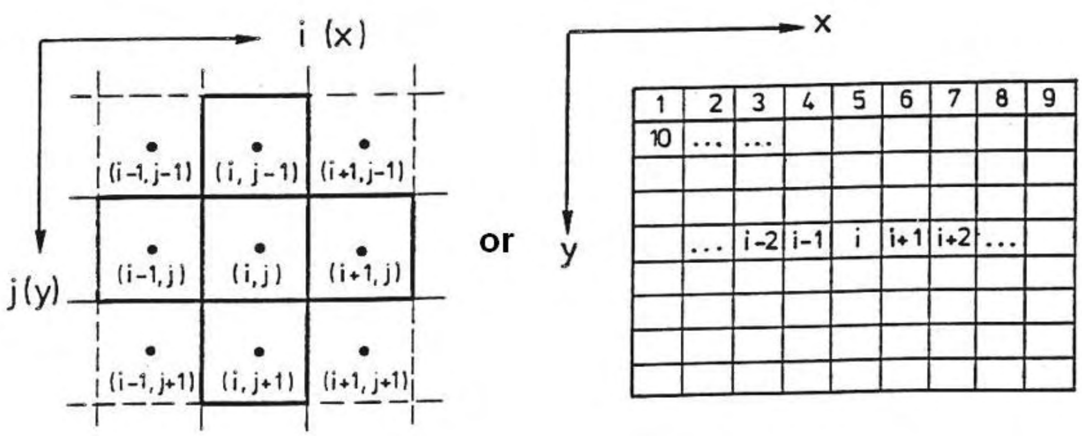
Note: This notation is used in MODFLOW!

Numbering of Nodes

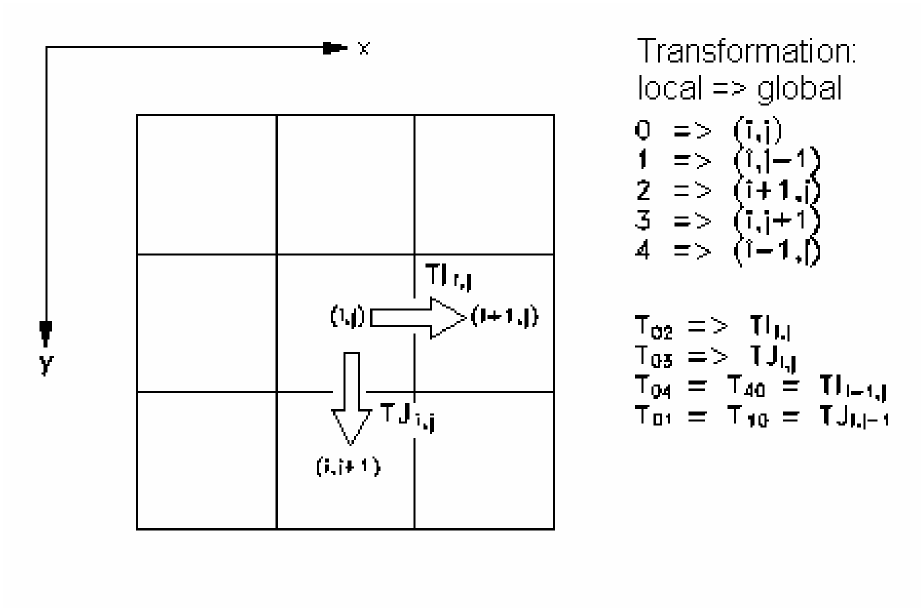
Local nomenclature of nodes



Globale nomenclature of nodes



Internodal Transmissivity Concept



Two possible averaging procedures

- **Arithmetic mean** e.g.

$$T_{10} = \frac{T_1 + T_0}{2}$$

- **Harmonic mean** e.g.

$$T_{10} = \frac{2T_1T_0}{T_1 + T_0}$$

Advantage of harmonic mean: incorporation of impervious boundaries.

Incorporation of anisotropy is simple as long as the coordinate axes are aligned with the principal axes of the transmissivity tensor.

Nodal Equation in Global Indices

$$S_{i,j}\frac{h_{i,j}(t+\Delta t)-h_{i,j}(t)}{\Delta t}=$$

$$\frac{TJ_{i,j-1}}{\Delta y^2}(h_{i,j-1}(t')-h_{i,j}(t'))+\frac{TI_{i,j}}{\Delta x^2}(h_{i+1,j}(t')-h_{i,j}(t'))+$$

$$\frac{TJ_{i,j}}{\Delta y^2}(h_{i,j+1}(t')-h_{i,j}(t'))+\frac{TI_{i-1,j}}{\Delta x^2}(h_{i-1,j}(t')-h_{i,j}(t'))+q_{i,j}$$

$$i=1,\ldots,Nx,\quad j=1,\ldots,Ny$$

Approximation of t'

- Explicit method: t' = t

$$\frac{T}{S}\left(\frac{\Delta t}{\Delta x^2}+\frac{\Delta t}{\Delta y^2}\right)\le\frac{1}{2}\quad !$$

restricted by stability criterion

- Implicit method: t' = t + Δt

- CRANK-NICOLSON-method:

$$h(t')=\frac{1}{2}(h(t)+h(t+\Delta t))$$

Approximation of dh/dt

Explicit method:

$$\left(\frac{\partial h}{\partial t}\right)_{n\,\Delta t} \approx \frac{h_{n+1} - h_n}{\Delta t}$$ forward difference

Implicit method:

$$\left(\frac{\partial h}{\partial t}\right)_{n\,\Delta t} \approx \frac{h_n - h_{n-1}}{\Delta t}$$ backward difference

$$\left(\frac{\partial h}{\partial t}\right)_{n\,\Delta t} \approx \frac{h_{(n+1/2)} - h_{n-1/2}}{\Delta t}$$ Crank–Nicolson

Organization of Program

- **Preprocessing**

  Data input

- **Computation**

  Calibration

  Prognostic simulation

- **Post processing**

  Graphical presentation of results

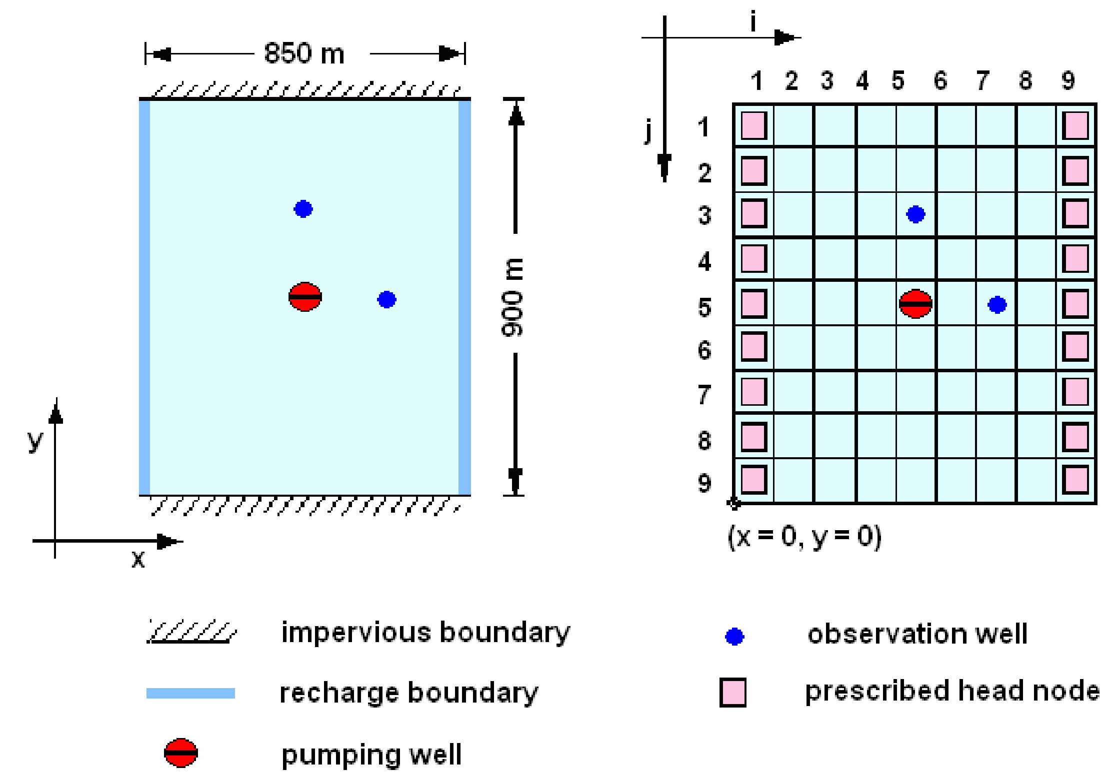
  Contour lines

  Time series plots

  Mass balances

  Pathlines, isochrones, velocity fields

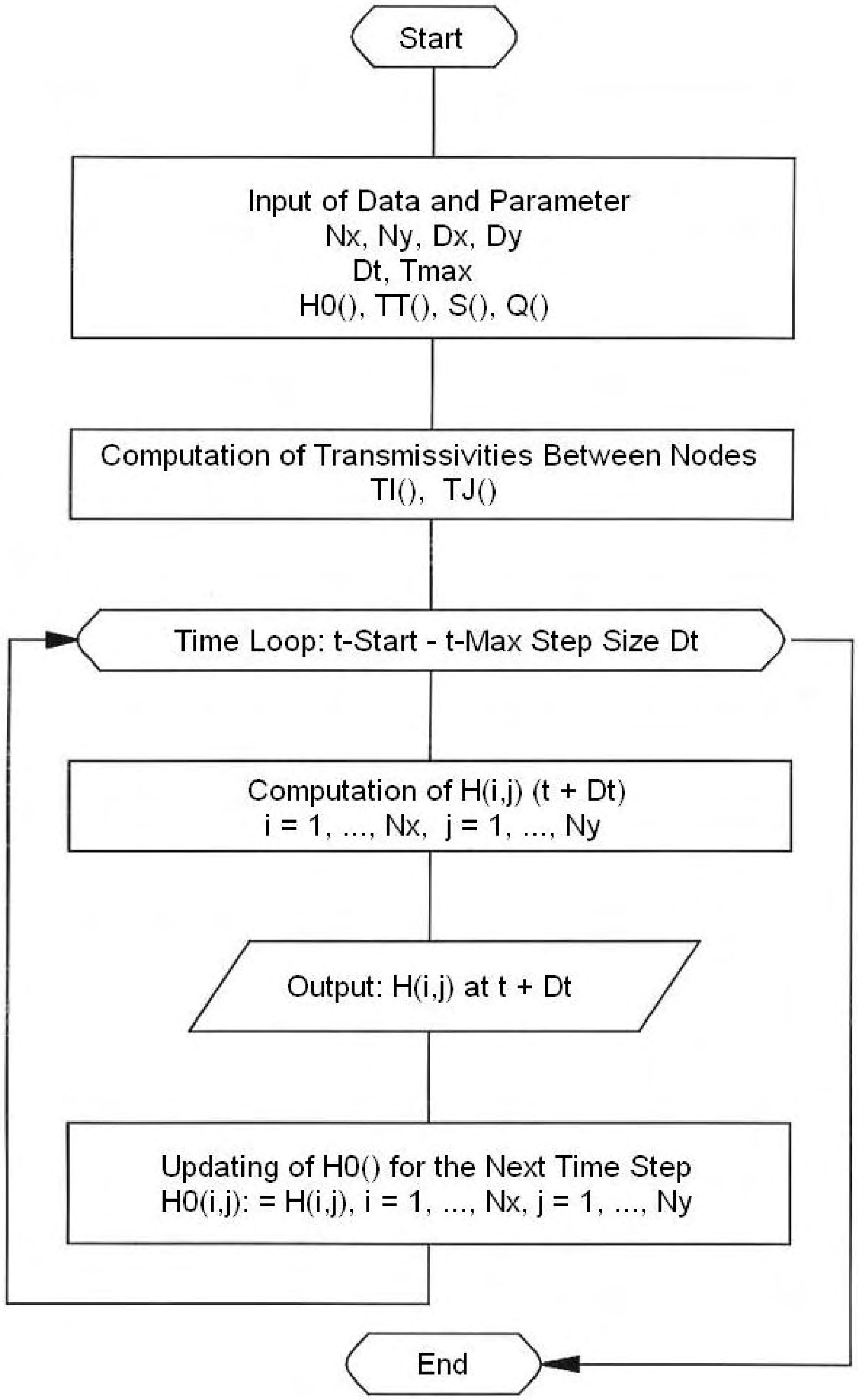
Problem Description: Explicit / Implicit Solution



Input data and parameters:

- Difference-grid: Nx = Ny = 9, $\Delta x = \Delta y = 100$ m
- Transmissivity T = 0.01 m^2/s
- Storage coefficient S = 0.0001
- Thickness of aquifer m = 20 m
- Discharge rate Q = - 0.1 m^3/s
- Initial heads at time t_0: h = 50 m
- Time parameters: Δt = 10 s, T-Max = 300 s

Flowchart for Explicit Solution



Program-Listing: EXPLICIT.BAS

```
================================================================================
'
'                            PROGRAM: EXPLICIT.BAS
'
'                      Programming language: MS-DOS-QBasic
'
'================================================================================

      DEFINT I-J, N

' Input of parameters and data. Values are read from data statements.

' Grid parameters

      READ Nx                  ' number of cells in x-direction
      READ Ny                  ' number of cells in y-direction
      READ Dx                  ' grid distance in x-direction
      READ Dy                  ' grid distance in y-direction

' Dimensioning of arrays. Note the index variables in BASIC arrays start from 0.
' Arrays TT, TI, TJ and H0 are thus dimensioned larger than the aquifer grid by
' two elements both in x- and y-direction. By this technique no special treatment
' need be given to nodal equations in which elements of those arrays with indices
' i = 0, j = 0, i = Nx+1, or j = Ny+1 appear. Their contribution will always be zero.

      OPTION BASE 0

      DIM TT(Nx + 1, Ny + 1)   ' local transmissivities
      DIM TI(Nx + 1, Ny + 1)   ' internodal transmissivities between nodes in x-direction
      DIM TJ(Nx + 1, Ny + 1)   ' internodal transmissivities between nodes in y-direction
      DIM H0(Nx + 1, Ny + 1)   ' initial heads at time t0
      DIM H(Nx, Ny)            ' heads at time t
      DIM S(Nx, Ny)            ' storage coefficients
      DIM Q(Nx, Ny)            ' recharges/discharges

' Time parameters

      READ Dt                  ' time increment
      READ Tmax                ' maximum time

' Initial heads

      FOR J = 1 TO Ny
       FOR I = 1 TO Nx
        READ H0(I, J)
       NEXT I
      NEXT J

' Local transmissivities

      FOR J = 1 TO Ny
       FOR I = 1 TO Nx
        READ TT(I, J)
       NEXT I
      NEXT J

' Storage coefficients

      FOR J = 1 TO Ny
       FOR I = 1 TO Nx
        READ S(I, J)
       NEXT I
      NEXT J

' Recharges/discharges
```

```
      FOR J = 1 TO Ny
       FOR I = 1 TO Nx
        READ Q(I, J)
       NEXT I
      NEXT J

' Calculating of internodal transmissivities from local transmissivities.
' By providing zero edges around matrix TT directional transmissivities
' TI(Nx,j) and TJ(i,Ny) automatically become zero. TI(0,j) and TJ(i,0)
' are zero as all variables in BASIC are initialized with 0.

      FOR J = 1 TO Ny
       FOR I = 1 TO Nx
        IF TT(I, J) + TT(I + 1, J) <> 0 THEN
         TI(I, J) = 2 * TT(I, J) * TT(I + 1, J) / (TT(I, J) + TT(I + 1, J))
        END IF
        IF TT(I, J) + TT(I, J + 1) <> 0 THEN
         TJ(I, J) = 2 * TT(I, J) * TT(I, J + 1) / (TT(I, J) + TT(I, J + 1))
        END IF
       NEXT I
      NEXT J

' Time loop

      Tstart = Dt

      FOR T = Tstart TO Tmax STEP Dt

' Computation and display of head distribution at time T

       CLS
       PRINT "HEAD DISTRIBUTION [M] AT TIME T ="; T; " S"
       PRINT

' Computation of heads H(I,J) at time T + Dt

       FOR J = 1 TO Ny
        FOR I = 1 TO Nx
         IF S(I, J) > 1 THEN
          H(I, J) = H0(I, J)
         ELSE
          T1 = TJ(I, J - 1) * (H0(I, J - 1) - H0(I, J)) / Dy / Dy
          T2 = TI(I, J) * (H0(I + 1, J) - H0(I, J)) / Dx / Dx
          T3 = TJ(I, J) * (H0(I, J + 1) - H0(I, J)) / Dy / Dy
          T4 = TI(I - 1, J) * (H0(I - 1, J) - H0(I, J)) / Dx / Dx
          H(I, J) = H0(I, J) + Dt / S(I, J) * (T1 + T2 + T3 + T4 + Q(I, J) / Dx / Dy)
         END IF
         PRINT USING "###.##  "; H(I, J);
        NEXT I
        PRINT
       NEXT J

' Updating of H0 for the next time step

       FOR J = 1 TO Ny
        FOR I = 1 TO Nx
         H0(I, J) = H(I, J)
        NEXT I
       NEXT J

' In the program re(dis)charges and boundary conditions are set at time
' t=0 and remain unchanged up to time TM. If they are time varying their
' actual values should be read in here in each time step in which their
' size changes.

       PRINT
       PRINT "PRESS ANY KEY TO CONTINUE ..."
       A$ = INPUT$(1)

      NEXT T
```

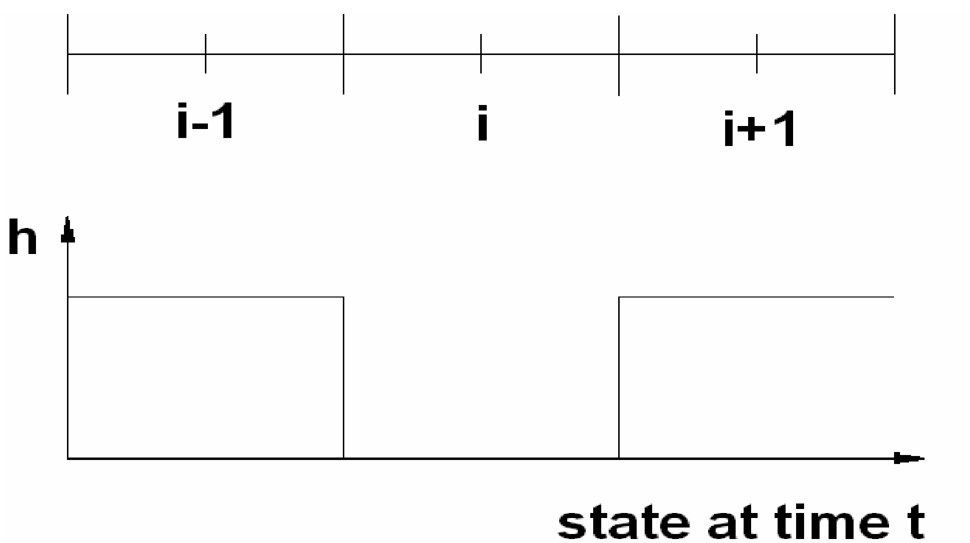
```
      PRINT
      PRINT "TIME T-MAX REACHED!"

END

'----------------------------  Input data   ------------------------------

' Number of nodes in x- and y-direction: Nx, Ny

      DATA  9, 9

' Grid distances in x- and y-direction: Dx, Dy (m)

      DATA 100,100

' Time parameters: Time increment Dt, maximum time Tmax (s)

      DATA  10, 300

' Matrix of initial heads: H0() (m)

      DATA   50, 50, 50, 50, 50, 50, 50, 50, 50
      DATA   50, 50, 50, 50, 50, 50, 50, 50, 50
      DATA   50, 50, 50, 50, 50, 50, 50, 50, 50
      DATA   50, 50, 50, 50, 50, 50, 50, 50, 50
      DATA   50, 50, 50, 50, 50, 50, 50, 50, 50
      DATA   50, 50, 50, 50, 50, 50, 50, 50, 50
      DATA   50, 50, 50, 50, 50, 50, 50, 50, 50
      DATA   50, 50, 50, 50, 50, 50, 50, 50, 50
      DATA   50, 50, 50, 50, 50, 50, 50, 50, 50

' Matrix of local transmissivities: TT() (m2/s)

      DATA  .01, .01, .01, .01, .01, .01, .01, .01, .01
      DATA  .01, .01, .01, .01, .01, .01, .01, .01, .01
      DATA  .01, .01, .01, .01, .01, .01, .01, .01, .01
      DATA  .01, .01, .01, .01, .01, .01, .01, .01, .01
      DATA  .01, .01, .01, .01, .01, .01, .01, .01, .01
      DATA  .01, .01, .01, .01, .01, .01, .01, .01, .01
      DATA  .01, .01, .01, .01, .01, .01, .01, .01, .01
      DATA  .01, .01, .01, .01, .01, .01, .01, .01, .01
      DATA  .01, .01, .01, .01, .01, .01, .01, .01, .01

' Matrix of storage coefficients: S() (-)

' Prescribed-potential boundary nodes are assigned arbitrary S-values
' larger than 1. Nodes that are outside the modelled aquifer are assigned
' storage coefficients S(i,j) = 0. At all other nodes S must be larger than
' 0 in the explicit solution procedure.

      DATA  2, 1E-4, 1E-4, 1E-4, 1E-4, 1E-4, 1E-4, 1E-4, 2
      DATA  2, 1E-4, 1E-4, 1E-4, 1E-4, 1E-4, 1E-4, 1E-4, 2
      DATA  2, 1E-4, 1E-4, 1E-4, 1E-4, 1E-4, 1E-4, 1E-4, 2
      DATA  2, 1E-4, 1E-4, 1E-4, 1E-4, 1E-4, 1E-4, 1E-4, 2
      DATA  2, 1E-4, 1E-4, 1E-4, 1E-4, 1E-4, 1E-4, 1E-4, 2
      DATA  2, 1E-4, 1E-4, 1E-4, 1E-4, 1E-4, 1E-4, 1E-4, 2
      DATA  2, 1E-4, 1E-4, 1E-4, 1E-4, 1E-4, 1E-4, 1E-4, 2
      DATA  2, 1E-4, 1E-4, 1E-4, 1E-4, 1E-4, 1E-4, 1E-4, 2
      DATA  2, 1E-4, 1E-4, 1E-4, 1E-4, 1E-4, 1E-4, 1E-4, 2

' Matrix of recharges (+)/discharges (-): Q() (m3/s)

      DATA  0,  0,  0,  0,  0,  0,  0, 0, 0
      DATA  0,  0,  0,  0,  0,  0,  0, 0, 0
      DATA  0,  0,  0,  0,  0,  0,  0, 0, 0
      DATA  0,  0,  0,  0,  0,  0,  0, 0, 0
      DATA  0,  0,  0,  0,-.1,  0,  0, 0, 0
      DATA  0,  0,  0,  0,  0,  0,  0, 0, 0
      DATA  0,  0,  0,  0,  0,  0,  0, 0, 0
      DATA  0,  0,  0,  0,  0,  0,  0, 0, 0
      DATA  0,  0,  0,  0,  0,  0,  0, 0, 0
```

Stability Criterion for Explicit Method

v. NEUMANN-criterion

$$\frac{T}{S}\left(\frac{\Delta t}{\Delta x^2}+\frac{\Delta t}{\Delta y^2}\right)\leq\frac{1}{2}$$

for explanation: 1-D-aquifer



Condition for length of time interval Δt:

$$h_i(t+\Delta t)\leq h_{i\pm1}(t)$$

("water can not flow uphill!")

Equation Systems

Explicit:

$$h_{i,j}(t+\Delta t) = f\,(h_{i-1,j}(t), (h_{i+1,j}(t), h_{i,j-1}(t), (h_{i,j+1}(t), h_{i,j}(t))$$

$$\text{for } i = 1, ..., Nx, \quad j = 1, ..., Ny$$

Implicit:

$$h_{i-1,j}(t+\Delta t)\,A_{i,j} + h_{i,j-1}(t+\Delta t)B_{i,j} + h_{i,j}(t+\Delta t)\,C_{i,j} + h_{i+1,j}(t+\Delta t)D_{i,j}$$
$$+ h_{i,j+1}(t+\Delta t)E_{i,j} = F_{i,j}(t)$$

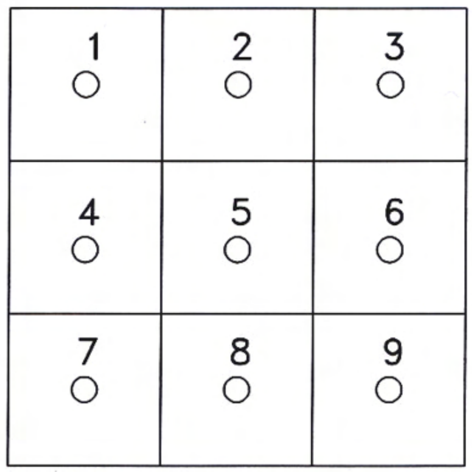
$$\text{or} : (i,j) \Rightarrow k = (j-1)\,Nx + i \qquad \text{for } i = 1, ..., N$$

$$\sum_{i=1}^{N} a_{k,l}\,h_l\,(t+\Delta t) = b_k \qquad \text{where } N = Nx\,Ny$$

$$\begin{array}{l} a_{11}h_1 + a_{12}h_2 + ... + a_{1N}h_N = b_1 \\ a_{21}h_1 + a_{22}h_2 + ... + a_{2N}h_N = b_2 \\ .... \quad .... \quad .... \quad .... \\ a_{N1}h_1 + a_{N2}h_2 + ... + a_{NN}h_N = b_N \end{array}$$

Solution of Flow Equation

Example: Model grid with 3 x 3 = 9 nodes

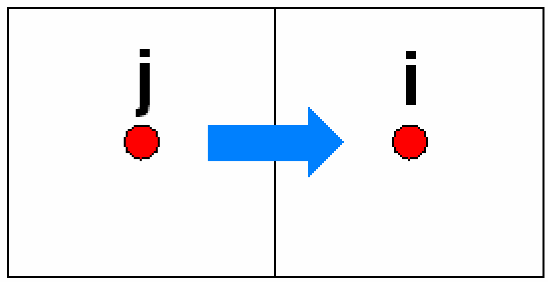


$$\sum_{i=1}^{n} a_{kl} \, h_l \, (t+\Delta t) = b_k \quad \text{where } n = Nx \times Ny$$

$$(a_{kl}) = \begin{bmatrix} x & x & 0 & x & 0 & 0 & 0 & 0 & 0 \\ x & x & x & 0 & x & 0 & 0 & 0 & 0 \\ 0 & x & x & 0 & 0 & x & 0 & 0 & 0 \\ x & 0 & 0 & x & x & 0 & x & 0 & 0 \\ 0 & x & 0 & x & x & x & 0 & x & 0 \\ 0 & 0 & x & 0 & x & x & 0 & 0 & x \\ 0 & 0 & 0 & x & 0 & 0 & x & x & 0 \\ 0 & 0 & 0 & 0 & x & 0 & x & x & x \\ 0 & 0 & 0 & 0 & 0 & x & 0 & x & x \end{bmatrix}$$

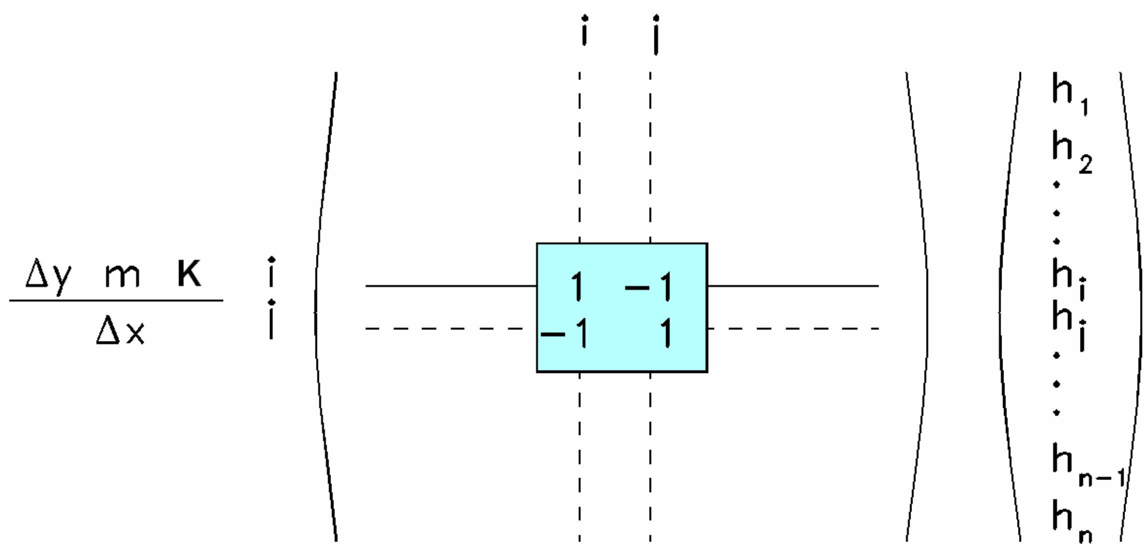
The coefficient matrix (a_{kl}) is a sparse matrix with a banded structure. The matrix is symmetric ($a_{kl} = a_{lk}$). Max. 5 coefficients $\neq 0$ in every row.

Form of System Matrix



$$\text{Darcy flux} = -\Delta y\, m\, \frac{h_j - h_i}{\Delta x} K = h_i\left(\frac{\Delta y\, T}{\Delta x}\right) - h_j\left(\frac{\Delta y\, T}{\Delta x}\right)$$

Symmetric matrix!



Solution Methods for Linear Equations

- **Direct solvers**

  GAUß-JORDAN

  LDU decomposition (e.g. CROUT-method)

  in case of symmetric matrices: CHOLESKY-method

  in case of tridiagonal matrices: THOMAS algorithm

- **Iterative solvers**

  point iteration: GAUß-SEIDEL + SOR (over relaxation)

  block iteration: IADI (Iterative Alternating Direction Implicit procedure)

  SIP: Strongly Implicit Procedure

  SOR: Slice Successive Over Relaxation

  PCG (Preconditioned Conjugate Gradient method)

  multi grid method

- **Additions for sparse matrices**

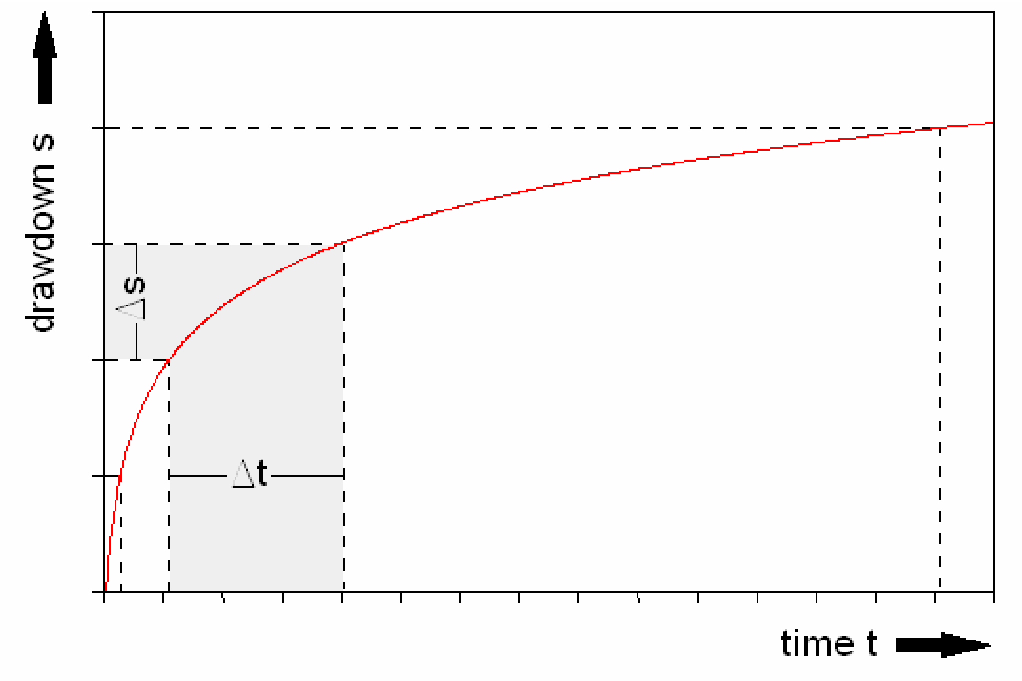
  use of band structure

  pointer vector or pointer matrix (skyline solver)

  frontal solver in combination with direct solvers

  compression of equation system

Selection of Time Steps



ISTEP	**Time**
1	**Δt**
2	**Δt + Δt x 1.2**
3	**Δt + Δt x 1.2 + (Δt x 1.2) x 1.2**
.	**.**
ISTEP	**$\Delta t\ (1 + 1.2^{1} + \ldots + 1.2^{(ISTEP-1)})$**
.	**.**
NSTEPS	**$\Delta t\ (1 + 1.2^{1} + 1.2^{2} + \ldots. + 1.2^{(NSTEPS-1)})$**

ISTEP: time increment number

NSTEPS: total number of time increments in simulation

Δt: initial time increment

Steady State: dh/dt = 0

2 Approaches

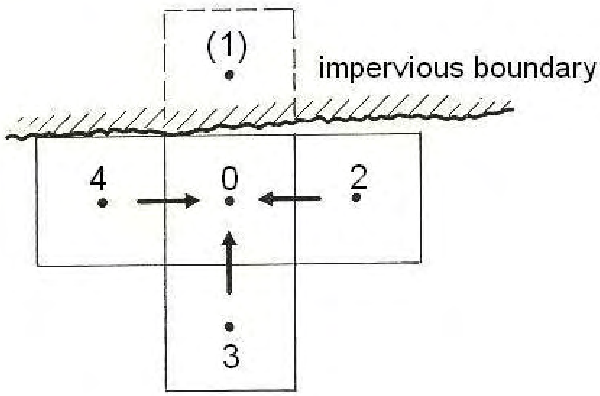
- Input of steady state boundary conditions as well as steady state in- and outflows. Perform computation over a long time until steady state conditions are reached.

- Elimination of storage term:

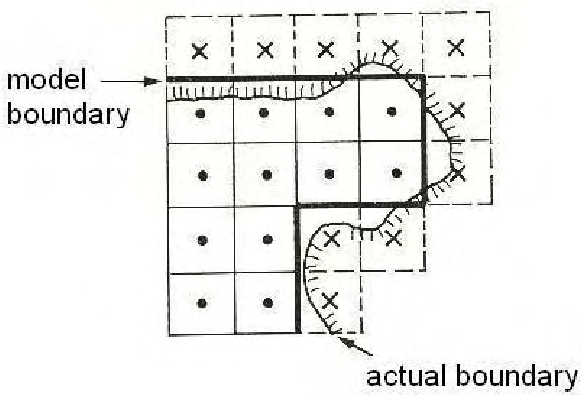
$$S_{i,j} \frac{h_{i,j}(t+\Delta t) - h_{i,j}(t)}{\Delta t}$$

Select either S = 0 or large time increment Δt. The unknowns of the equation system are now the heads $h_{i,j}$ (t + Δt). That means that only the implicit solution scheme can be used.

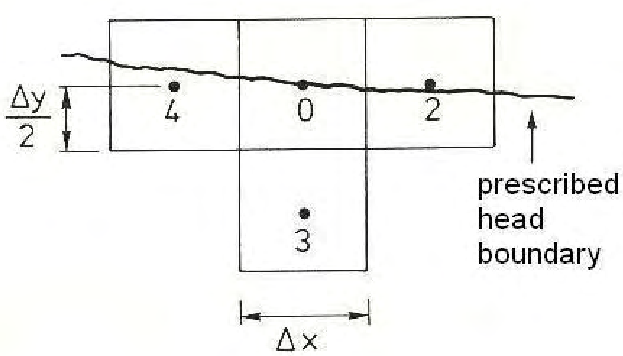
Positioning of Boundary Nodes



Second kind boundaries (example 1)

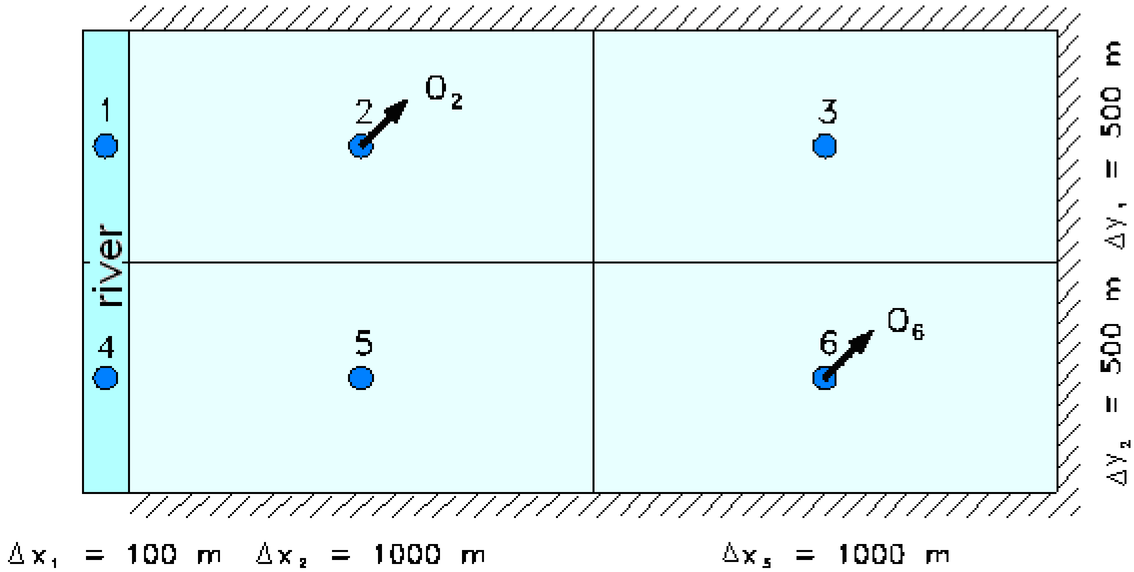


Second kind boundaries (example 2)



First kind boundaries

Steady flow in a confined aquifer



Plan view of model area and finite difference grid

Input data

Transmissivities:

$T_1 = T_2 = T_3 = 0.05 \text{ m}^2/\text{s}$

$T_4 = T_5 = T_6 = 0.01 \text{ m}^2/\text{s}$

Pumping rates:

$Q_2 = -0.001 \text{ m}^3/\text{s}$

$Q_6 = -0.005 \text{ m}^3/\text{s}$

Groundwater recharge:

$Q_R = 1 \cdot 10^{-8} \text{ m}^3/\text{s} \cdot \text{m}^2 = 10 \text{ l/s} \cdot \text{km}^2$

Prescribed heads:

$h_1 = h_4 = 10 \text{ m}$

Compute for steady state conditions the heads h_2, h_3, h_5, h_6 at nodes 2, 3, 5 and 6. Is there a risk that polluted river water gets into the wells?

Solution

Water balances for nodes 2, 3, 5 and 6

Cell 2: $Q_{12} + Q_{52} + Q_{32} + Q_R + Q_2 = 0$,
Cell 3: $Q_{23} + Q_{63} + Q_R = 0$,
Cell 5: $Q_{45} + Q_{25} + Q_{65} + Q_R = 0$,
Cell 6: $Q_{56} + Q_{36} + Q_R + Q_6 = 0$.

Example for the computation of in-/outflows for cell 2

$$Q_{12} = T_{12} \frac{h_1 - h_2}{\frac{\Delta x_1}{2} + \frac{\Delta x_2}{2}} \Delta y_1 \quad \text{where} \quad T_{12} = \frac{(\Delta x_1 + \Delta x_2)\, T_1 T_2}{T_1 \Delta x_2 + T_2 \Delta x_1}$$

$Q_{12} = 0.454545 – 0.045455\ h_2$.
$Q_{52} = 0.033333\ h_5 – 0.033333\ h_2$,
$Q_{32} = 0.025000\ h_3 – 0.025000\ h_2$.
$Q_R = Gw_{recharge} \cdot \Delta x_2 \cdot \Delta y_1 = 1 \cdot 10^{-8} \cdot 1000 \cdot 500 = 0.005\ m^3/s$.
$Q_2 = -0.001\ m^3/s$.

Balance equations:

Cell 2: $0.458545 – 0.103788\ h_2 + 0.025000\ h_3 + 0.033333\ h_5 = 0$.
Cell 3: $0.005000 + 0.025000\ h_2 – 0.058333\ h_3 + 0.033333\ h_6 = 0$,
Cell 5: $0.095909 + 0.033333\ h_2 – 0.047424\ h_5 + 0.005000\ h_6 = 0$,
Cell 6: $0.000000 + 0.033333\ h_3 + 0.005000\ h_5 – 0.038333\ h_6 = 0$.

4 equations with 4 unknowns:

$-0.103788\ h_2 + 0.025000\ h_3 + 0.033333\ h_5 + 0.000000\ h_6 = -0.458545$,
$0.025000\ h_2 – 0.058333\ h_3 + 0.000000\ h_5 + 0.033333\ h_6 = -0.005000$,
$0.033333\ h_2 + 0.000000\ h_3 – 0.047424\ h_5 + 0.005000\ h_6 = -0.095909$,
$0.000000\ h_2 + 0.033333\ h_3 + 0.005000\ h_5 – 0.038333\ h_6 = 0.000000$.

System of linear equations

$$\begin{vmatrix} -0.103788 + 0.025000 + 0.033333 + 0.000000 \\ 0.025000 - 0.058333 + 0.000000 + 0.033333 \\ 0.033333 + 0.000000 - 0.047424 + 0.005000 \\ 0.000000 + 0.033333 + 0.005000 - 0.038333 \end{vmatrix} \begin{vmatrix} h_2 \\ h_3 \\ h_5 \\ h_6 \end{vmatrix} = \begin{vmatrix} -0.458545 \\ -0.005000 \\ -0.095909 \\ 0.000000 \end{vmatrix}$$

$$[A] \times [h] = [B]$$

[A] = coefficient matrix, [h] = variable matrix, [B] = constant matrix

Iterative solution of equations using the GAUß-SEIDEL method:

$h_2 = 0.240876\ h_3 + 0.321164\ h_5 + 4.418093,$
$h_3 = 0.428574\ h_2 + 0.571426\ h_6 + 0.085715,$
$h_5 = 0.702872\ h_2 + 0.105432\ h_6 + 2.022373,$
$h_6 = 0.869564\ h_3 + 0.130436\ h_5.$

Initial guess for iteration: $h_3 = h_5 = h_6 = 10$ m.

	1. Iteration	2. Iteration	3. Iteration		20. Iteration	21. Iteration	22. Iteration
h_2	10.04	10.11	10.15	....	10.24	10.24	10.24
h_3	10.10	10.19	10.26	....	10.42	10.43	10.43
h_5	10.30	10.19	10.23	....	10.32	10.32	10.32
h_6	10.11	10.19	10.25	....	10.41	10.41	10.41

Result: $h_2 = 10.24$ m, $h_3 = 10.43$ m, $h_5 = 10.32$ m, $h_6 = 10.41$ m.

2-D Flow Equation: Unconfined Aquifer

∇-Notation

$$\nabla((h-b)K\nabla h)+q=S_y\frac{\partial h}{\partial t}$$

where $\nabla=(\partial/\partial x,\ \partial/\partial y)$

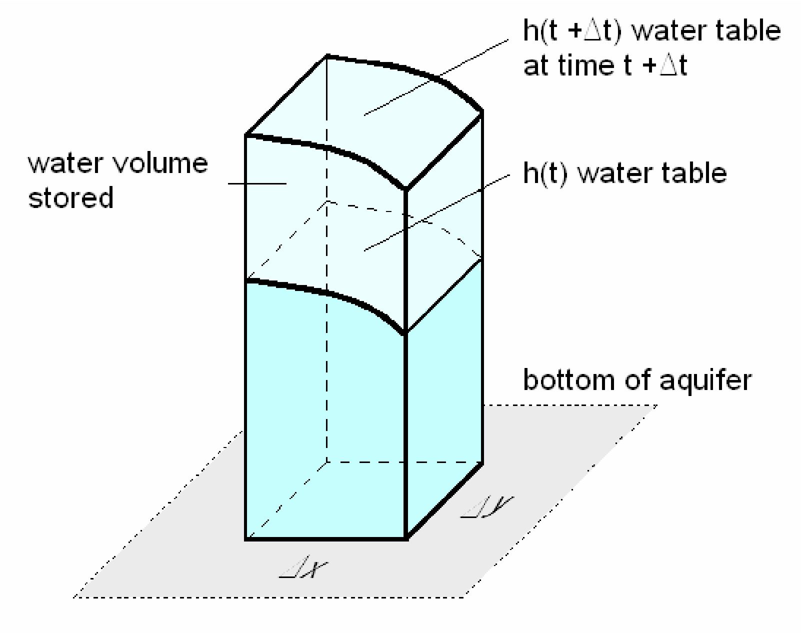
$\partial/\partial n$-Notation

$$\frac{\partial}{\partial x}((h-b)K\frac{\partial h}{\partial x})+\frac{\partial}{\partial y}((h-b)K\frac{\partial h}{\partial y})+q=S_y\frac{\partial h}{\partial t}$$

$$T=(h-b)K$$

Unconfined ("Phreatic") Aquifer

Storage mechanism in the horizontally 2-D model of the unconfined aquifer



Two changes compared to confined aquifer:

$$T \Rightarrow K\ (h - b)$$
$$S \Rightarrow S_y + (S) \qquad S_y >> S$$

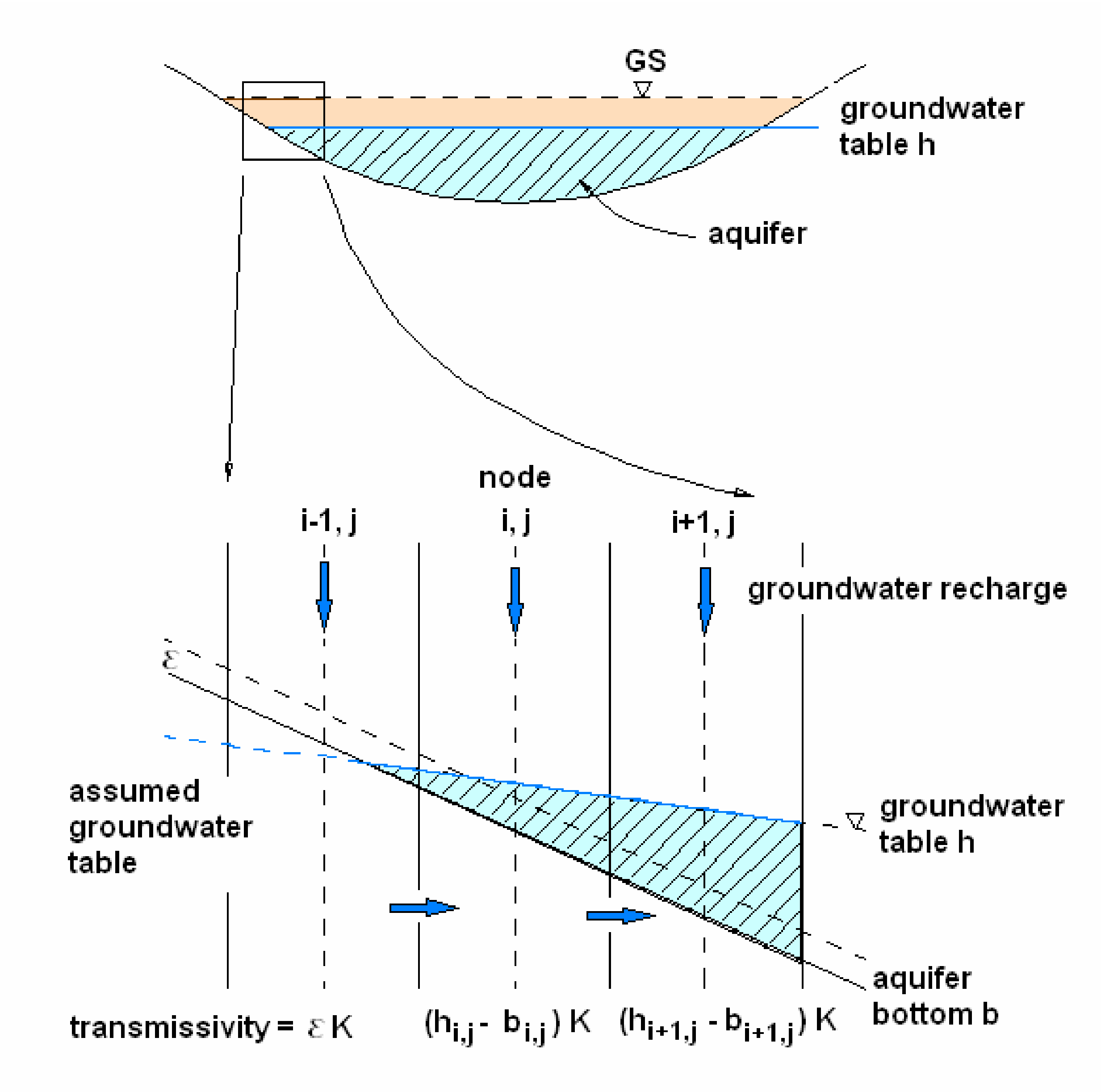
Transmissivities between nodes:

$$TI_{i,j} = KI_{i,j}\ \sqrt{(h_{i+1,j} - b_{i+1,j})\ (h_{i+1,j} - b_{i+1,j})}$$
$$TJ_{i,j} = KJ_{i,j}\ \sqrt{(h_{i,j+1} - b_{i,j+1})\ (h_{i+1,j} - b_{i+1,j})}$$

Non linear in h! Iteration required

$$q = -TI_{i,j}\ \Delta y\ \frac{h_{i,j+1} - h_{i,j}}{\Delta x}$$

Falling-dry of Nodes in Unconfined ("Phreatic") Aquifer Model



2-D Flow Equation: Leaky Confined Aquifer

∇-Notation

$$\nabla(T\nabla h) + q + l_1(h_1 - h) = S\,\frac{\partial h}{\partial t}$$

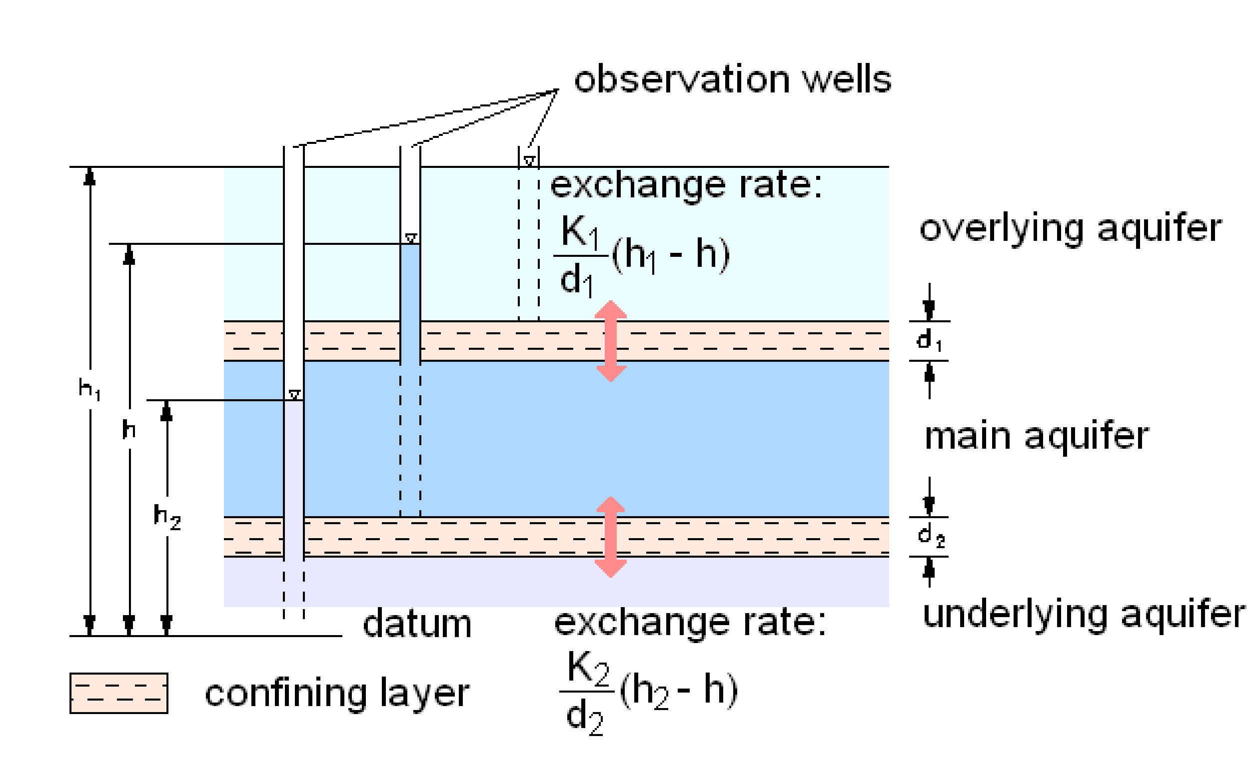
where $\quad \nabla = (\partial/\partial x,\ \partial/\partial y)$

∂ / ∂n-Notation

$$\frac{\partial}{\partial x}\left(T\frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(T\frac{\partial h}{\partial y}\right) + q + l_1(h_1 - h) = S\,\frac{\partial h}{\partial t}$$

$l_1(h_1 - h)$: leakage flow

Leaky Confined Aquifer



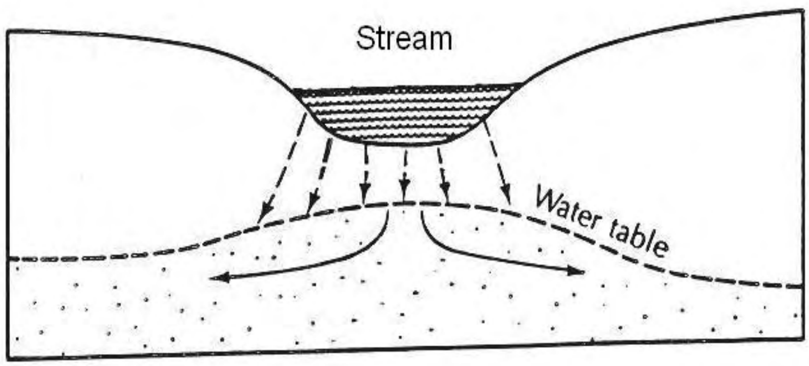
Exchange flow between main aquifer and overlying aquifer:

$$q = \frac{K_1}{d_1}(h_1 - h) \qquad \left(\frac{L^3}{TL^2}\right)$$

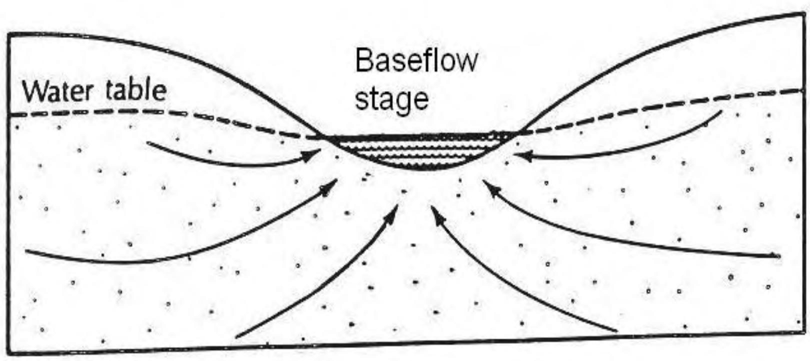
K_1: vertical hydraulic conductivity of semi pervious layer
d_1: thickness of semi pervious layer

$$\frac{K}{d} = l: \quad \text{leakage factor}$$

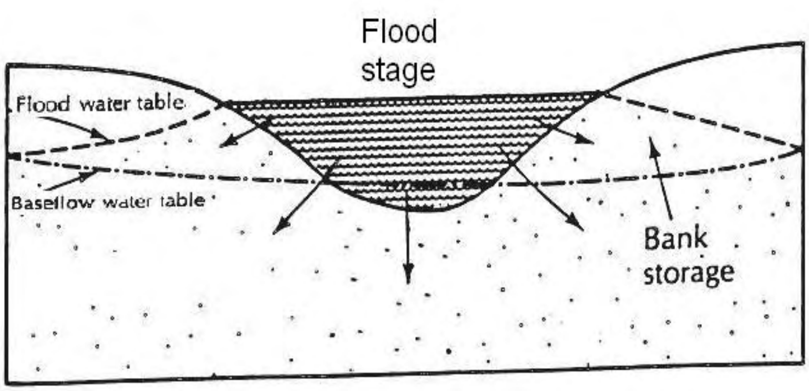
Cross Sections of Gaining and Losing Streams



A losing stream

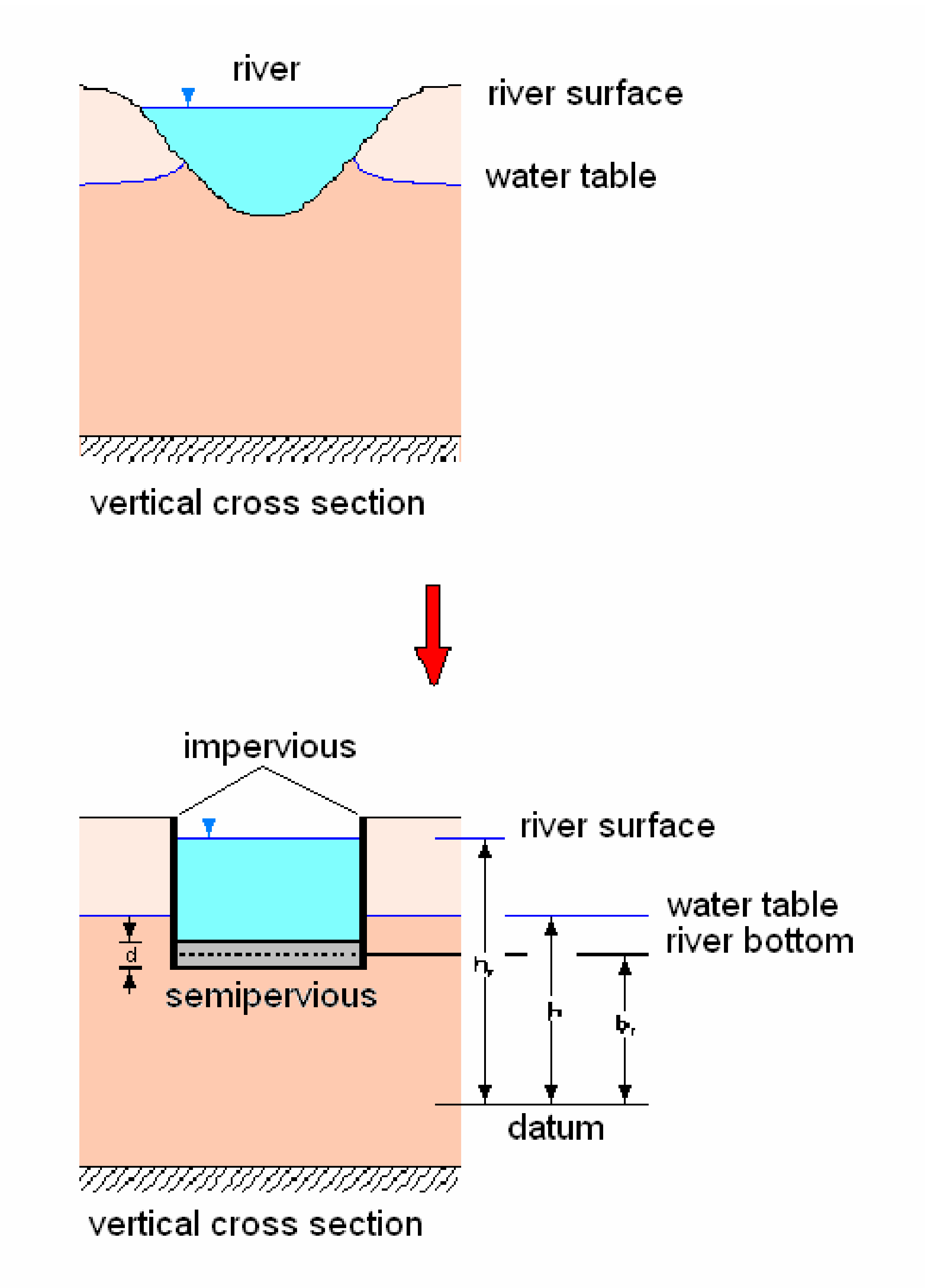


A gaining stream

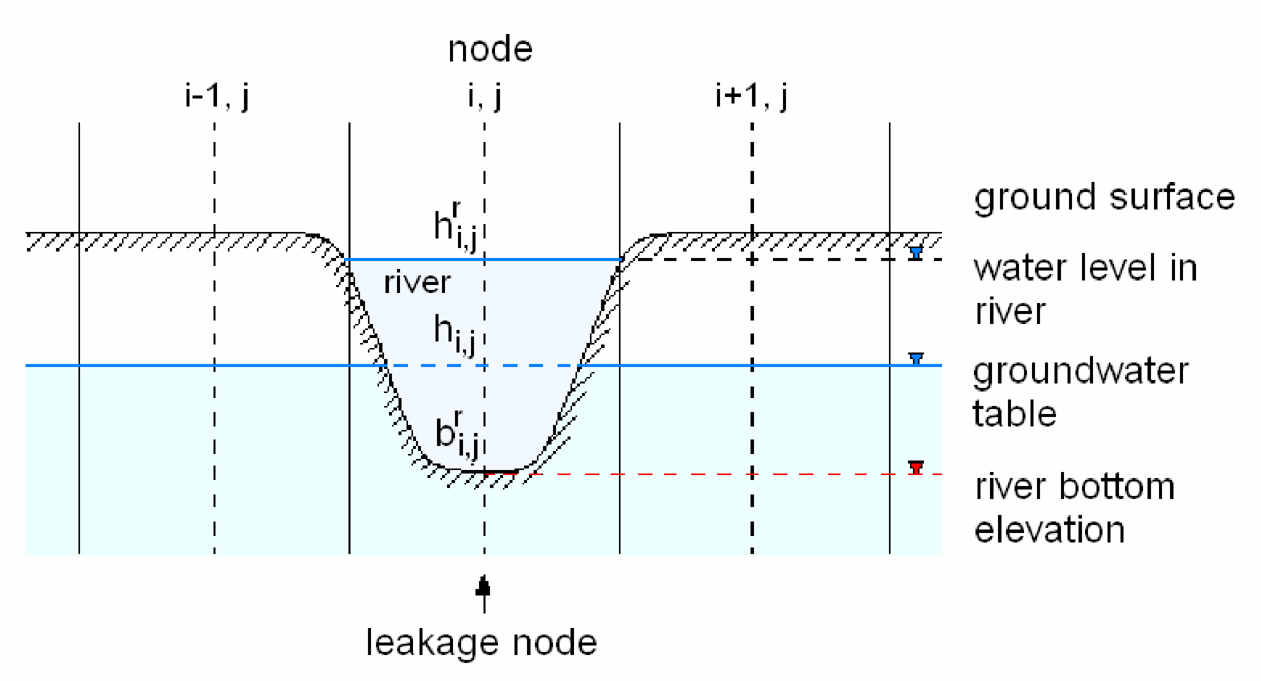


A stream which is gaining during low flow periods but which may temporarily become a losing stream during flood stage

Application of the Leaky Principle to River Ex- and Infiltration



Leaky from Surface Water Bodies



$$q_{i,j} = \begin{cases} l_{i,j}(h^r_{i,j} - h_{i,j}) & \text{if } b^r_{i,j} < h_{i,j} \\ l_{i,j}(h^r_{i,j} - b^r_{i,j}) & \text{if } b^r_{i,j} > h_{i,j} \end{cases}$$

q: flow rate per unit area (m/s)

Exchange rate:

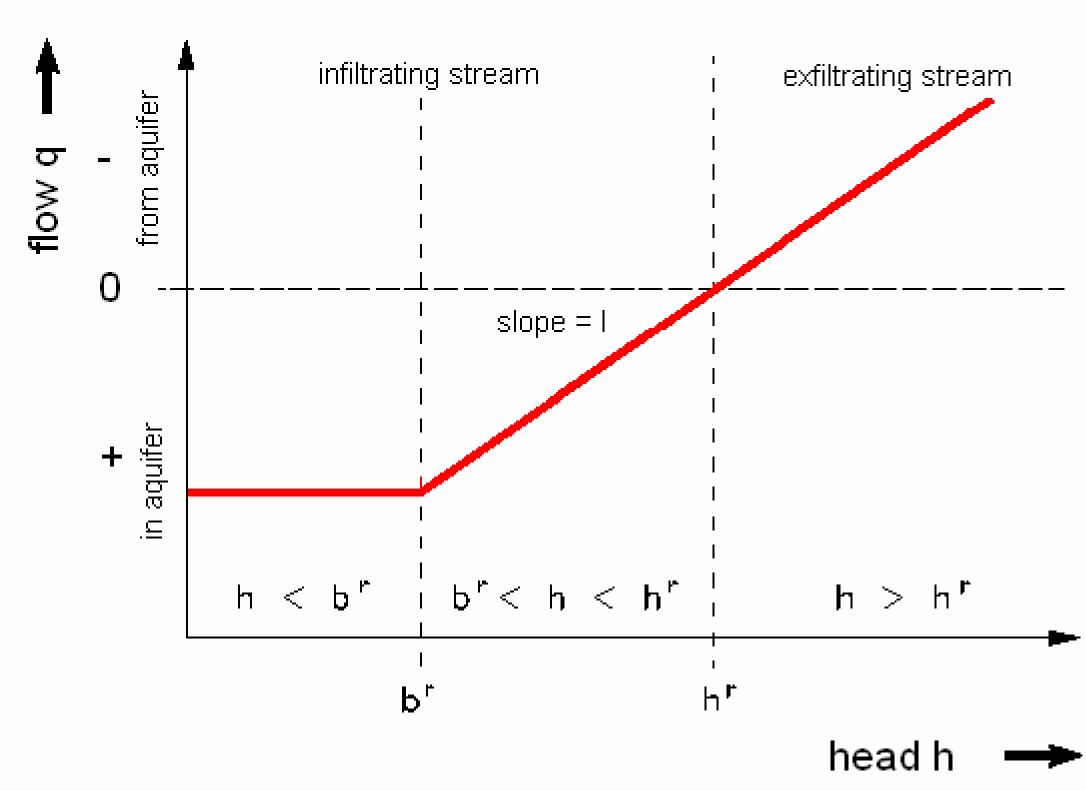
- if exchange area = cell area:

$$Q_{i,j} = q_{i,j}\,\Delta x\,\Delta y$$

- if exchange area < cell area $\Delta x\ \Delta y$ => correction of l

$$l \Rightarrow l\frac{A}{\Delta x\,\Delta y}$$

Leakage from a Stream as Function of Head



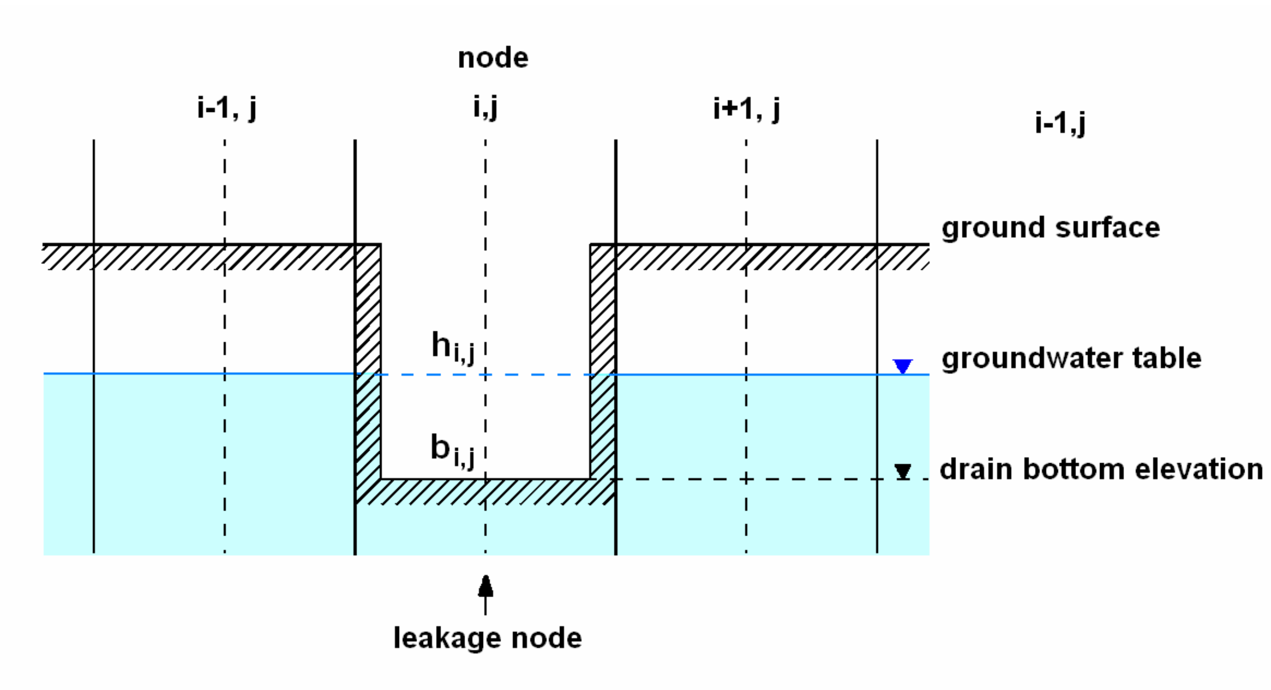
h^r: water level in river, b^r: river bottom elevation, l: leakage factor

$$q = f(h)$$

$$\text{Case 1:} \quad q_{i,j} = l_{i,j}\,(h^r_{i,j} - h_{i,j}) \qquad \text{if } b^r_{i,j} < h_{i,j}$$

$$\text{Case 2:} \quad q_{i,j} = l_{i,j}\,(h^r_{i,j} - b^r_{i,j}) \qquad \text{if } b^r_{i,j} > h_{i,j}$$

Simulation of Drain Node by the Leakage Principle



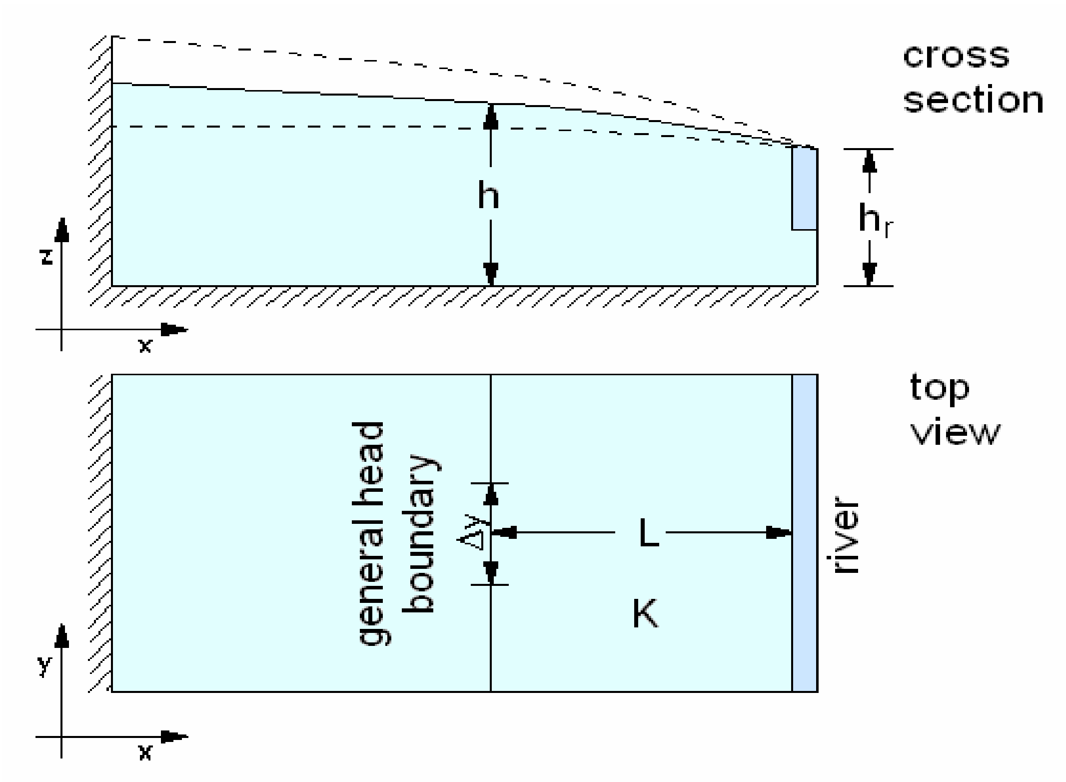
Exchange between surface water and aquifer

$$q_{i,j} = \begin{cases} l_{i,j}(h^r_{i,j} - h_{i,j}) & \text{if } b^r_{i,j} < h_{i,j} \\ l_{i,j}(h^r_{i,j} - b^r_{i,j}) & \text{if } b^r_{i,j} > h_{i,j} \end{cases}$$

For $h^r_{i,j} = b^r_{i,j}$ we obtain:

$$q_{i,j} = \begin{cases} l_{i,j}(b_{i,j} - h_{i,j}) & \text{if } b_{i,j} < h_{i,j} \\ 0 & \text{if } b_{i,j} > h_{i,j} \end{cases}$$

General Head Boundary



$$q = -l\,(h_r - h), \qquad Q = q\,m\,\Delta y, \qquad l = \frac{K}{L}$$

$l \Rightarrow 0$: impervious boundary

$l \Rightarrow$ large : prescribed head

Note ASM: l must be modified because ASM expects an exchange area $\Delta x\ \Delta y$:

- boundary parallel to x-axis: l => l m/Δy
- boundary parallel to y-axis: l => l m/Δx

Set h-elevation of river bottom < aquifer bottom!

3-D Flow Equation (Confined Aquifer)

1. Continuity

$$S_0 \frac{\partial h}{\partial t} = -\nabla \vec{v}_D + q_0$$

2. DARCY'S-law

$$\vec{v}_D = -\mathbb{K}\,\nabla h$$

$$\Rightarrow \quad S_0 \frac{\partial h}{\partial t} = \nabla(\mathbb{K}\,\nabla h) + q_0$$

Partial differential equation of 2^{nd} order

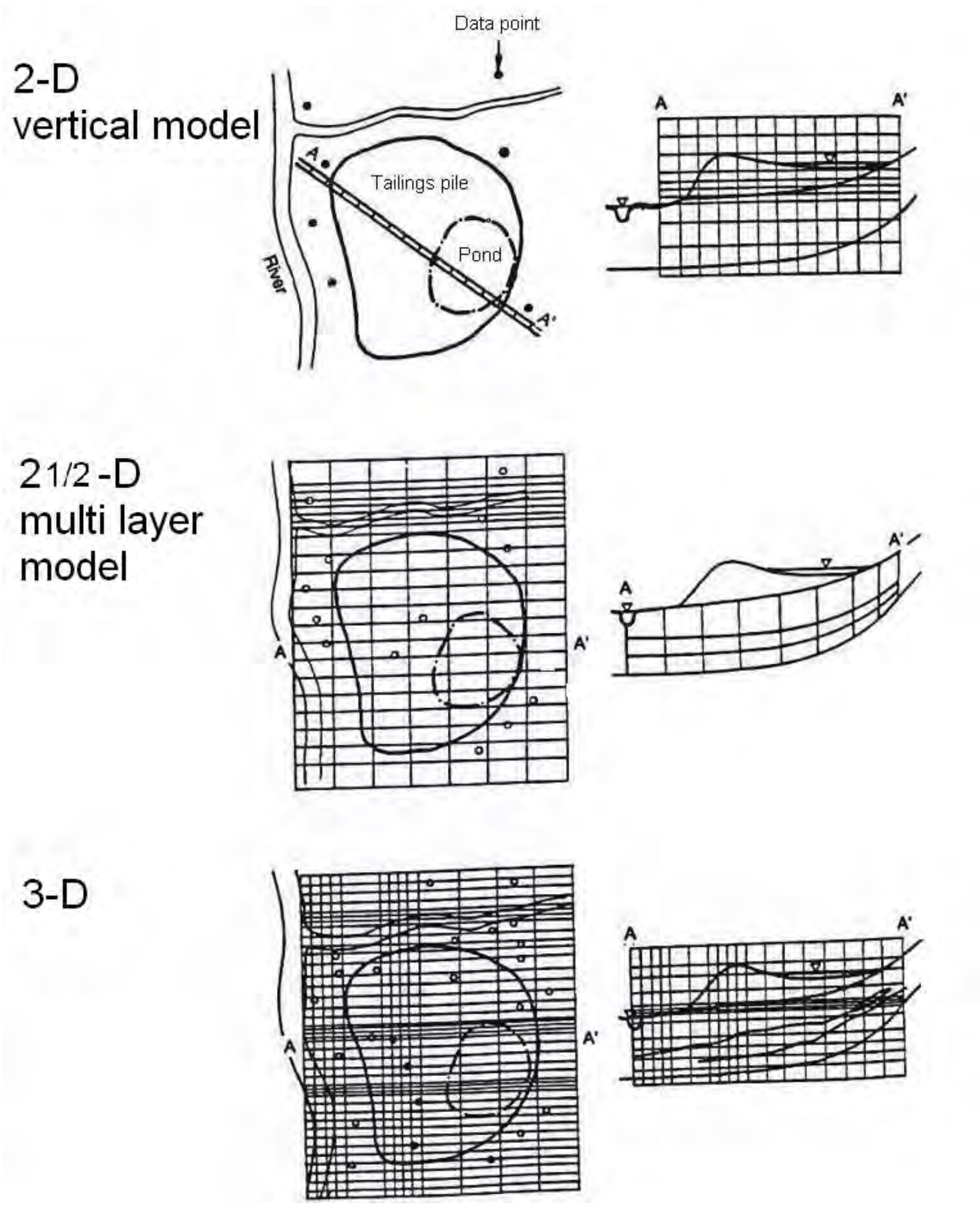
Required for solution:

- boundary conditions
- initial conditions

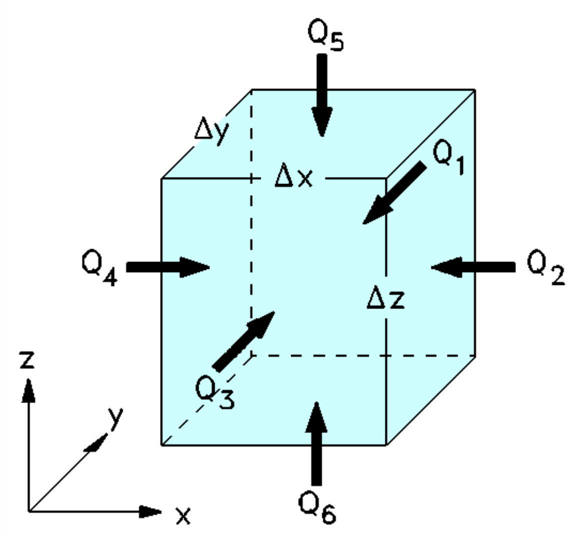
Solution: h = f (x, y, z, t)

2-D-Vertical ⇨ 2 ½-D ⇨ 3-D-Model

Phase **Model Area (top view)** **Numerical Model (cross section)**



Water Balance around one Cell



Water balance:

$$Q_1 + Q_2 + Q_3 + Q_4 + Q_5 + Q_6 = S_0 \, \Delta z \, \Delta x \, \Delta y \, \frac{\partial h}{\partial t}$$

Difference compared to 2-D:

$$Q_5 = Q_6 = 0, \; \Delta z = 0$$

Equation system 2-D (isotropic or II principal axes)

$$\begin{pmatrix} \text{max.5} \\ \text{coeff.} \neq 0 \\ \text{per row} \end{pmatrix} \begin{pmatrix} . \\ h_i \\ . \end{pmatrix} = \begin{pmatrix} . \\ . \\ . \end{pmatrix}$$

Equation system 3-D (isotropic or II principal axes)

$$\begin{pmatrix} \text{max.7} \\ \text{coeff.} \neq 0 \\ \text{per row} \end{pmatrix} \begin{pmatrix} . \\ h_i \\ . \end{pmatrix} = \begin{pmatrix} . \\ . \\ . \end{pmatrix}$$

Fully anisotropic situation 2-D: 9 coefficients, 3-D: 27 coefficients

New Terms Q5, Q6

3-D Formulation

$$Q_5 = \frac{h_{i,j,k} - h_{i,j,k+1}}{z_{k+1} - z_k} K_z \; \Delta x \; \Delta y$$

where $$\frac{K_z}{z_{k+1} - z_k} = l_{i,j,k}$$

"2 ½-D" Formulation

$$Q_5 = (h_{i,j,k} - h_{i,j,k+1})\, l_{i,j,k} \; \Delta x \; \Delta y$$

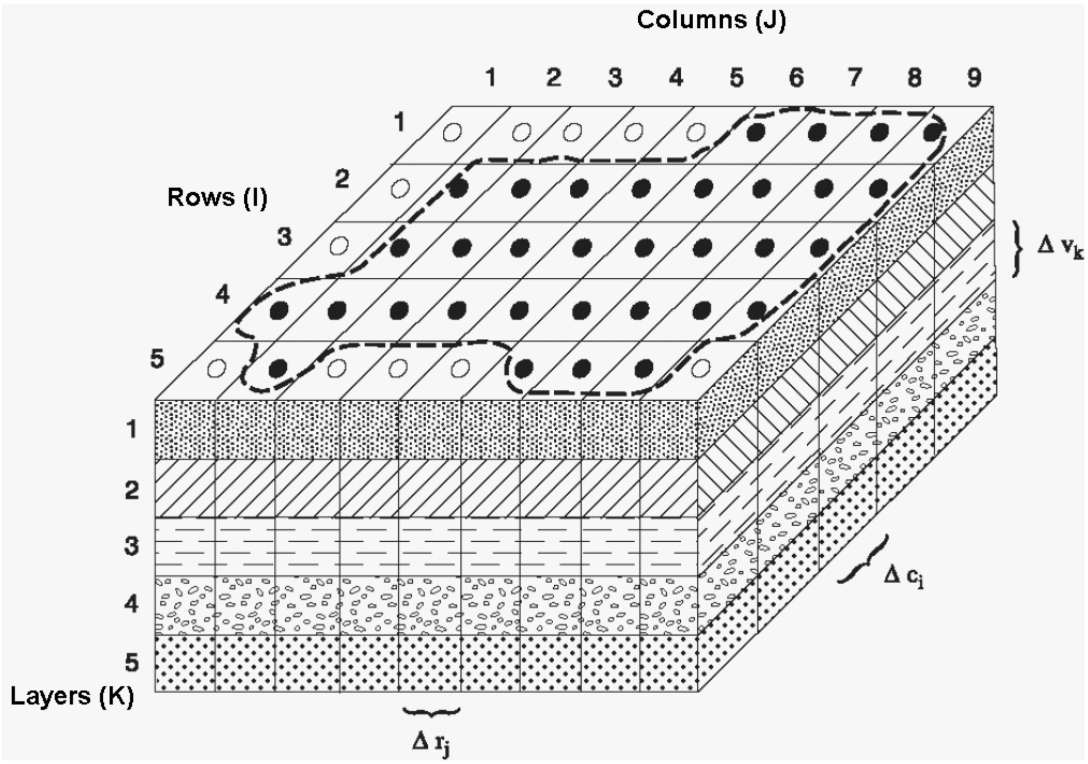
$$\Uparrow$$

leakage factor

Advantages:

- aquitard need not be modeled explicitly (gap)
- discretization parallel to stratigraphy more economical

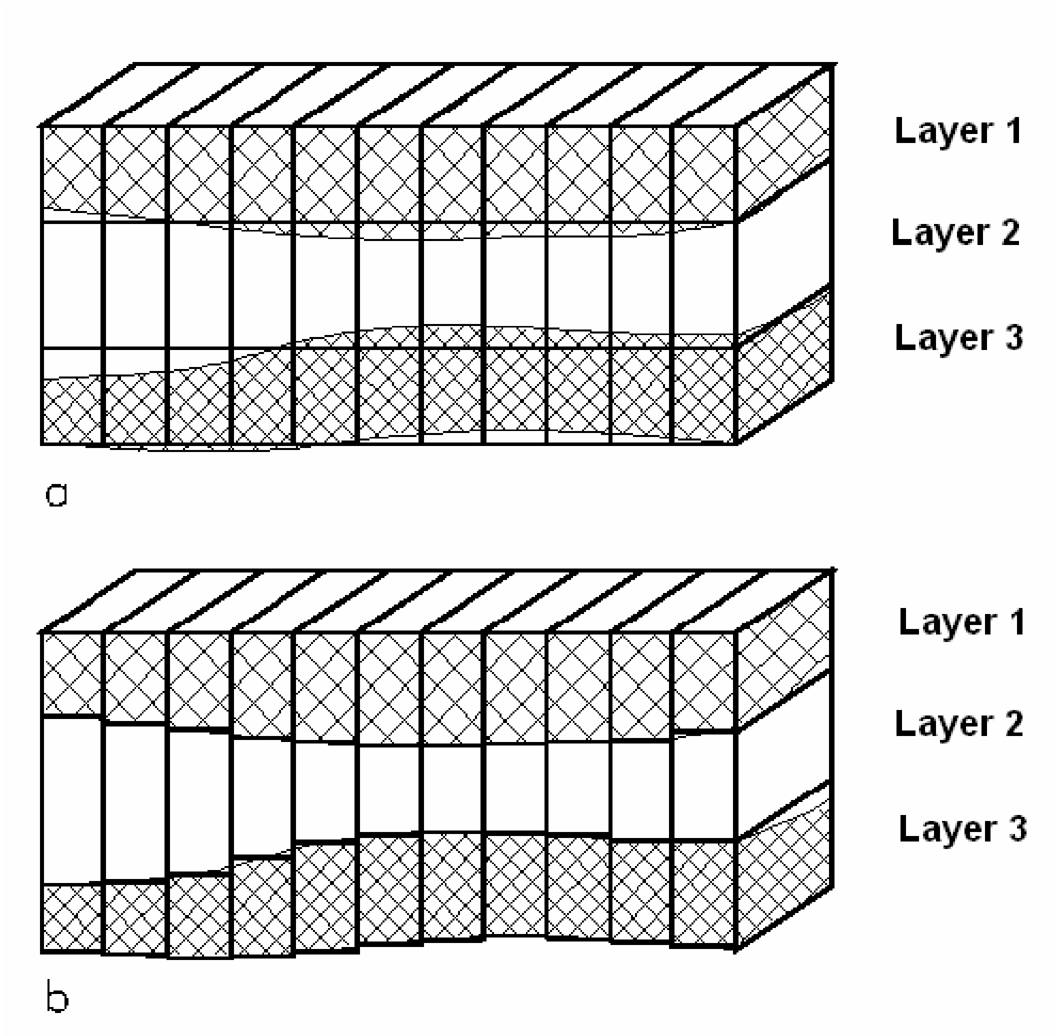
Discretization Scheme: MODFLOW



Columns (J)	correspond to x-coordinate
Rows (I)	correspond to y-coordinate
Layers (K)	correspond to z-coordinate

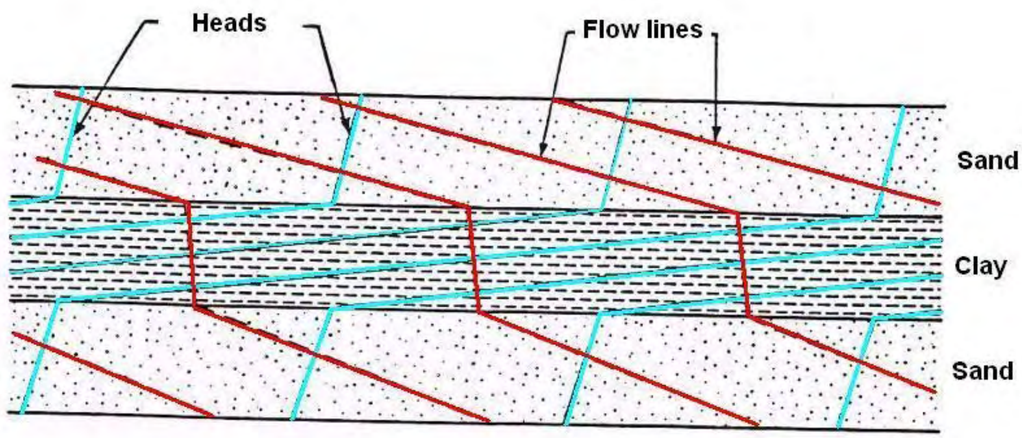
Note: The convention in MODFLOW is to number layers from the top down.

Schemes of Vertical Discretization



a) Aquifer cross section with rectilinear grid superimposed
b) Aquifer cross section with deformed grid superimposed

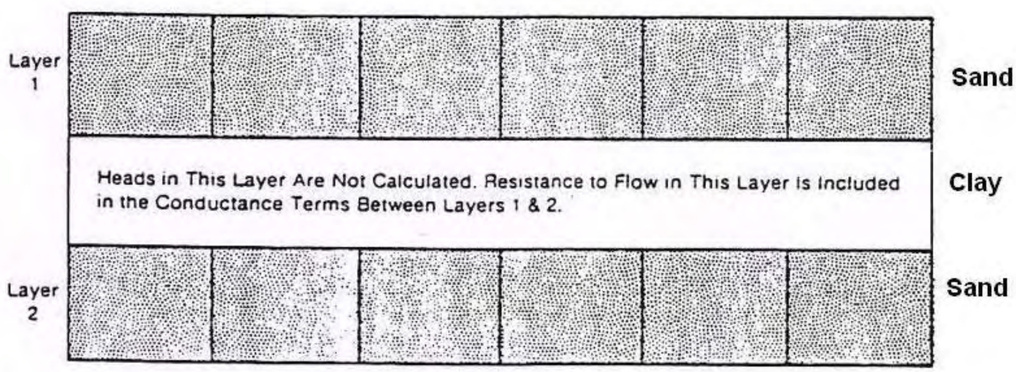
2 ½-D Model: Simulation of Low Conductivity Layer



Flow pattern in a cross section consisting of 2 high conductivity units separated by a low conductivity unit.

Heads in aquifer almost vertical, flow lines almost horizontal!

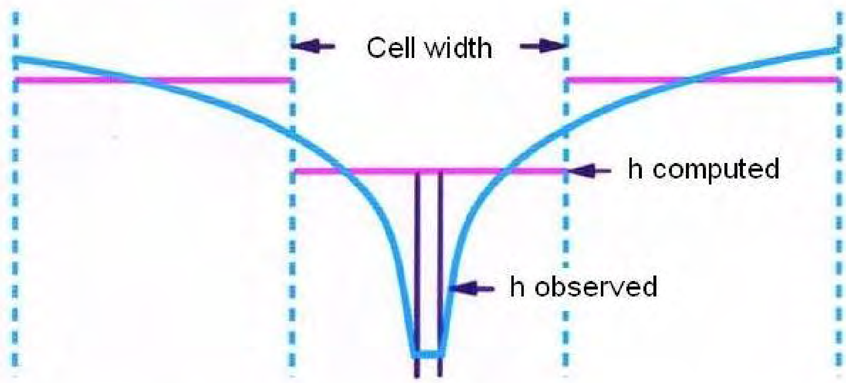
Heads in aquitard almost horizontal, flow lines almost vertical!



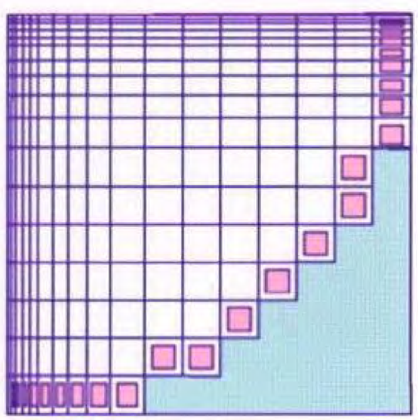
A cross section in which a low conductivity unit is represented by the conductance between model layers.

Note: Using the leakage principle the aquitard must not be modeled explicitly (only valid for flow!)

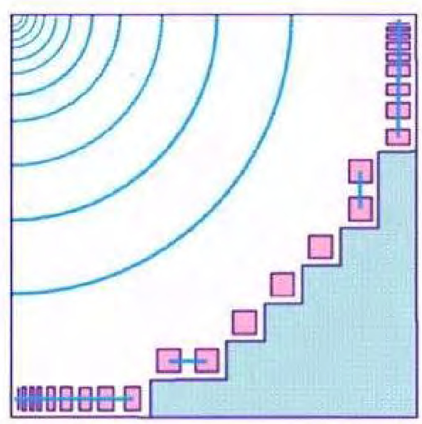
Simulation of Well Drawdown



Comparison of computed and observed head within a well cell



Finite difference grid



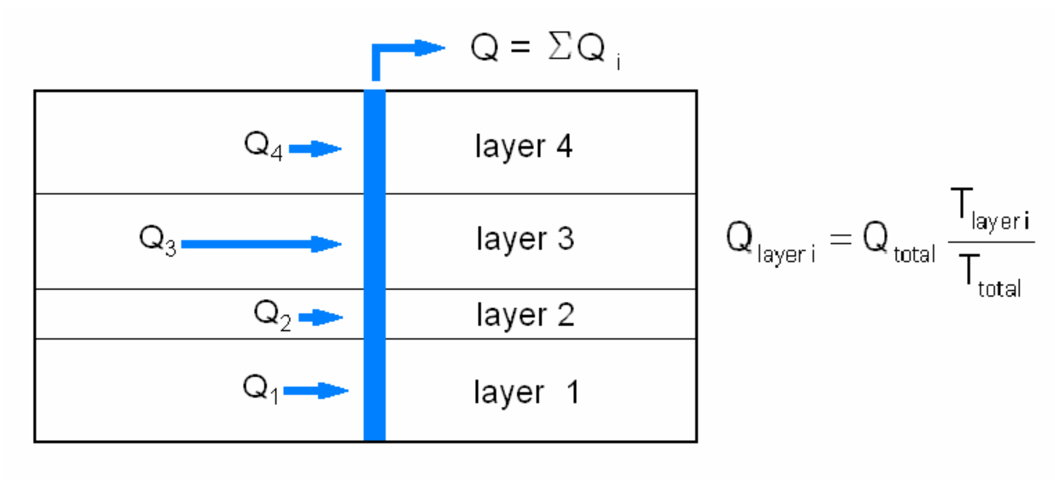
Simulated head distribution

Note: Well loss!

Wells in 3-D-Model

- Grid refinement in horizontal direction
- Distribution of total discharge to different layers

  - Proportional to transmissivities of layers

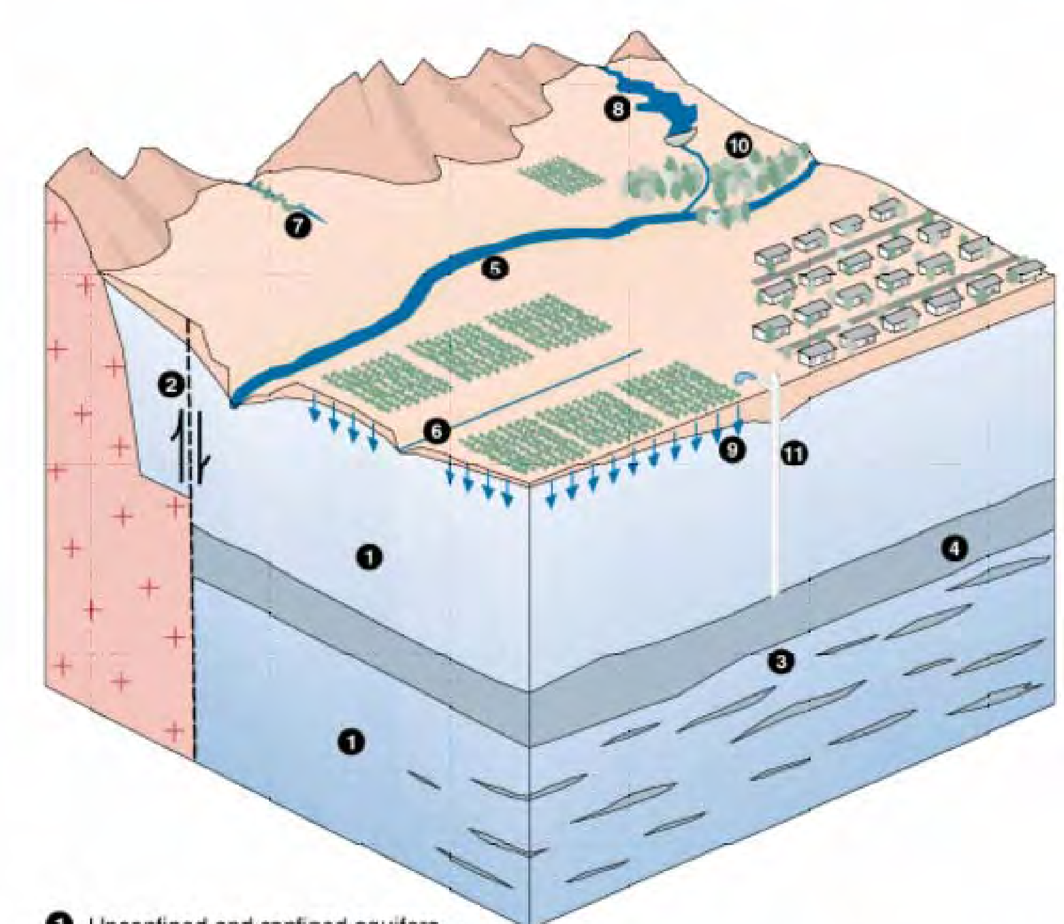


  - Total discharge in 1 cell, but high vertical hydraulic conductivity in well cells

- Falling dry of nodes leads to in-stabilities!

  Way out → adjustment of pumping rate

Features of an Aquifer System that can be Simulated by MODFLOW



1. Unconfined and confined aquifers—Ground-water flow and storage changes
2. Faults and other barriers—Resistance to horizontal ground-water flow
3. Fine-grained confining units and interbeds
4. Confining units—Ground-water flow and storage changes
5. Rivers—Exchange of water with aquifers
6. Drains and springs—Discharge of water from aquifers
7. Ephemeral streams—Exchange of water with aquifers
8. Reservoirs—Exchange of water with aquifers
9. Recharge from precipitation and irrigation
10. Evapotranspiration
11. Wells—Withdrawal or recharge at specified rates

Solute Transport Modeling

Pollutants

- **Bacterial contamination**

- **Inorganic pollutants**

  - Nitrate
  - Heavy metals
    e.g. lead, cadmium, mercury, arsenic ...
  - Radio nuclides

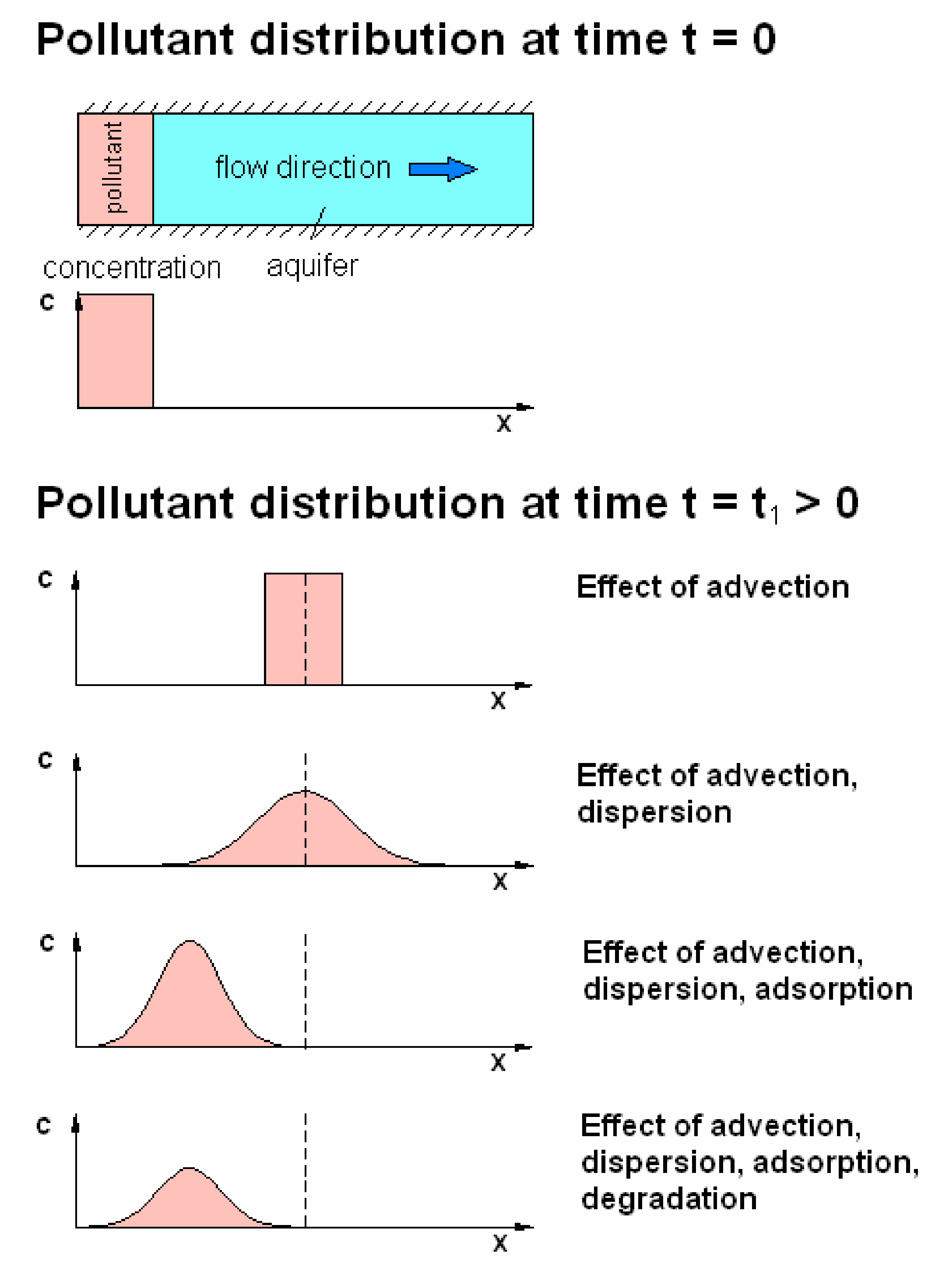
- **Organic pollutants**

  - Oil products
  - Chlorinated hydrocarbons
    e.g. tetrachlorethene, trichlorethene, ...
  - Aromatic hydrocarbons
    e.g. benzene, toluene, xylene, ...
  - Polycyclic aromatic hydrocarbons
    e.g. naphthalene, ...
  - Pesticides (diverse chemical compounds)
    e.g. atrazine, ...

Risk of Pollutants

- Produced in big quantities
- Persistent (no decay)
- High solubility
- Non absorbent (high mobility)
- Toxic

Representation of Transport Processes



Transport Mechanism

- **Advection**

  Dissolved solids are carried along with the average velocity of flowing groundwater

- **Molecular diffusion**

  Transport by concentration gradients (FICK'S law)

- **Dispersion**

  Spreading of pollutants due to heterogeneity of flow field (small scale dispersion, macro dispersion)

- **Adsorption**

  Adsorption of pollutants onto the surfaces of the mineral grains in the aquifer

- **Chemical and biochemical reactions**

  Chemical and biological decay and transformation processes

- **Radioactive decay in case of radioactive substances**

DARCY Velocity – Pore Velocity

- **DARCY velocity v_f**

Relevant for mass balances

$$v_f = -K \frac{dh}{dn}$$

The DARCY velocity is related to the total cross sectional area.

- **Pore velocity u**

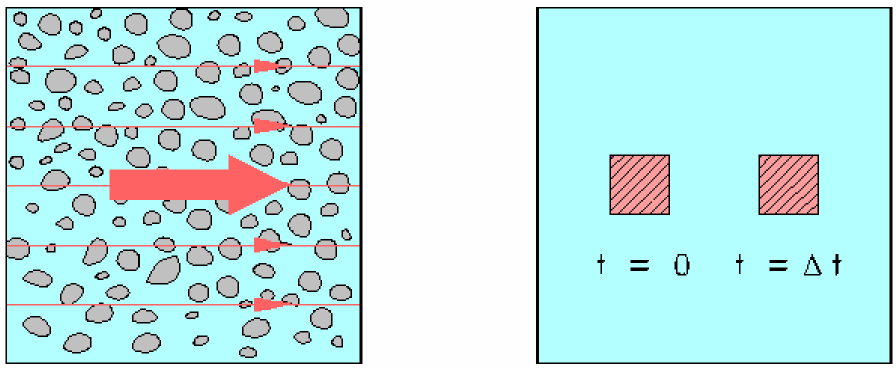
Relevant for transport time

$$u = \frac{v_f}{n_f}$$

The pore velocity is restricted to the effective cross section. Therefore it is larger than the DARCY velocity by the factor $1/n_f$.

Advection

Displacement of pollutants in the average direction of groundwater flow



Average pore velocity and average pathlines

Advective transport of an ideal tracer

Advective pollutant flux through unit area vertical to flow direction:

$$\vec{j}_{adv} = \vec{u}\, n_f\, c = \vec{v}_f\, c$$

$\vec{j}_{adv}$: mass flux (M/L^2T)

$\vec{u}$: pore velocity (L/T)

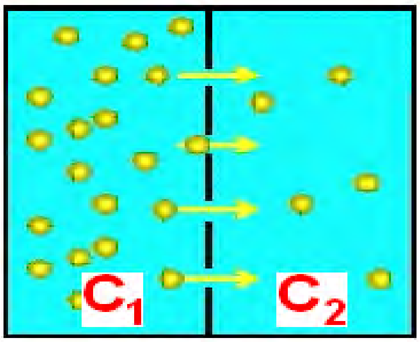
n_f : effective porosity (-)

c : pollutant concentration (M/L^3)

Note: Convection = motion of fluids due to temperature gradients

Molecular Diffusion

Solvent moves by concentration gradient. Transport due to BROWNIAN molecular motion.



$C_1 > C_2$

$u = 0$!

Diffuse pollutant flux (FICK´s law):

$$\vec{j}_D = -D_m \frac{\partial c}{\partial n}$$

taking into account the effective flow area

$$\vec{j}_D = -nD_m \frac{\partial c}{\partial n}$$

$\vec{j}_D$: diffusive mass flux (M/L^2T)

D_m : diffusion coefficient (L^2/T)

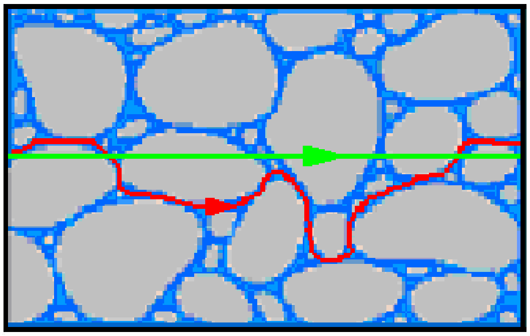
$\partial c/\partial n$: concentration gradient ($M/L^3/L$)

n : porosity (-)

For u > 0.1 m/d diffusive flux can usually neglected!

Tortuosity

In porous medium diffusion is not as effective as in open water. Solute only moves through pores.



— straight line distance (L)

— actual length of flow path (Le)

$$D_m = \tau D_0 \qquad \tau = L/Le$$

where :

τ : tortuosity of the porous medium $(-)$

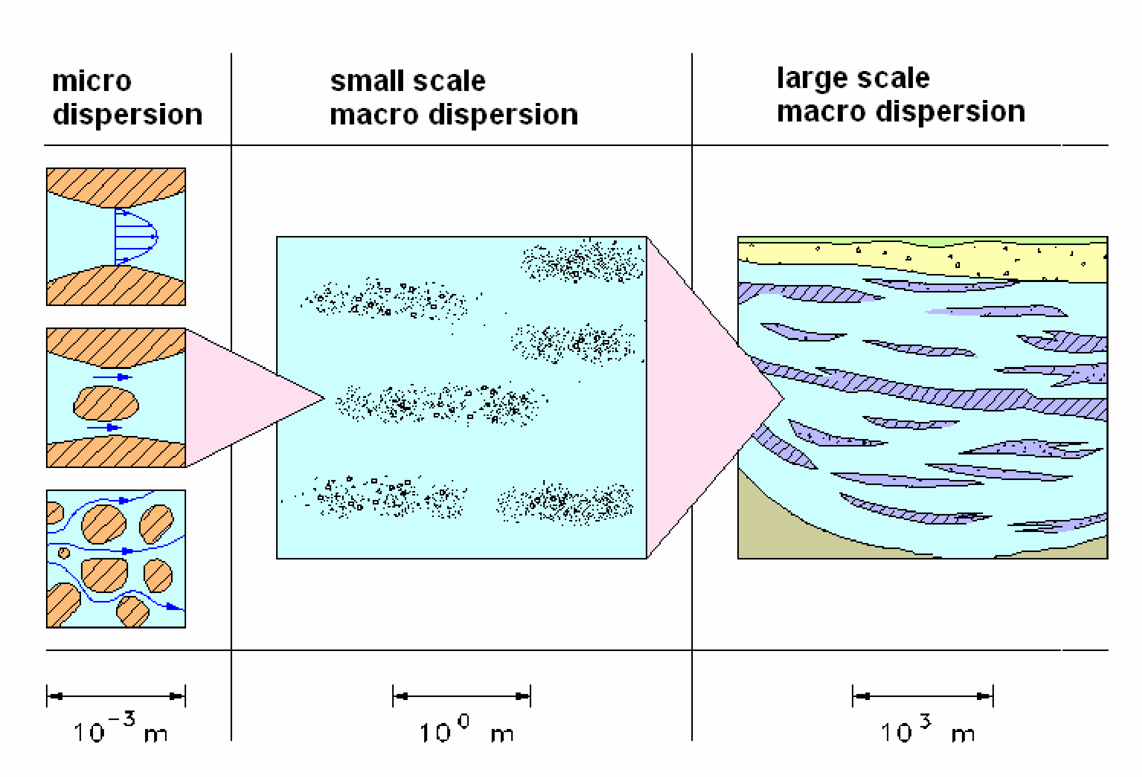
D_0 : free solution diffusion coefficient (L^2/T)

D_m : effective diffusion coefficient (L^2/T)

$D_0 \approx 10^{-9}$ m²/s for water

Typical values for $\tau : 0.56 - 0.88$

Causes for Velocity Variations at Various Spatial Scales

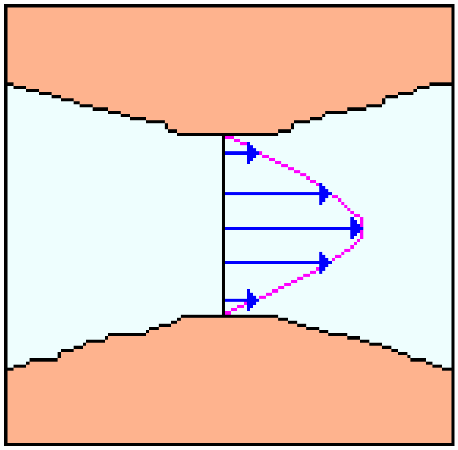


2 Kinds of Dispersion

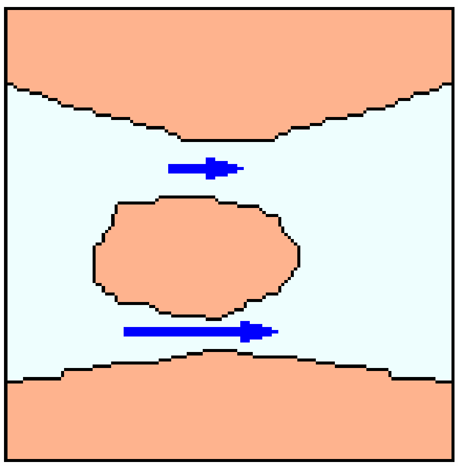
- micro dispersion

- macro dispersion
    - small scale
    - large scale

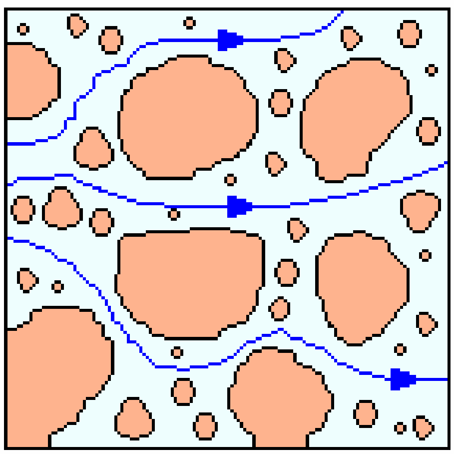
Micro Dispersion



Velocity profile across a single pore

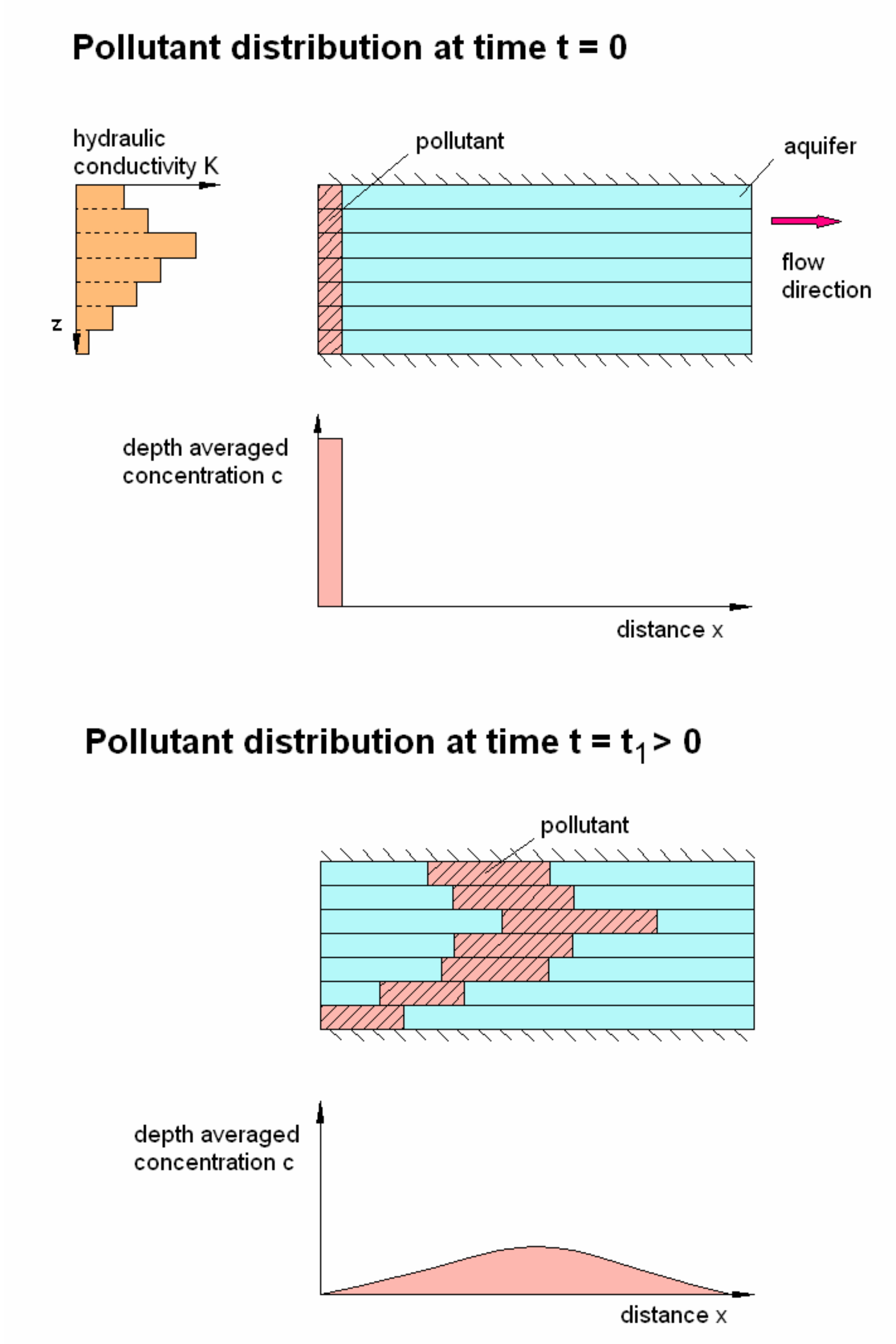


Velocity variations from pore to pore



Flowlines within a porous medium

Impact of Macro Dispersion



Dispersion created by layered heterogeneities in hydraulic conductivity on the migration of a solute

Dispersion Model

In analogy to molecular diffusion (FICK´s law)

$$\vec{j}_D = -D\nabla c \quad \text{where} \quad D = \begin{pmatrix} D_L & 0 \\ 0 & D_T \end{pmatrix}$$

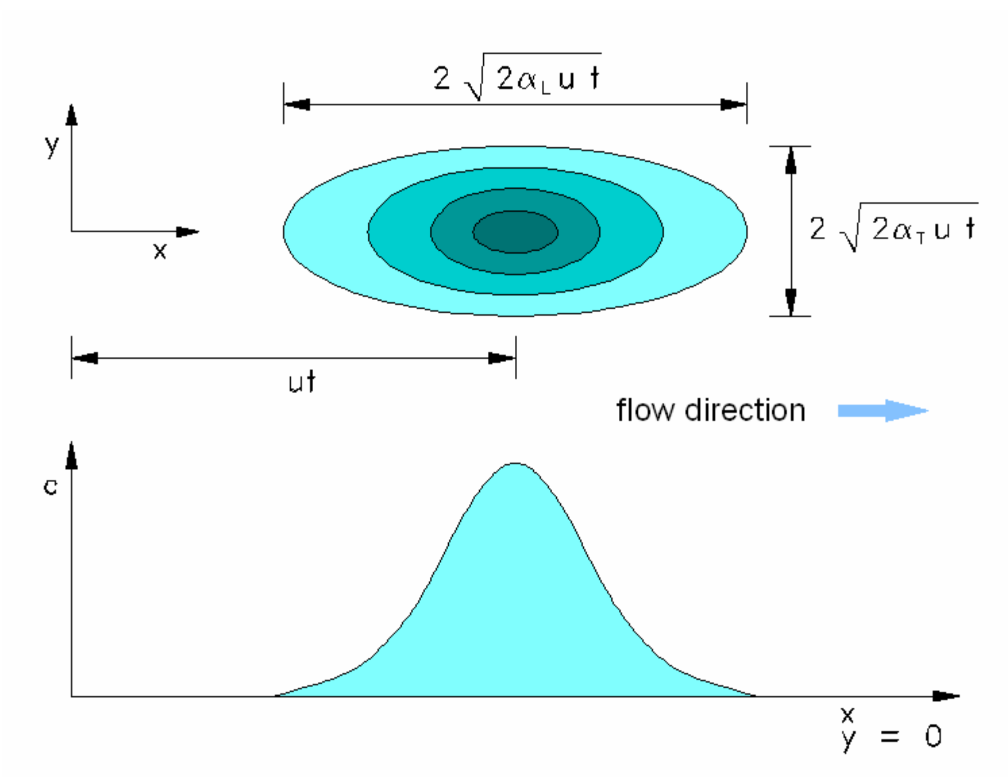
resp.

$$\vec{j}_L = -n_f D_L \frac{\partial c}{\partial s_L} \quad \text{and} \quad \vec{j}_T = -n_f D_T \frac{\partial c}{\partial s_T}$$

D_L : longitudinale dispersion coefficient (L^2/T)

D_T : transverse dispersion coefficient (L^2/T)

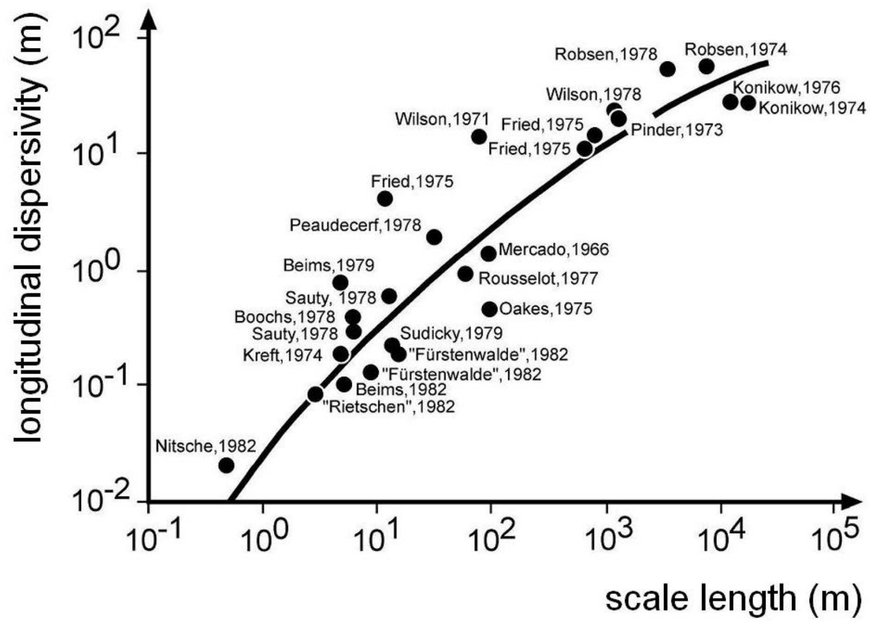
$$D_L = \alpha_L |\vec{u}| \quad , D_T = \alpha_T |\vec{u}|, \quad \text{with constant } \alpha_L \text{ and } \alpha_T$$



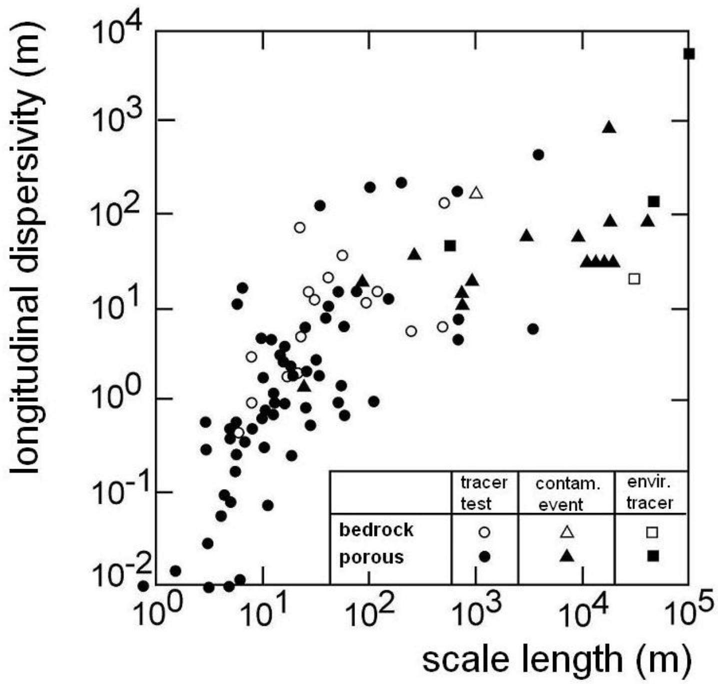
$$\sigma_L^2 = 2 D_L t, \quad \sigma_T^2 = 2 D_T t$$

Scale Dependence of Longitudinal Dispersivity

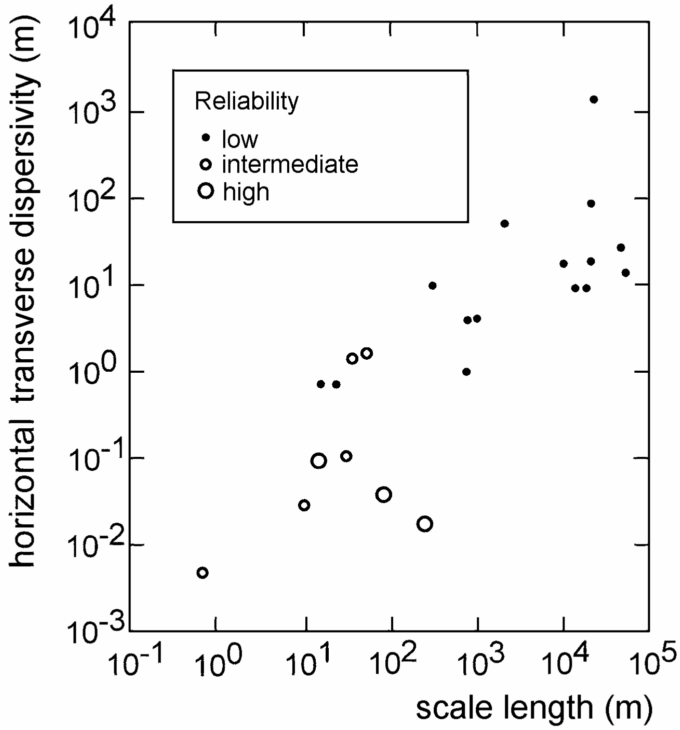
BEIMS, 1983

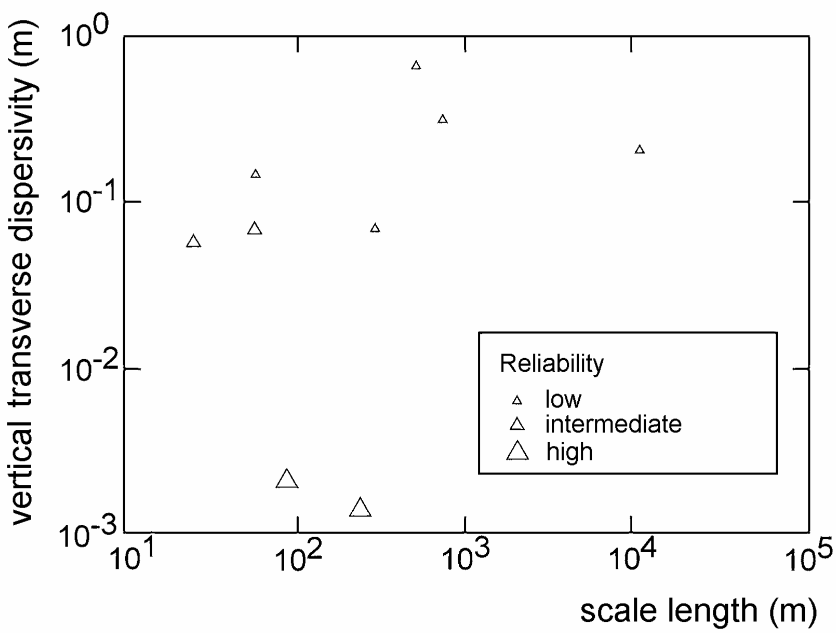


GELHAR et al., 1985



Scale Dependence of Transverse Dispersivity





How can we explain the Scale Effect of Dispersion?

- **At small scale (lab scale) dispersion due to diffusion, pore size distribution and pore size geometry.**

  Tortuosity and microscopic variations within a pore and between pores.

- **At field scale dispersion due to variations in stratigraphy, lithology, and permeability.**

  Heterogeneity in K and n_f

Scale Dependence of Longitudinal Dispersivity

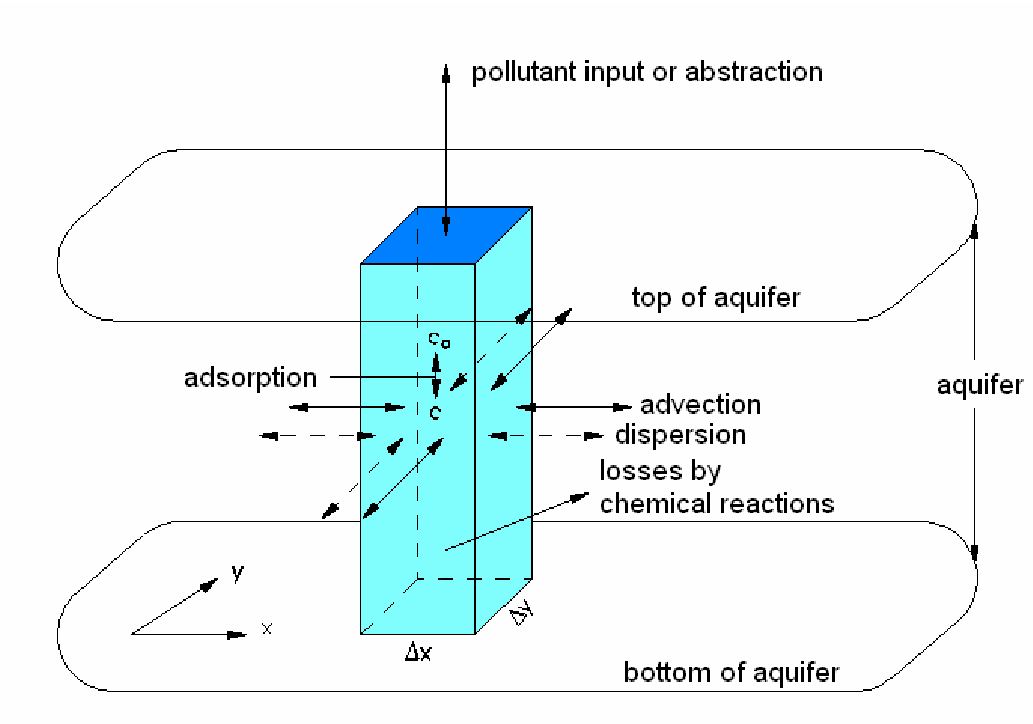
- **α_L is a measure of the heterogeneity and correlation length of a porous medium**

- **$\alpha_L >> \alpha_T$**

- **Laboratory experiments: $\alpha_T/\alpha_L \approx 0.1$**

- **Field studies: α_T/α_L from 0.001 to 0.3**

Transport Equation



$$\frac{\partial c}{\partial t} = -\nabla \cdot \left(\vec{j}_{adv}\right) - \nabla \cdot \left(\vec{j}_{diff}\right) - \nabla \cdot \left(\vec{j}_{disp}\right) \pm S$$

$$\Uparrow \qquad\qquad \Uparrow \qquad\qquad \Uparrow$$

$$\vec{u}c \qquad -D_m \nabla c \qquad -D\nabla c$$

Temporal change in concentration	Advection	Diffusion	Dispersion	Sources and Sinks

Solution 2-D: c = f (x, y, t)

Required: Initial and boundary conditions

1-D Transport Equation

$$D\frac{\partial^2 c}{\partial x^2} - u\frac{\partial c}{\partial x} = \frac{\partial c}{\partial t}$$

A measure for the ratio of advective/dispersive transport is given by the PECLET-number:

$$Pe = \frac{L\,u}{D_L} = \frac{L\,u}{\alpha_L\,u}$$

where L: typical length scale of transport phenomenon

$$Pe = 0, \quad \text{pure dispersive transport}$$
$$Pe = \infty, \quad \text{pure advective transport}$$

The transport equation is a hyperbolic **P**artial **D**ifferential **E**quation

Neglecting the advective term the transport equation becomes a parabolic PDE. Then it is of the same type as the flow equation.

$$D\frac{\partial^2 h}{\partial x^2} = \frac{\partial h}{\partial t} \quad \text{where } D = \frac{T}{S}, \text{("diffusivity" of aquifer)}$$

Boundary Conditions

1. type (Dirichlet): $\quad c\,(\text{boundary}) = f\,(t)$

2. type (Neumann): $\quad \dfrac{\partial c}{\partial n}(\text{boundary}) = f\,(t)$

3. type (Cauchy): $\quad \alpha\, c\,(\text{boundary}) + \beta\,\dfrac{\partial c}{\partial n}(\text{boundary}) = f\,(t)$

Physical meaning

1. type: specifies advective flux over boundary.

$$u_n\, c$$

2. type: specifies diffusive/dispersive flux over boundary.

$$-D\,\frac{\partial c}{\partial n}$$

3. type: specifies total flux over boundary.

$$u_n\, c \; - D\,\frac{\partial c}{\partial n}$$

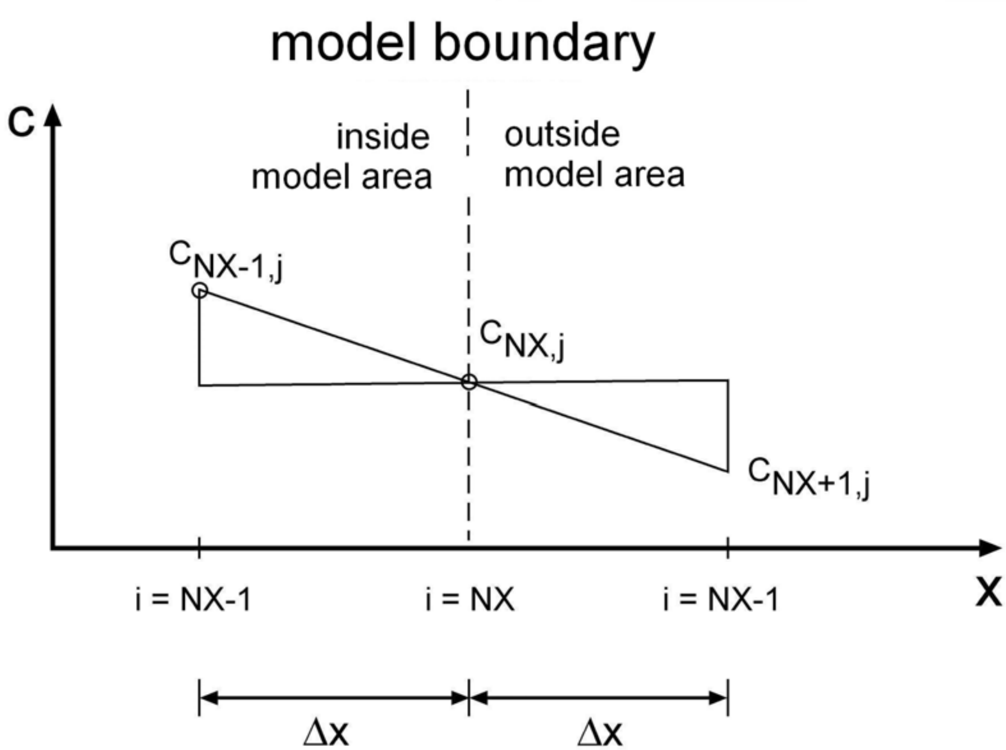
Initial Conditions

Concentration distribution c (x, y, t) at time t_0

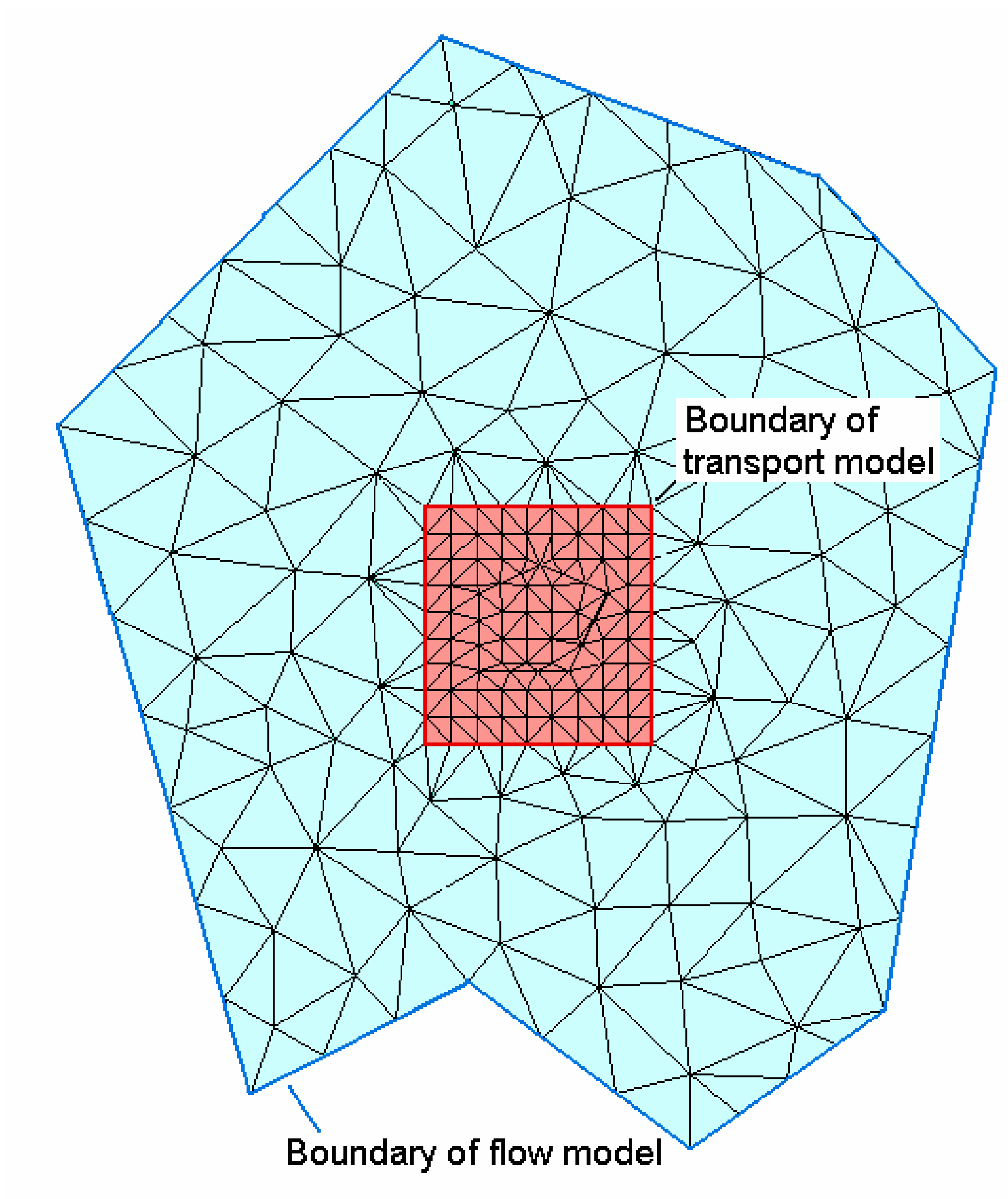
Choice of Boundary Conditions

- If model area is large enough to contain the total plume: 1. type boundary everywhere (c(boundary) = 0.
- At impervious boundaries: 2. type boundary: $\partial c/\partial n(\text{boundary}) = 0$.
- Transmission boundary: Extrapolate gradient beyond boundary.

$$\frac{c_{Nx,j} - c_{Nx-1,j}}{\Delta x_{Nx-1}} = \frac{c_{Nx+1,j} - c_{Nx,j}}{\Delta x_{Nx}}$$



Embedding of a Transport Model in a Flow Model



Refined grid for the transport model within a coarse grid for the flow model.

Solution Methods for the Transport Equation

Analytical Solutions:

- Simple flow conditions
- Simple boundary and initial conditions
- Assumption of homogeneity

Neglecting Diffusion / Dispersion:

- Pathlines
- Concentrations along pathlines
- Traveltimes and isochrones

Numerical Solution of Complete Equation:

- Grid methods:

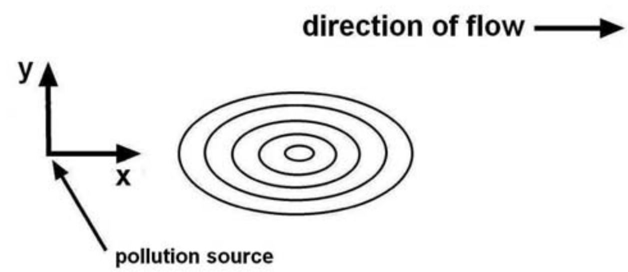
  Finite-Differences-, Finite-Volume-, Finite-Elements-method

- Particle-tracking methods:

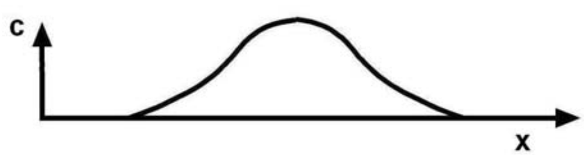
  Method of characteristics, Random-Walk-method

Instantaneous Pollutant Injection into Parallel Constant Flow

Injection: $t = 0$, $x = 0$, $y = 0$



lines of equal concentration at time t > 0



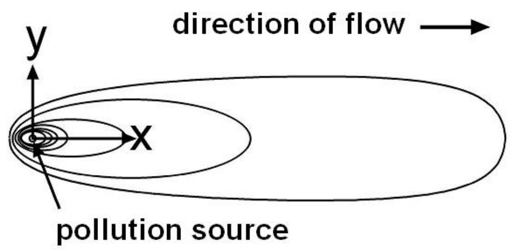
axial concentration distribution at time t > 0

Analytical solution:

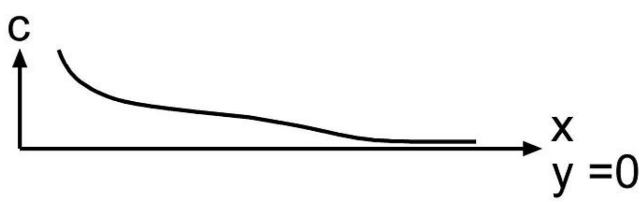
$$c(x,y,t) = \frac{\Delta M}{4\,\pi\,n_f\,m\,u\,\sqrt{\alpha_L\,\alpha_T}\;t}\,\exp\left(-\frac{\left(x - \frac{u}{R}\,t\right)^2}{4\,\alpha_L\,\frac{u}{R}\,t} - \frac{y^2}{4\,\alpha_T\,\frac{u}{R}\,t} - \lambda\,t\right)$$

Permanent Pollutant Injection into Parallel Constant Flow

Injection: t = 0, x = 0, y = 0



lines of equal concentration at time t > 0



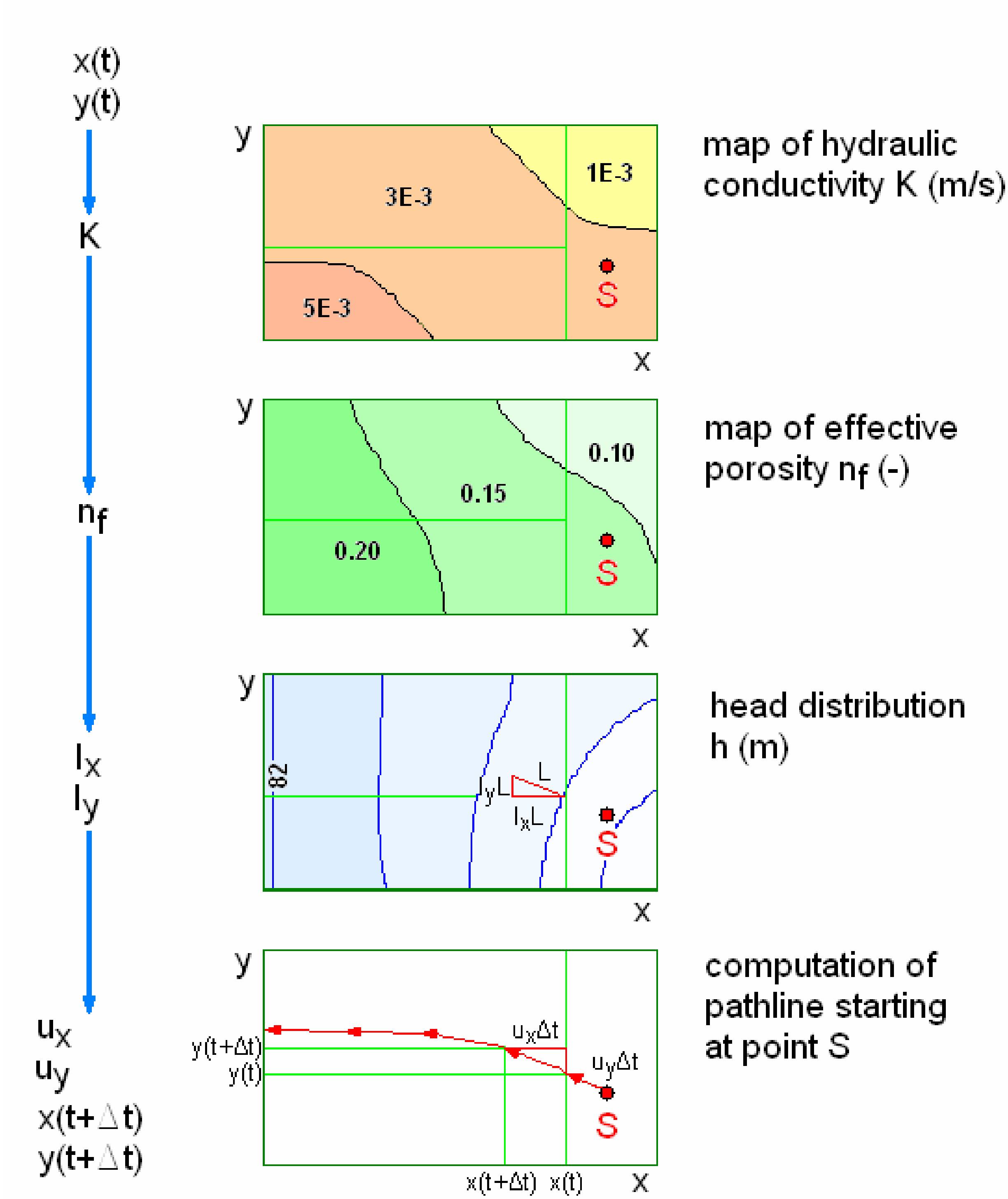
axial concentration distribution a time t > 0

Analytical solution:

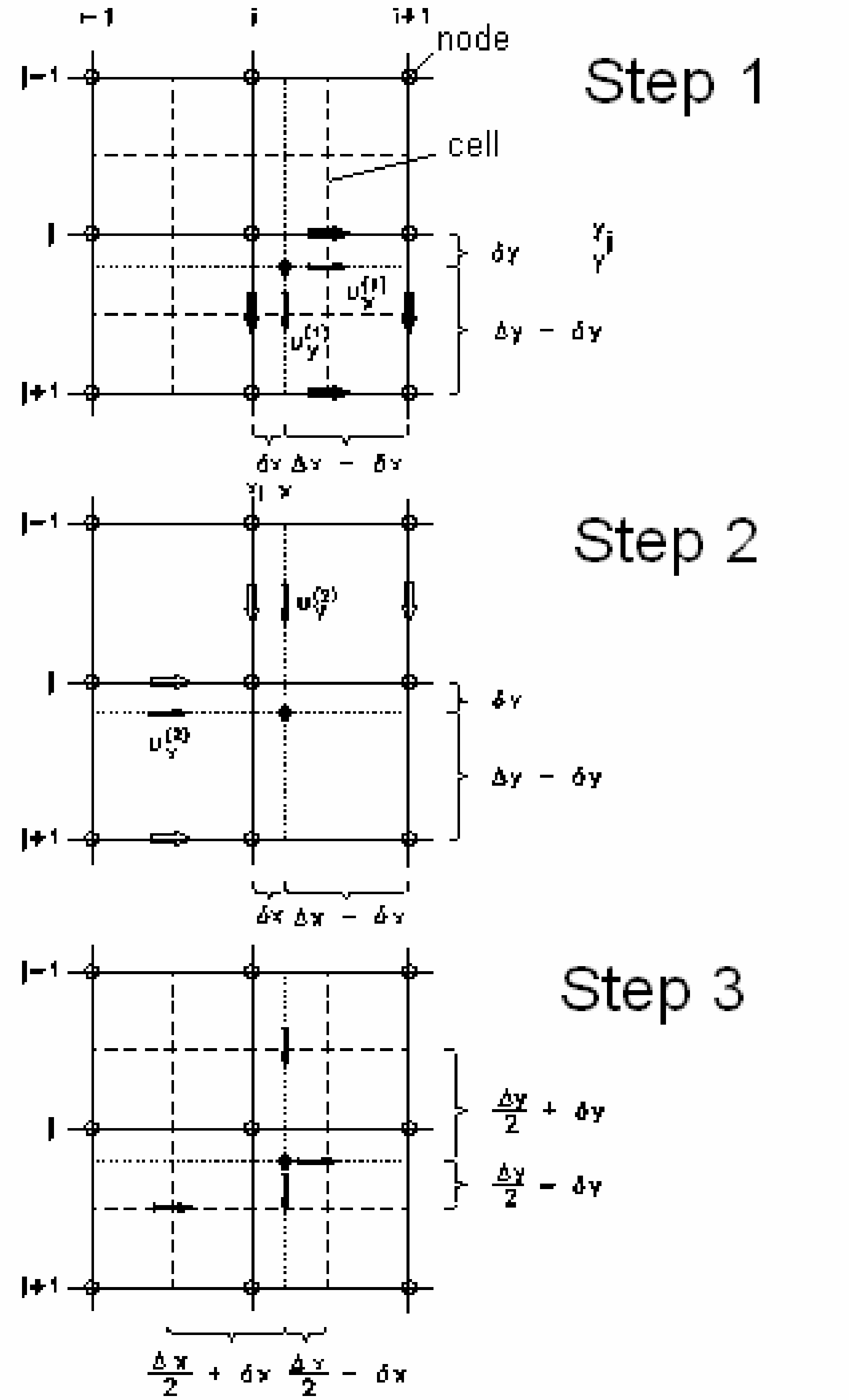
$$c(x,y,t) = \frac{\dot{M}}{4\, n_f\, m\, u \sqrt{\pi\, \alpha_T \gamma}} \exp\left(\frac{x - r\,\gamma}{2\,\alpha_L}\right) \frac{1}{\sqrt{r}}\, \mathrm{erfc}\left(\frac{r - \frac{u}{R}\, t\, \gamma}{2\sqrt{\alpha_L \frac{u}{R} t}}\right)$$

$$r = \sqrt{x^2 + y^2 \frac{\alpha_L}{\alpha_T}}\,, \qquad \gamma = \sqrt{1 + 4\,\alpha_L\, \lambda\, \frac{R}{u}}$$

Construction of Pathlines

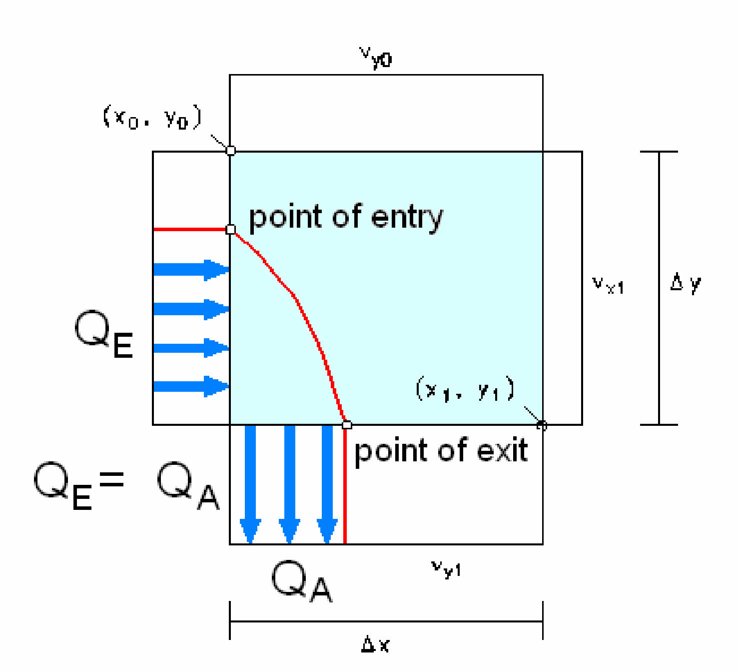


PRICKETT'S Method



Velocity interpolation after PRICKETT et al. (1981).

POLLOCK's Method



Given: Flow distribution along cell boundary. No sinks and sources in the interior.

Pathline: For point of entry the point of exit follows immediately from continuity. Interpolation between the points is made on the basis of linear interpolation of velocities v_x in x-direction v_y in y-direction. Analytical solution exists.

$$v_x = a_x (x - x_1) + v_{x1}$$

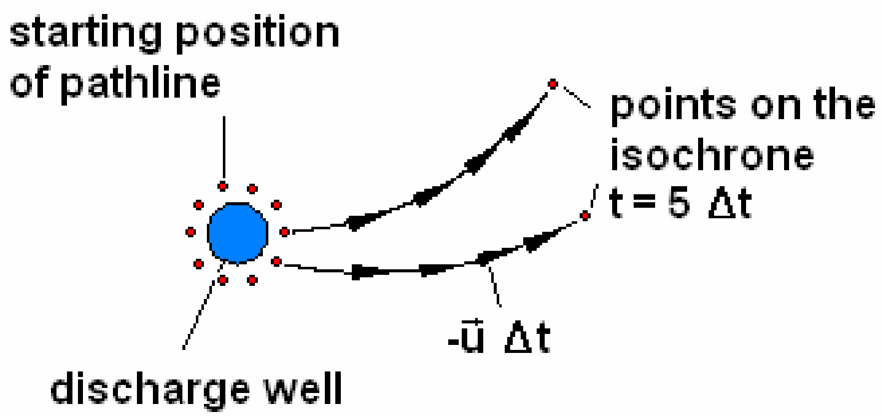
$$v_y = a_y (y - y_1) + v_{y1}$$

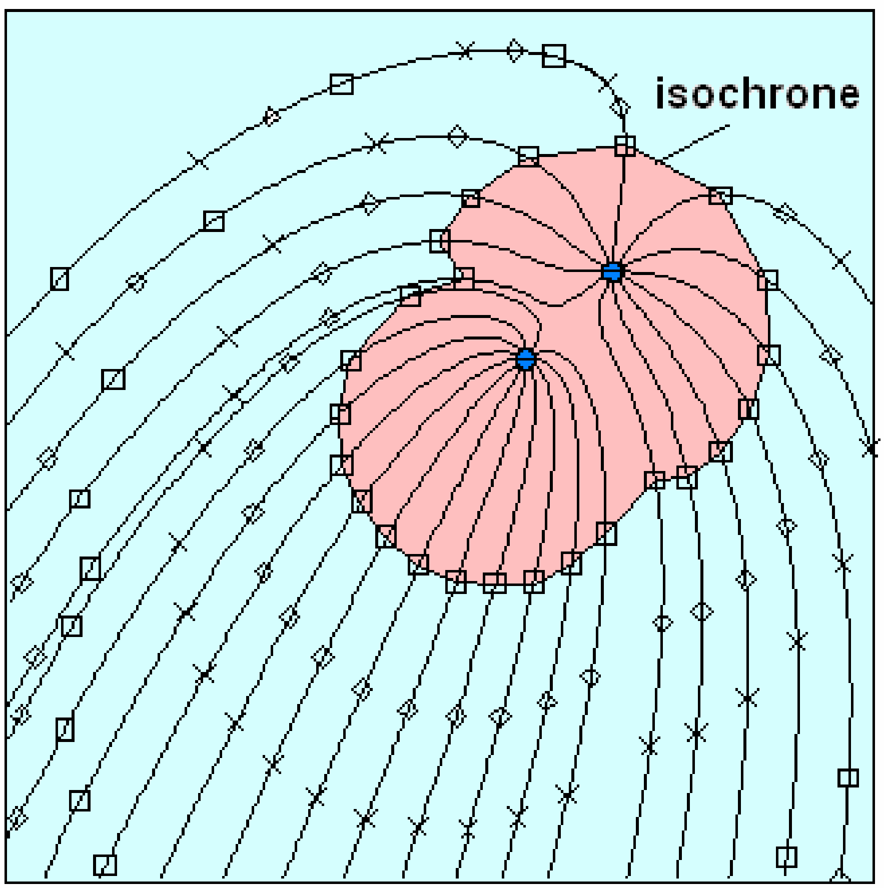
$$x(t_2) = x_1 + \frac{1}{a_x} (v_{xp}(t_1)\, e^{a_x \Delta t} - v_{x1})$$

$$y(t_2) = y_1 + \frac{1}{a_y} (v_{yp}(t)\, e^{a_y \Delta t} - v_{y1})$$

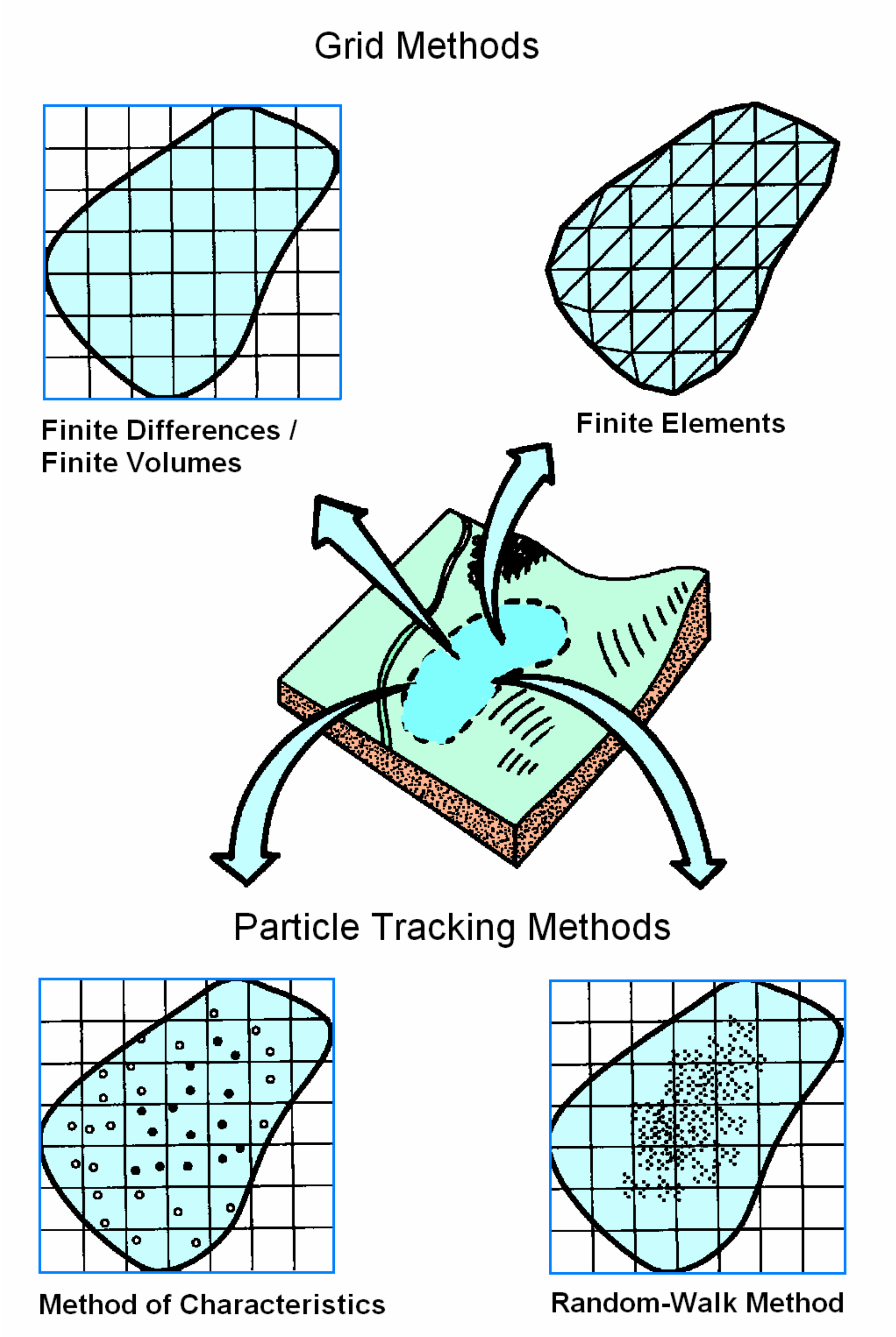
$$\text{where} \quad a_x = \frac{v_{x2} - v_{x1}}{\Delta x}, \quad a_y = \frac{v_{y2} - v_{y1}}{\Delta y}$$

Numerical Computation of Isochrones

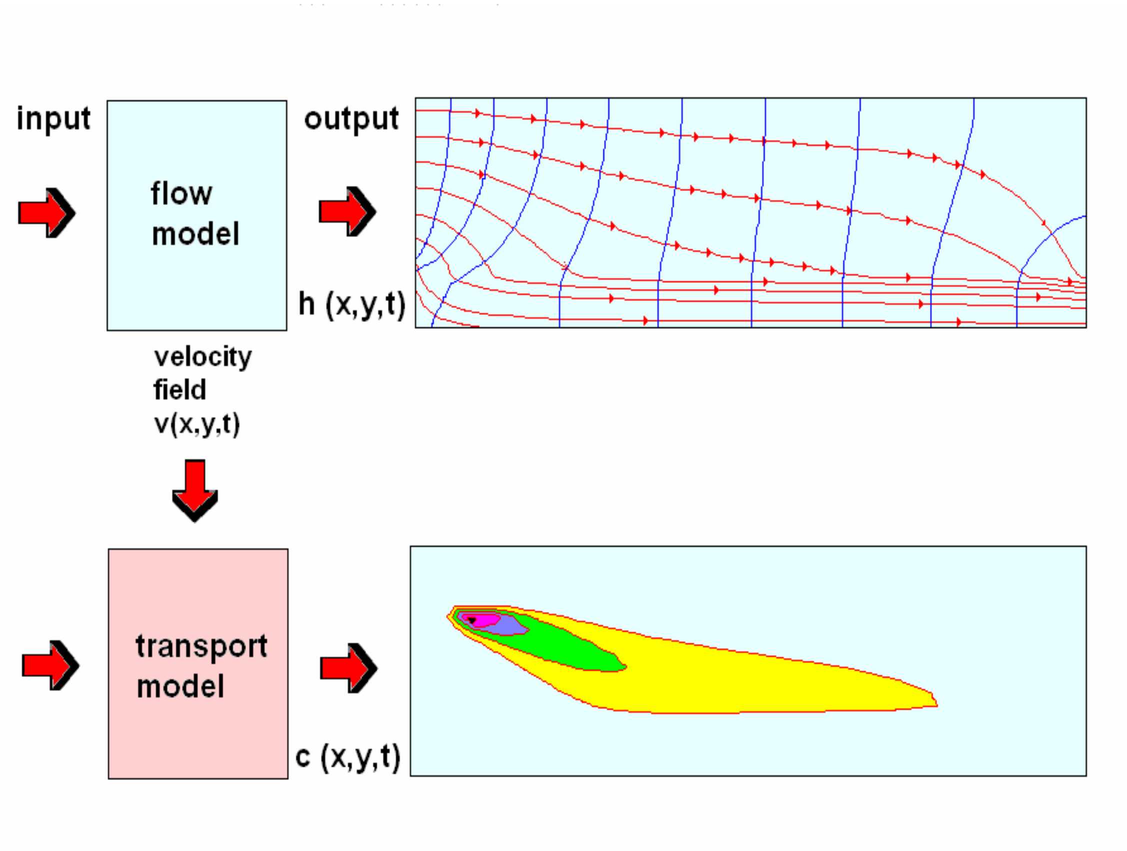




Numerical Solution Methods

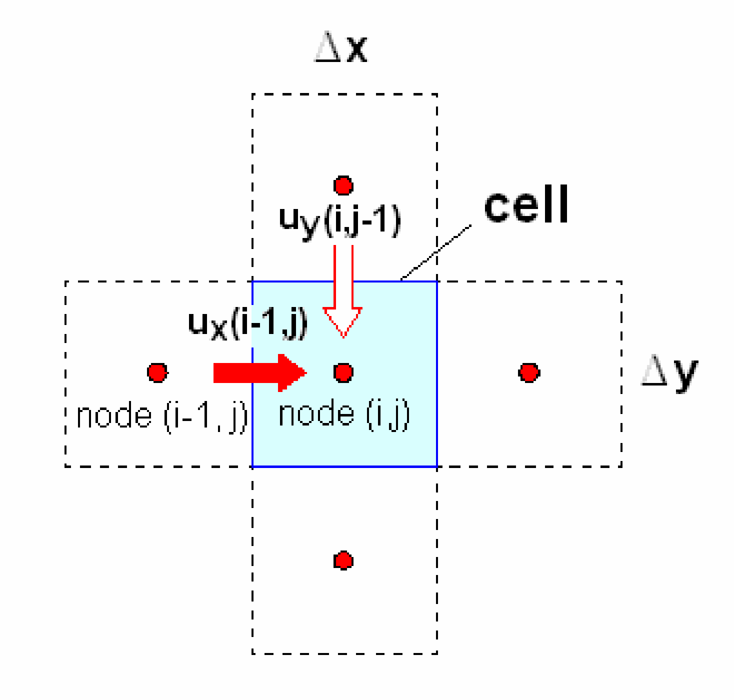


Relation between Groundwater Flow and Solute Transport Models



Note: In case of hydrodynamic inactive pollutants flow and transport processes are not coupled!

Advection: Mass Balance over Time Interval (t, t + Δt)



Advective input from cell (i-1,j) to cell (i,j)

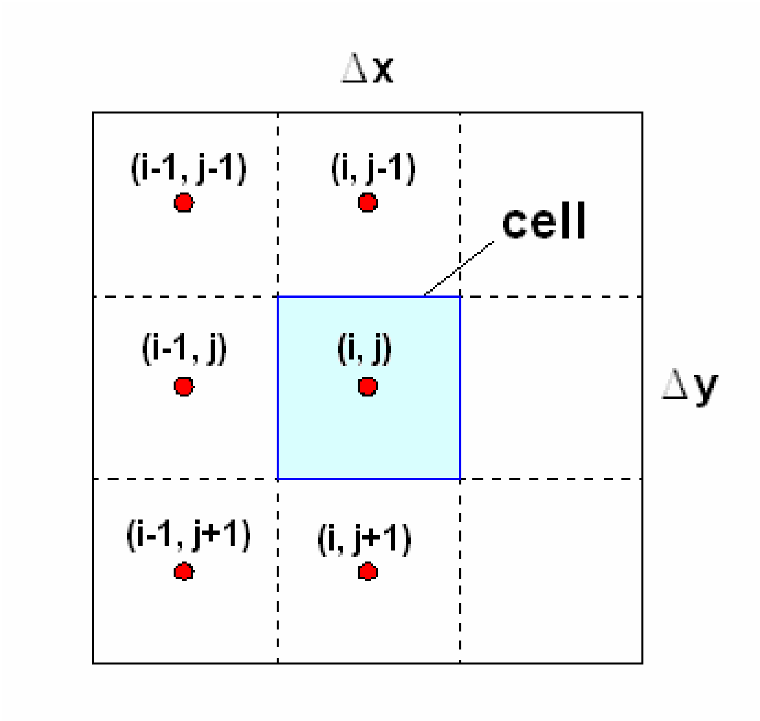
$$\Delta t\, u_x(i-1, j)\, m\, \Delta y\, n_f\, c$$

Concentration (c) at what time and at which node ?

1. $c = c(t)$ $\Rightarrow$ explicit
2. $c = c(t + \Delta t)$ $\Rightarrow$ implicit
3. $c = c_{i-1,j}$ $\Rightarrow$ upwind
4. $c = \frac{1}{2}(c_{i-1,j} + c_{i,j})$ $\Rightarrow$ central

Note: "Upwind" if advection dominates
"Central" if dispersion dominates

Dispersion: Mass Balance over Time Interval (t, t + Δt)



Dispersive flux from cell (i-1,j) to cell (i,j)

1. $-\Delta t\, D_{xx}\, m\, \Delta y\, n_f\, \dfrac{c(i,j)-c(i-1,j)}{\Delta x}$

2. $-\Delta t\, D_{xy}\, m\, \Delta y\, n_f\, \dfrac{(c(i-1,j+1)-c(i-1,j-1))+(c(i,j+1)-c(i,j-1))}{2\, \Delta y\, 2}$

(1) $c = c(t)$ $\Rightarrow$ explicit

(2) $c = c(t+\Delta t)$ $\Rightarrow$ implicit

or

$c = \kappa\, c(t) + (1-\kappa)\, c(t+\Delta t)$ $(\kappa = 1/2 \Rightarrow$ Crank–Nicolson$)$

Equation Systems Transport

Explicit:

$$c_{i,j}(t+\Delta t) = f\,(c_{i,j}(t), c_{i-1,j}(t), c_{i+1,j}(t), c_{i-1,j-1}(t), c_{i+1,j-1}(t), \\ c_{i-1,j+1}(t), c_{i+1,j+1}(t), c_{i,j-1}(t), c_{i,j+1}(t))$$

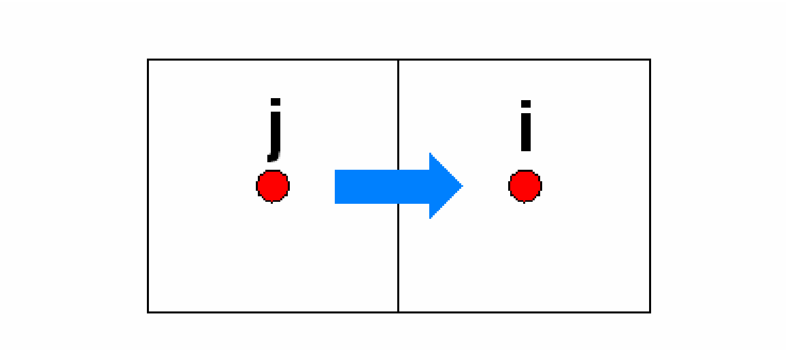
Implicit:

$$\begin{aligned}
&A_{i,j}\ c_{i,j}(t+\Delta t) + B_{i,j}\ c_{i-1,j}(t+\Delta t) + C_{i,j}\ c_{i+1,j}(t+\Delta t) + \\
&D_{i,j}\ c_{i-1,j-1}(t+\Delta t) + E_{i,j} c_{i+1,j-1}(t+\Delta t) + F_{i,j} c_{i-1,j+1}(t+\Delta t) + \\
&G_{i,j}\ c_{i+1,j+1}(t+\Delta t) + H_{i,j}\ c_{i,j-1}(t+\Delta t) + I_{i,j}\ c_{i,j+1}(t+\Delta t) \\
&= K_{i,j}
\end{aligned}$$

or after transformation to single indices:

$$\sum_{j=1}^{N} A_{i,j}\ c_j(t+\Delta t) = B_i, \qquad i = 1, ..., N$$

Form of System Matrix due to Advection



$$\text{Advective flux} = -u\,\Delta y\, m\, n_f\, c'(t')$$

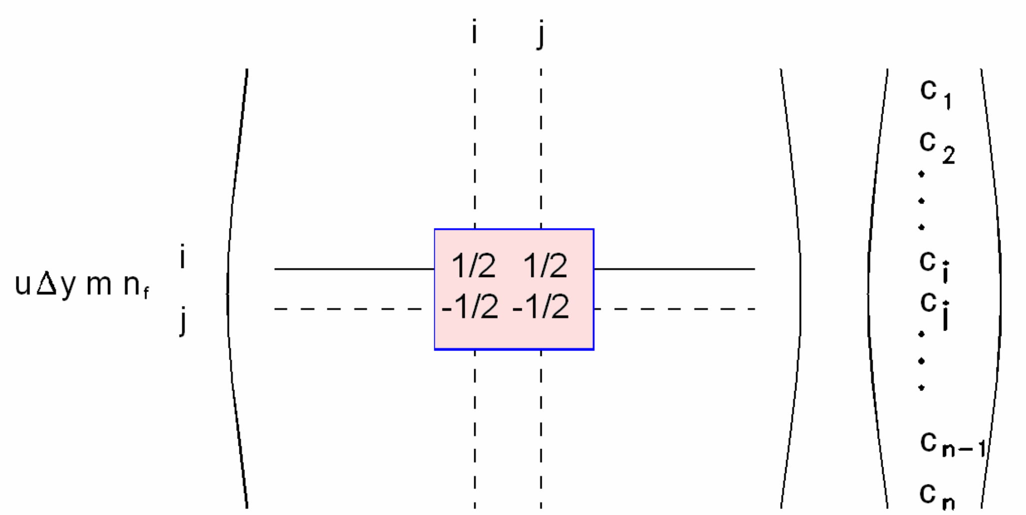
upwind : $\quad c' = c_j$

central : $\quad c' = (c_i + c_j)/2$

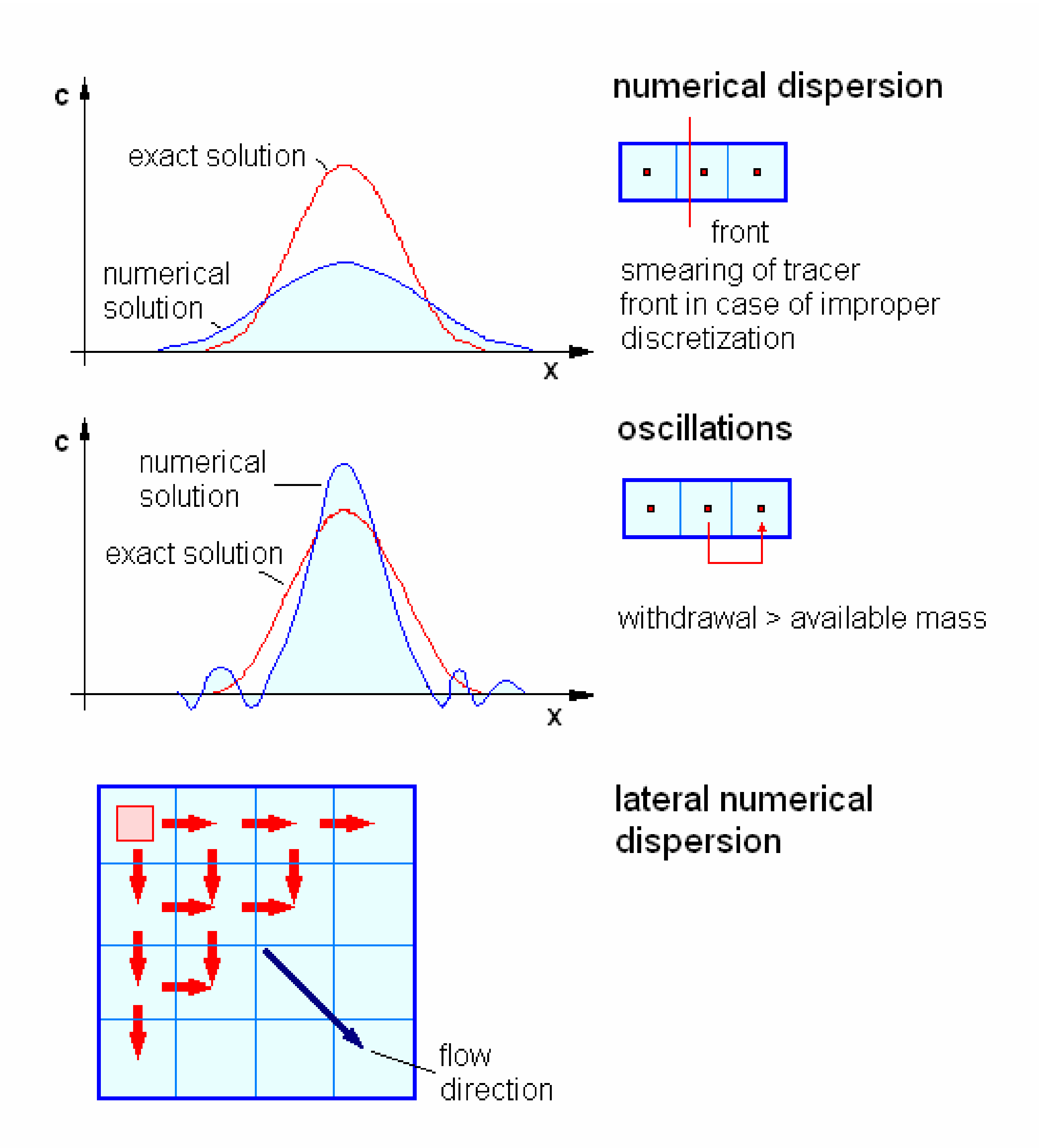
explicit : $\quad t' = t$

implicit : $\quad t' = t + \Delta t$

Asymmetric matrix!



Numerical Dispersion



Numerical Dispersion:

Rules for discretization

- **Courant number:**

$$Co_x = \left|\frac{u_x \Delta t}{\Delta x}\right|, \quad Co_y = \left|\frac{u_y \Delta t}{\Delta y}\right|$$

$$Co_x \le 1, \quad Co_y \le 1 \quad (\text{better}: Co_x + Co_y < 1)$$

(advection => small time steps required)

- **Grid Peclet number:**

$$Pe_x = \left|\frac{u_x \Delta x}{D_{xx}}\right| = \left|\frac{\Delta x}{\alpha_L}\right|, \quad Pe_y = \left|\frac{u_y \Delta y}{D_{yy}}\right| = \left|\frac{\Delta y}{\alpha_T}\right|$$

$$Pe_x \le 2, \quad Pe_y \le 2 \quad (\Delta\Delta \le 2\alpha_L)$$

(dispersion => small cells required)

- **Requirement for the adequate resolution of a plume in transverse direction:**

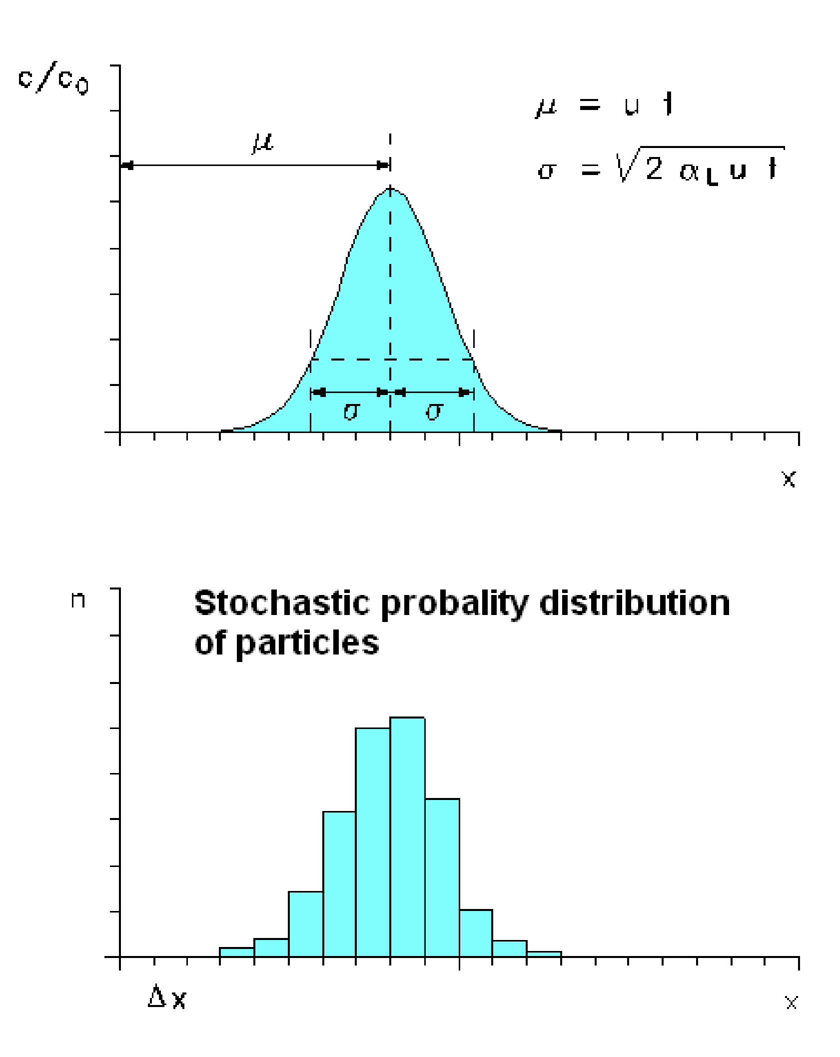
$$\Delta x = \alpha_T \quad \text{near the pollutant source}$$

Random Walk Method

Basic Idea

- Particle tracking method
- Each particle is assigned the same fixed mass
- Advective transport is simulated by moving particles along pathlines
- Dispersive transport is simulated by superimposing the advective particle movement with a random movement possessing properties that correspond to the properties of the dispersive process
- Sources and sinks are modeled by adding and annihilating particles
- The concentration distribution is obtained by overlaying a grid, counting the number of particles per grid cell, and dividing the total mass of the particles by the corresponding water volume

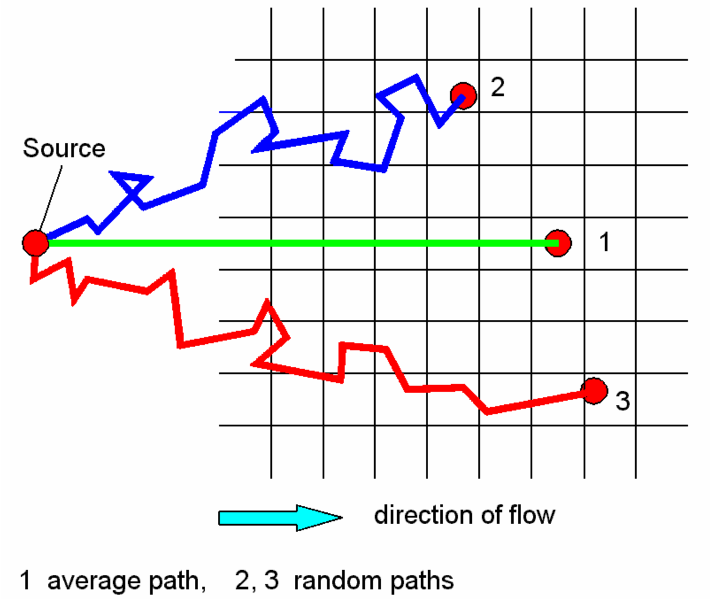
Interpretation of Concentration Distribution by Probability Distribution



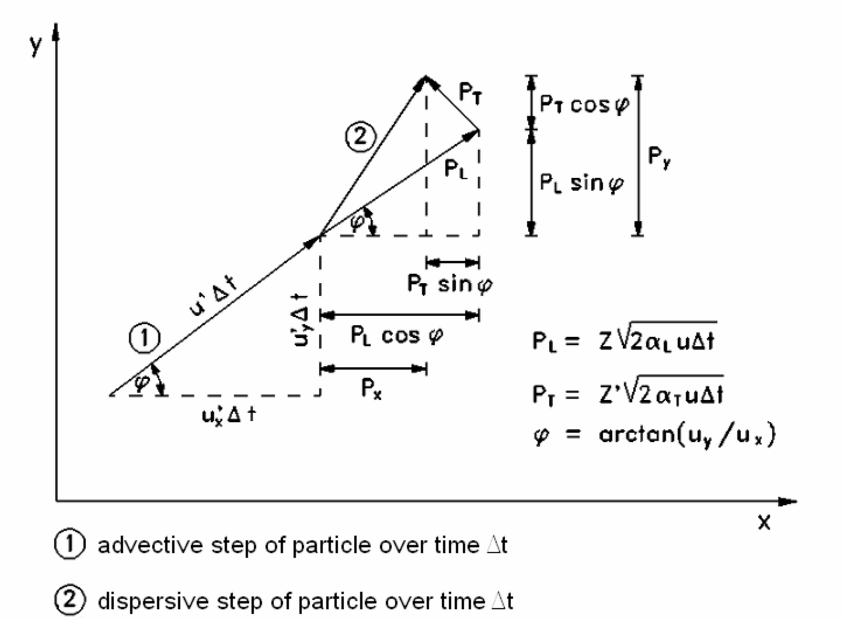
$$c(x,t) = \frac{\Delta M}{2\,A\,n_f\,\sqrt{\pi\,\alpha_L\,u\,t}}\,\exp\left(-\frac{(x - u\,t)^2}{4\,\alpha_L\,u\,t}\right)$$

$$c(x,t) = \frac{\Delta M}{N\,A\,n_f\,\Delta x}\,n\,(x - 0.5\,\Delta x\,,\,x + 0.5\,\Delta x\,,\,t)$$

Example of 2-D Random Paths



Tensorial Properties of Dispersive Displacement



Random Walk Method

Advantages

- No numerical dispersion
- Most powerful method for extreme anisotropy of dispersion
- Parallel computing possible
- Zero dispersivity yields pathlines
- Generalizable to non-Fickian behavior

Disadvantages

- Stochastic fluctuations
- Low local concentrations insignificant
- Many particles required
- Total flux boundaries difficult to model
- Nonlinear chemistry not possible

Basis of Method of Characteristics

$$\frac{\partial c}{\partial t} + u_x \frac{\partial c}{\partial x} + u_y \frac{\partial c}{\partial y} = \nabla (\mathbb{D}\,\nabla c) + S$$

$$\Updownarrow$$

$$\frac{dc\,(x(t), y(t))}{dt} = \nabla (\mathbb{D}\,\nabla c) + S$$

$$(x(t), y(t)) \quad \text{pathline from:}$$

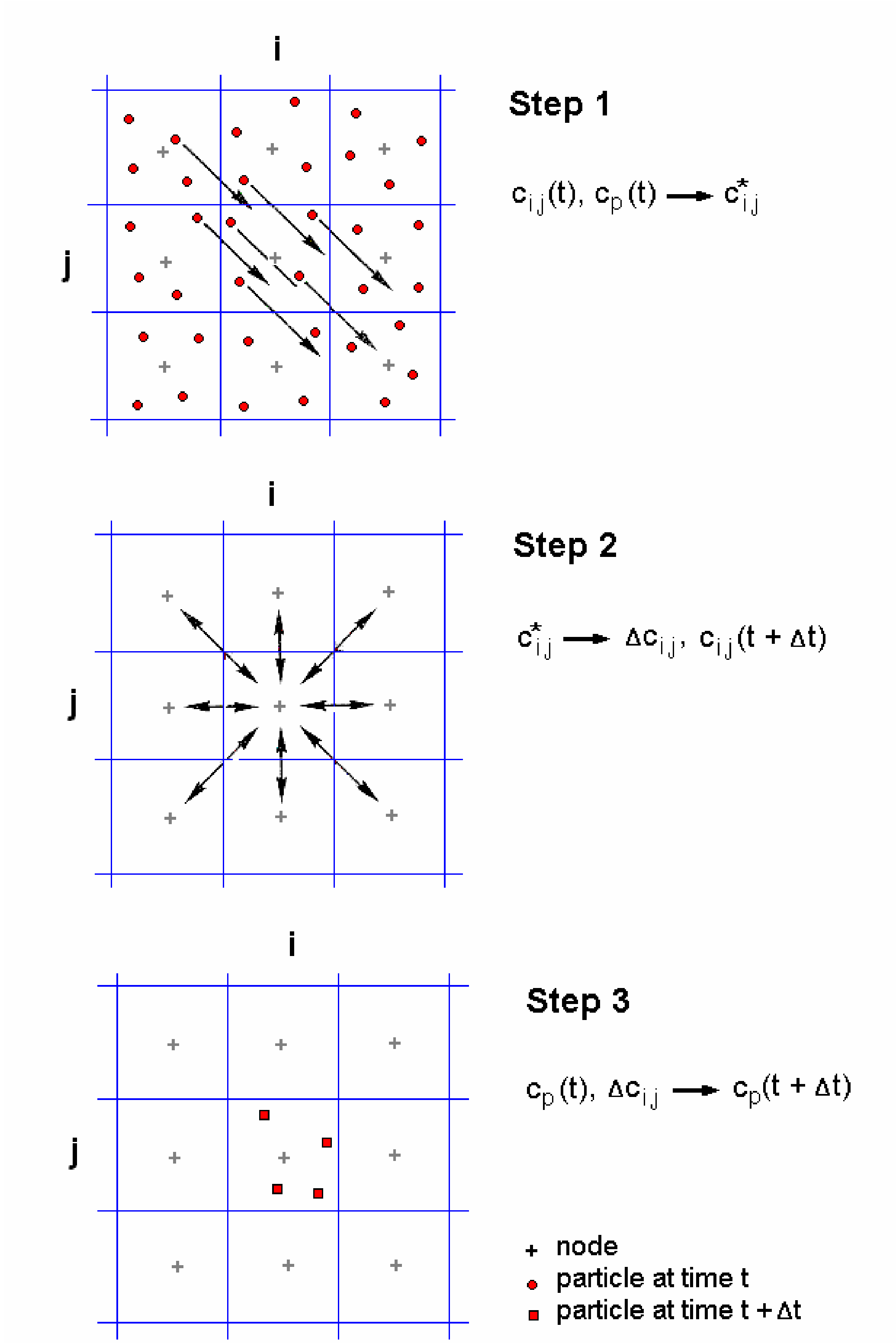
$$u_x = \frac{dx(t)}{dt}$$

$$u_y = \frac{dy(t)}{dt}$$

Implementations:

- **moving grids**
- **particle tracking**

Computational Steps in the Method of Characteristics



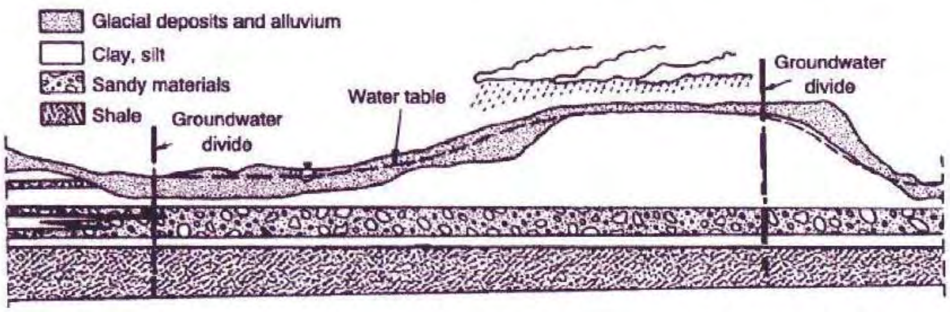
Process of Modeling

Process of Modeling

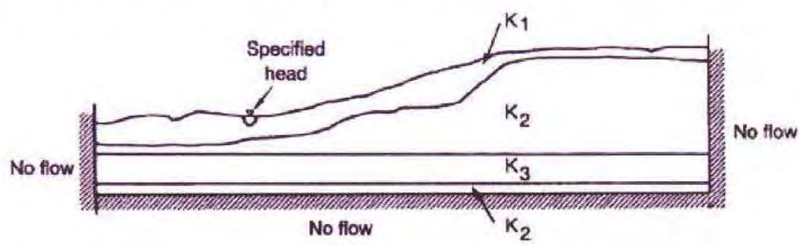
- Model objectives
- Collection and interpretation of data
- Development of hydrogeological model
- Choice of model type
- Modeling software selection / programing
- Model design
- Model calibration
- Sensitivity analysis
- Model validation
- Model application and performance of prognostic runs
- Analysis of results
- Iteration of any of the steps above
- Post-auditing

Process of Modeling

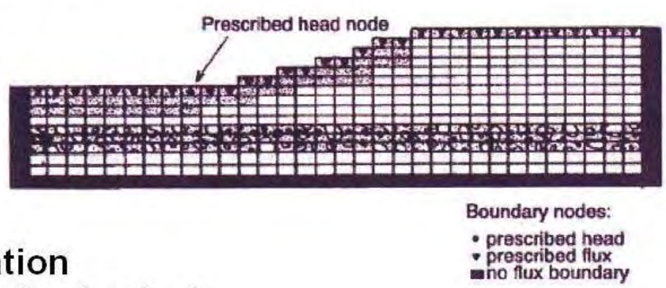
Collection and Interpretation of Data



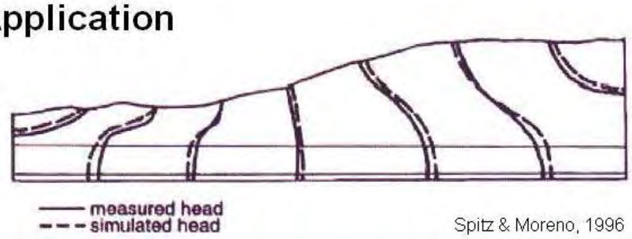
Development of the Hydrogeological Model



Model Design



Calibration
Sensitivity Analysis
Validation
Model Application



Spitz & Moreno, 1996

Analysis of Results
Post-Auditing

Model Objectives

- **Identification of question(s) to be answered**
- **Defining the purpose of the model**

Note: The modeling objectives will profoundly impact the modeling effort required.

Collection and Interpretation of Data

- Understanding the natural system
- Input data for flow models
- Input data for transport models

Input Data for Flow Models

- **Geometry:**

  shape of model area
  elevation of aquifer bottom and top
  thickness of aquifer

- **Aquifer parameters:**

  hydraulic conductivity / transmissivity
  specific storage / storage coefficient

- **Inflows / outflows**

  well discharge / recharge
  groundwater recharge by precipitation
  boundary flows
  ex- / infiltrations from surface water bodies

- **Prescribed heads**

- **Observed discharges**

  e.g. spring discharge etc.

Input Data for Transport Models

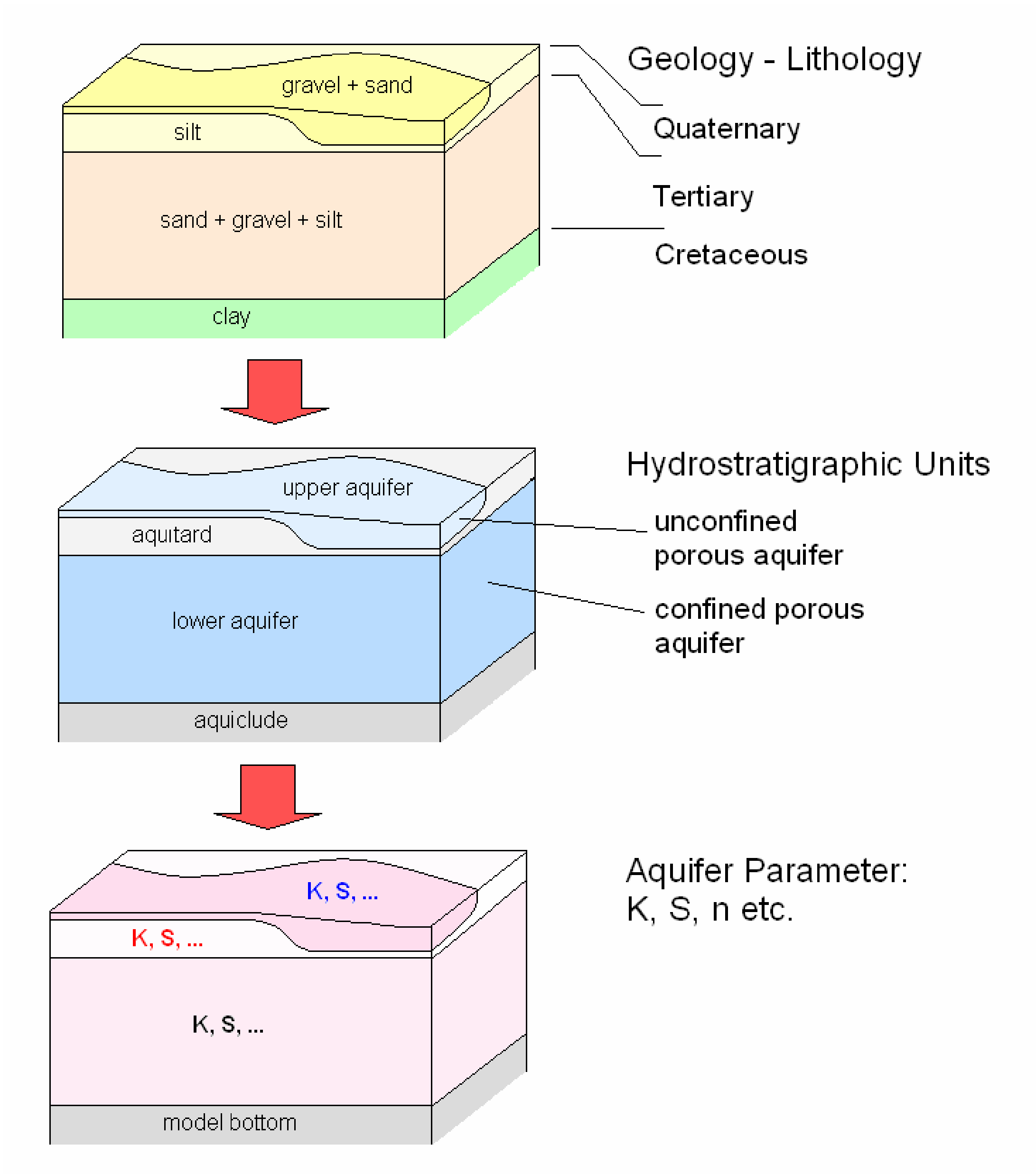
- **effective porosity**
- **dispersivities**
- **input and abstraction of pollutants**
- **decay constant**
- **adsorption parameters**

Development of the Hydrogeological Model (Conceptual Model)

- **Characterizing aquifers (simplification)**
- **Identifying of hydrostratigraphic (hydrogeological units)**
- **Identifying system boundaries, choice of model domain (horizontal, vertical)**
- **Defining boundary conditions and initial conditions (hints for model boundaries)**
- **0-D-Balances**

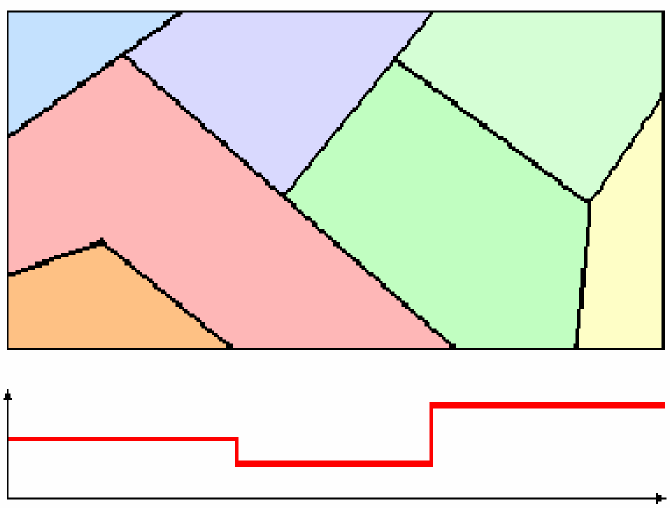
Note: Experience needed. Mistakes in the hydrogeological (conceptual) model can not be corrected in model calibration!

Steps in the Development of the Hydrogeological Model

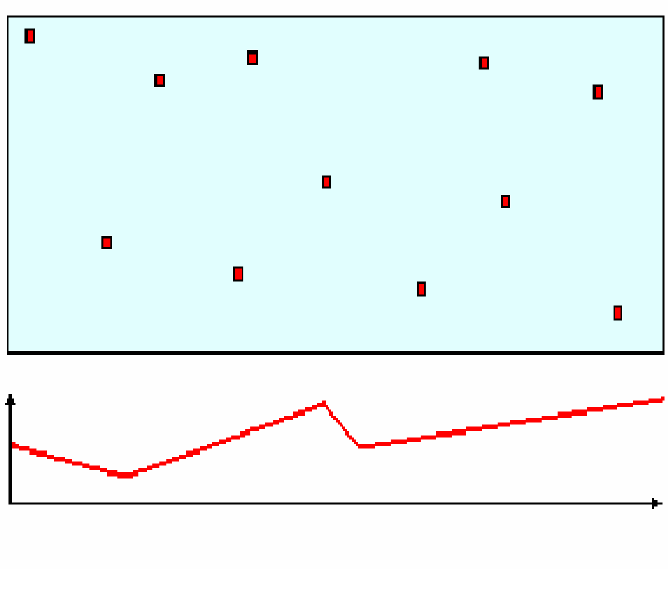


Concepts for Parameterization of Spatial Structures

Reduction of degree of freedom by:



Zonation (N zones)

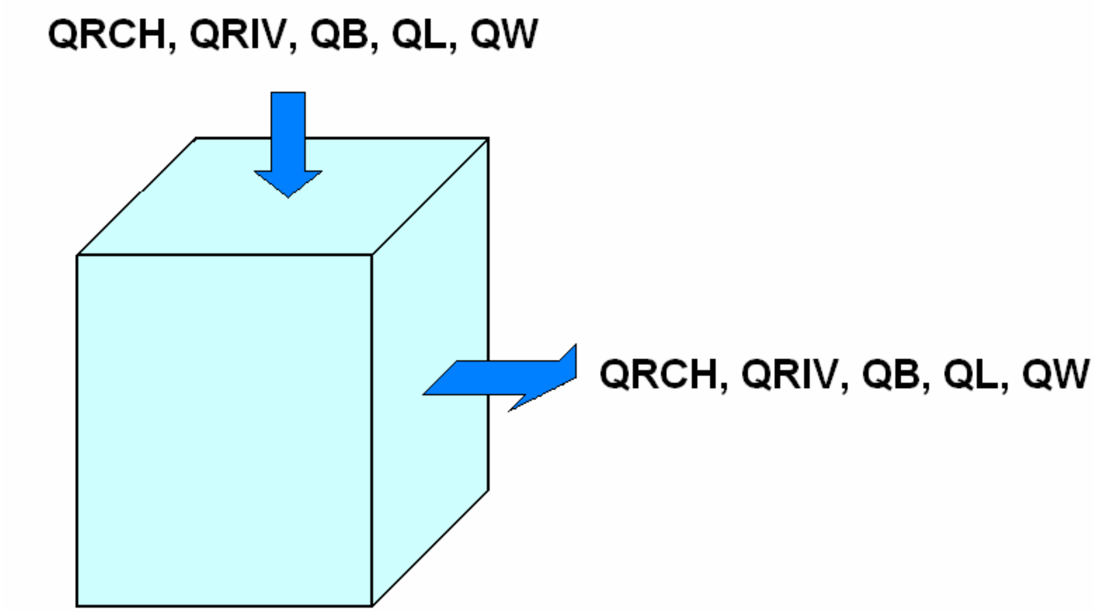


Interpolation and pivot points

Rules for Model Boundaries

- **Make use of natural hydrogeological boundaries (e.g. rivers, groundwater divides)**
- **Use as few prescribed heads as possible**
- **Use prescribed heads at downstream boundaries. In the upstream use flux boundaries**
- **Make use of general head boundaries in case of distant prescribed heads**
- **If you use streamline boundaries in connection with wells, make sure that total discharge in the stream tube is much larger than well discharge**

Water Balance Model (Box Model)



Change in Storage =

$$(\pm \mathbf{QRCH} \ \pm \mathbf{QRIV} \pm \mathbf{QB} \pm \mathbf{QL} \pm \mathbf{QW})\ \Delta \mathbf{t}$$

QRCH: natural groundwater recharge or discharge
QRIV: exchange with surface water bodies
QB: subsurface flow over boundary
QL: leakage flow from and to adjacent aquifers
QW: infiltration or exfiltration (e.g. wells)

Note: The 0-D water budget of an aquifer is a prerequisite for every groundwater flow model!

Choice of Model Type

- **Physical options**
- **Dimensionality**
- **Space and time**
- **Solution method**

Modeling Software Selection / Programing

You must convince yourself that the code is verified. If you write a program, then you have to verify it.

Model Design (Input Parameters)

Puts the hydrogeological model in a form suitable for modeling

- **Input parameters for flow models**
- **Input parameters for transport models**
- **Design of model grid**
- **Selecting of time discretization**
- **Use of GIS**

Design of Model Grids

- Locate well nodes near the physical location of a single pumping well or center of a well field.

- Use variable grid distances. For distant boundaries the grid may be expanded. But avoid large spacing next to small ones.

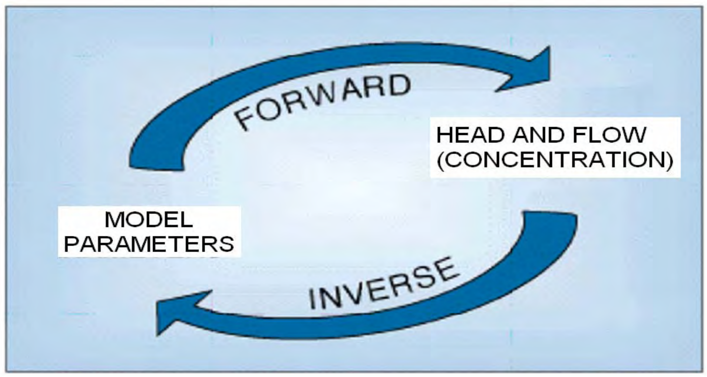
- Nodes should be closer together in areas where there are large spatial changes in transmissivity or hydraulic head.

- Align axes of grid with the major directions of anisotropy (that is, orientate grid with the major trends)

Model Calibration

- **Forward ("direct") problem / inverse problem**
- **Simulation of historical records**
- **Calibration steps**
- **Rules for manual calibration**
- **Identification problem of steady state calibration (non uniqueness)**
- **Calibration of 3-D models**
- **Trial and error**
- **Automatic calibration**

Forward and Inverse Approaches



Forward ("Direct") Problem

Given: parameters, boundary and initial conditions
Wanted: head / flow distribution (or concentration)

Usually parameters are not known completely! Therefore a calibration (i.e. completion of parameters) using measurements of heads / flows (or concentration) is required.

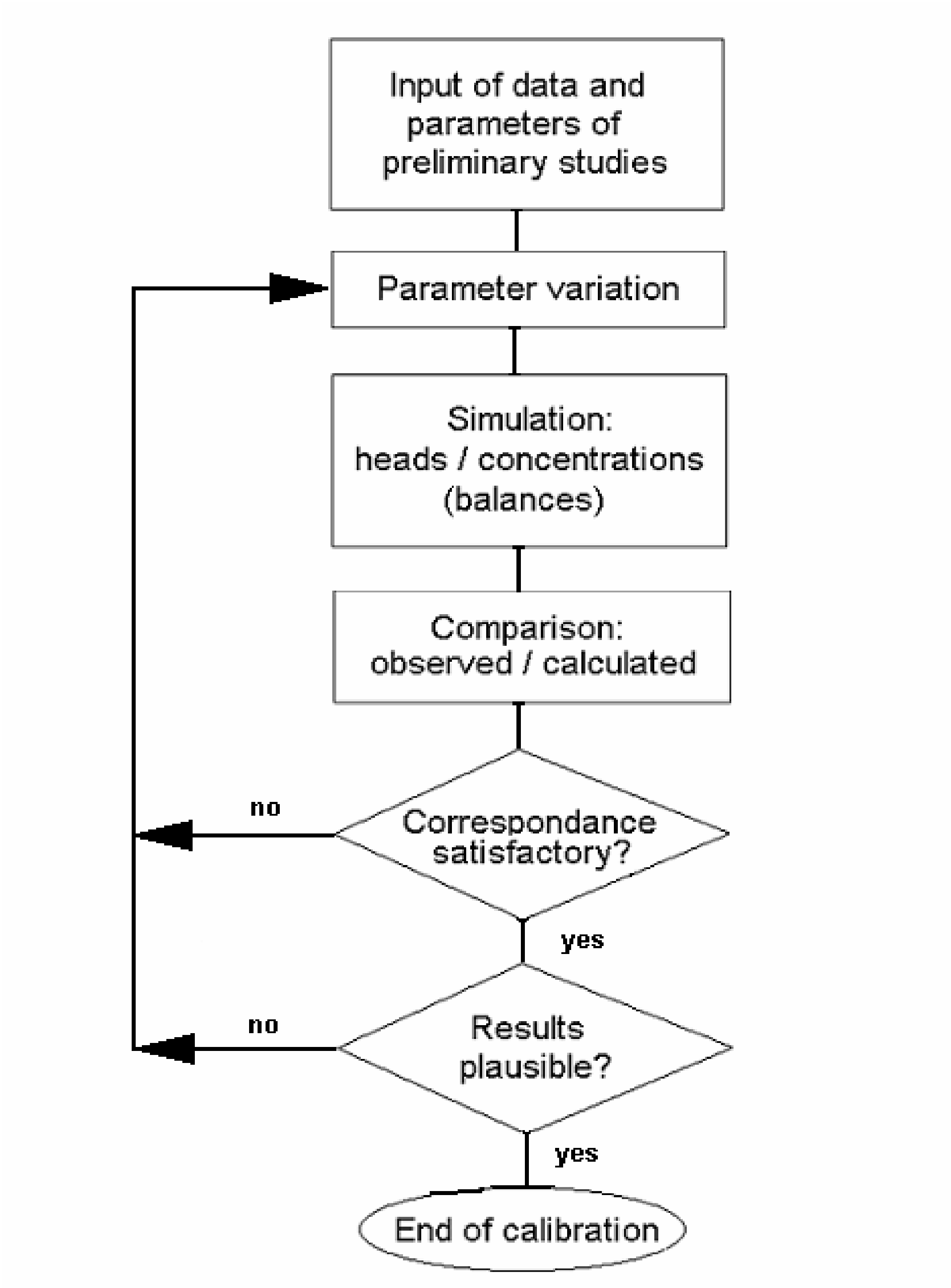
Inverse Problem

Given: heads / flows, (concentrations)
Wanted: parameter distribution

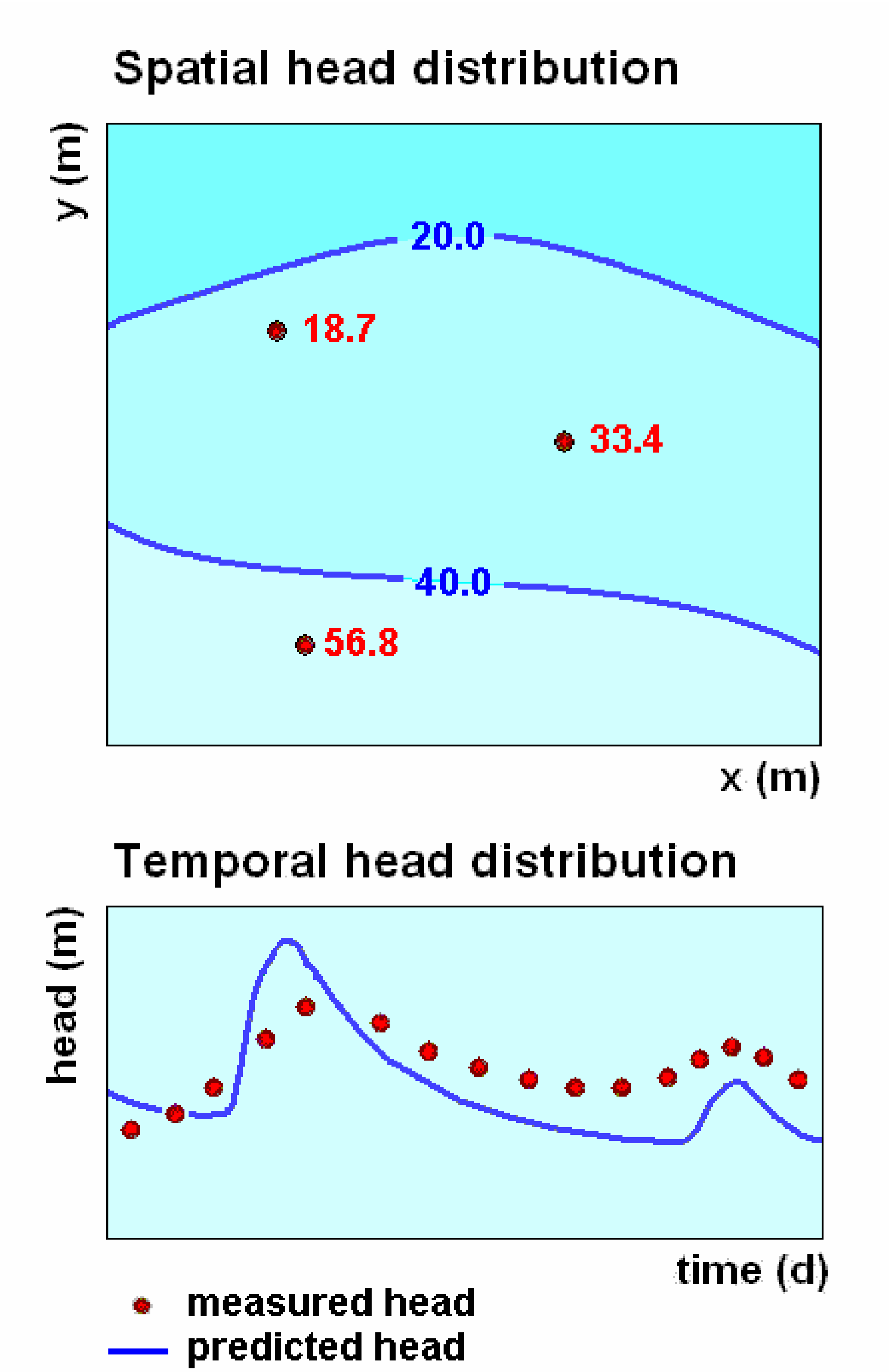
Problem: ill-posedness
No unique solution may exist
Measurement errors make result unreliable

Ways out: Reduction of degrees of freedom and regression
Introduction of "a priori" knowledge
Joint use of head, flow and / or concentration measurements
Estimation of uncertainty

Flowchart: Model Calibration



Comparison of Measured and Predicted Heads

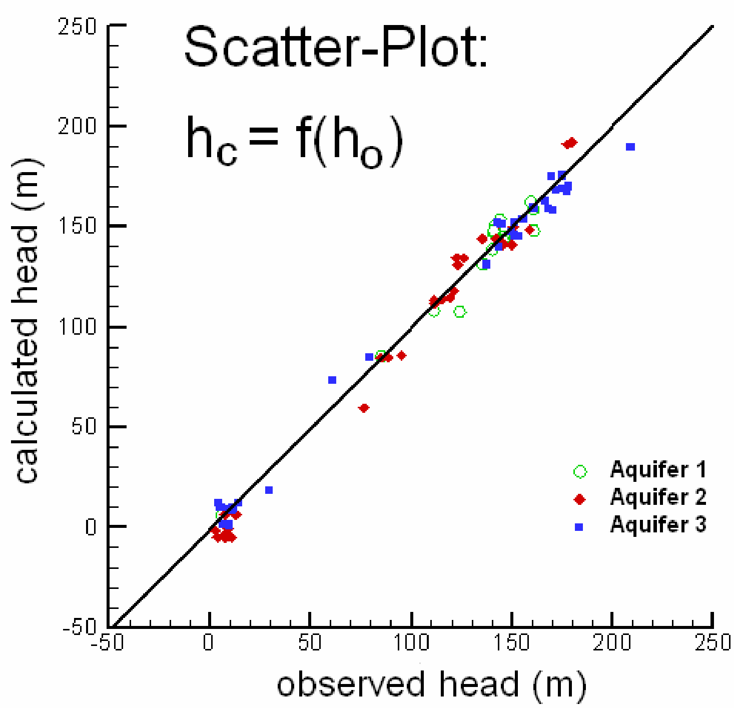


Rules for Manual Calibration

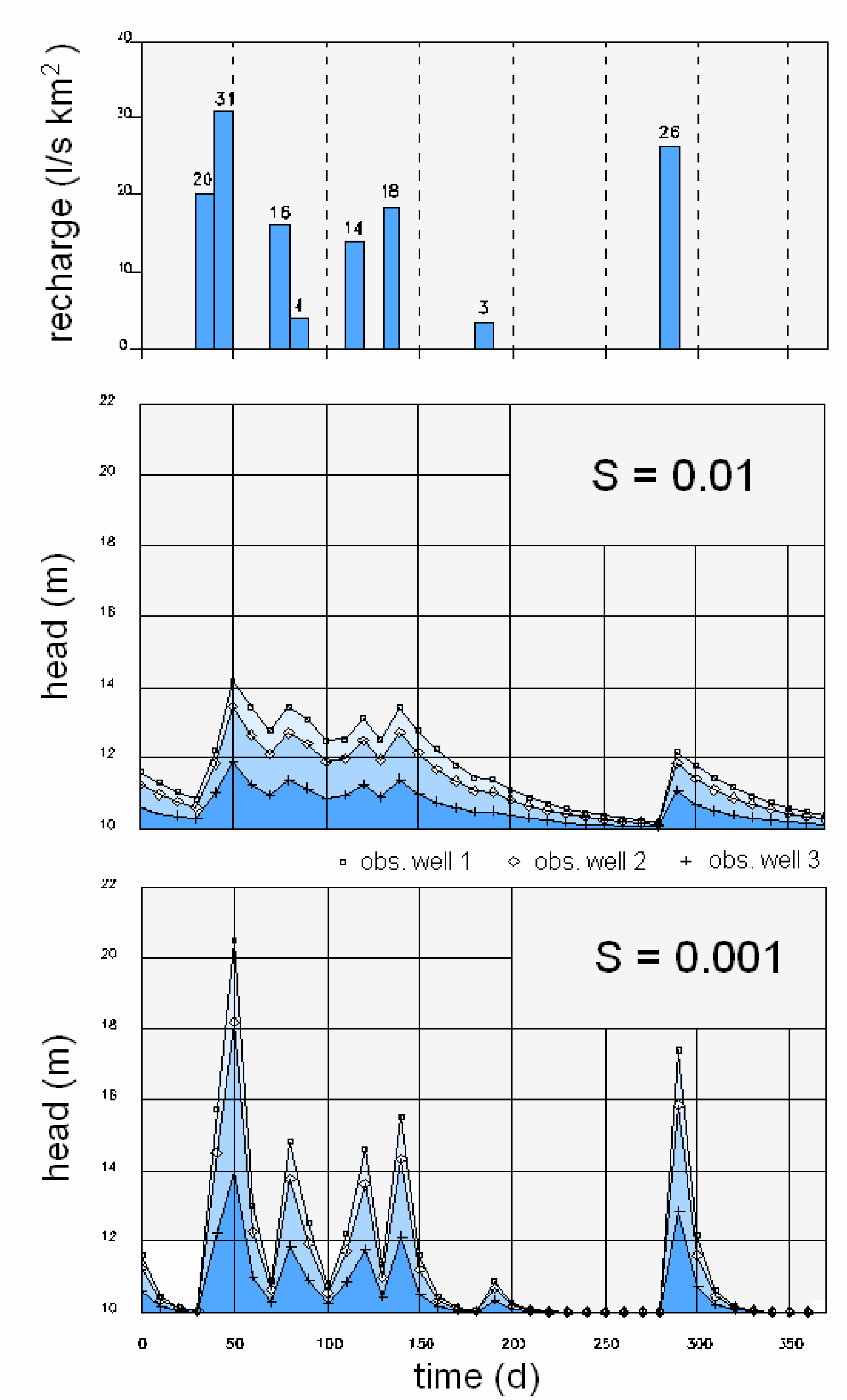
- Change only one parameter per model run
- Make a documentation of each model run
- Estimate goodness of fit objectively e.g. by computation of Mean Square Deviation

$$MSD = \frac{1}{n} \sum_{i=1}^{n} (h_i^{observed} - h_i^{calculated})^2$$

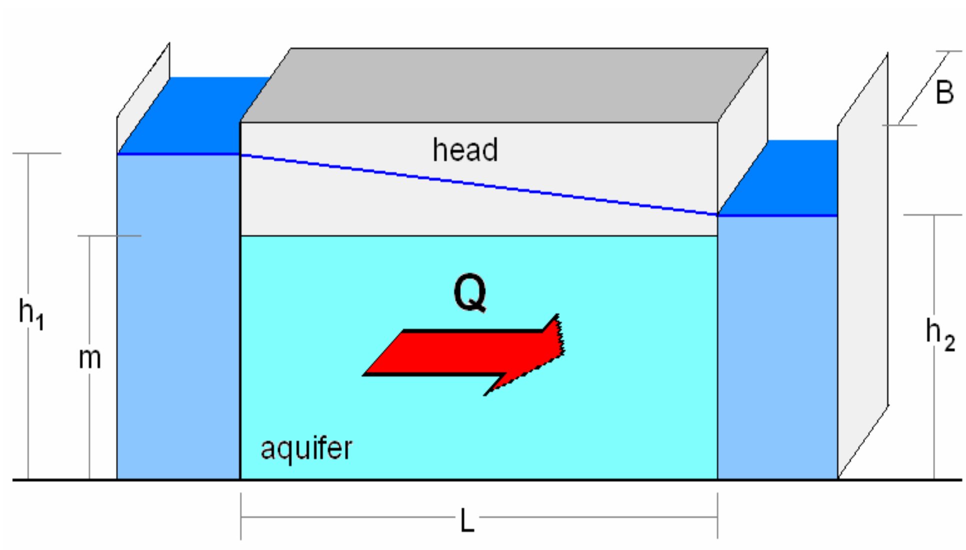
- Plot of $h_{calculated} = f(h_{observed})$



Effects on Storage Coefficients



Non Uniqueness of the Inverse Problem



$$Q = B\ T\ (h_1 - h_2)/L$$

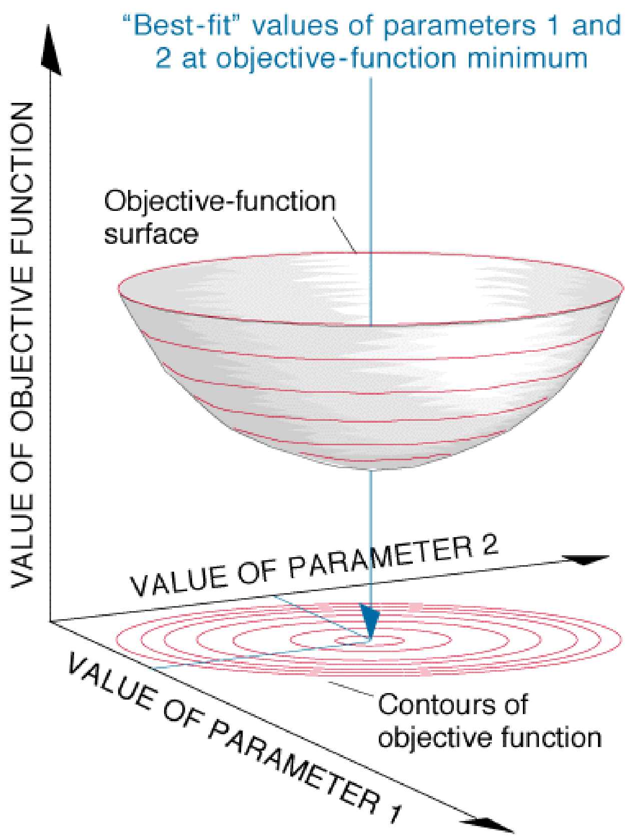
Where: Q: discharge
B: width
T: transmissivity
h: head
L: length

Identification problem of steady state calibration.

Every T leads to the same head distribution, only Q varies!

Parameter Optimization

$$\chi^2 = \sum (s_{calculated} - s_{observed})^2 \Rightarrow \text{Minimum}$$



Example of an objective function and „best fit" parameter values for a linear problem with two parameters

Optimization algorithm e.g.:

- NEWTON-RAPHSON-method
- GAUß-NEWTON-method
- MARQUARDT-LEVENBERG-method

Sensitivity Analysis

Purpose: The sensitivity analysis involves a perturbation of model parameters to see how much the results (head, concentration) change. This is compared to the uncertainty of parameters.

Use of the results of a sensitivity analysis

- Identify sensitive input parameters for the purpose of guiding additional field data collection

- Define parameters to be used in uncertainty analysis

Note: If the model output changes a lot within the uncertainty range of parameters, you are in way much trouble!

Model Validation

Purpose: To get greater confidence in model predictions by demonstrating that the calibrated model is an adequate representation of the physical system.

- Successfully predict alternate conditions

  To calibrate using steady state data and validate using transient data
  To calibrate using a part of a transient data set. Use the remainder of the data set for validation.

- Successfully predict existing conditions

  To validate using comparison data, which are not employed in the calibration process (only useful if there are sufficient data and one does not need the entire data for the calibration)

- Compare the model predictions with the results of other models

  This method validates the numerical (computer code) but not the conceptual model

- Predict conditions for locations beyond the existing monitoring network or at future times, to validate the model when additional fieldwork is undertaken

Model Application and Performance of Prognostic Runs

Analysis of Results

Iteration of any of the Steps above

Post-Auditing

Come back later and see how you did it. Adjust model as necessary.

Epilogue

Modeling under Uncertainty

- **Worst case analysis**
- **Scenario techniques**
- **Sensitivity analysis**
- **Stochastic modeling**

How do we know a Solution is Correct?

- **Numeric:**
  - **Successive refinement**
  - **Choice of two independent methods (e.g. Random Walk, FD in transport)**
  - **Comparison with approximations (e.g. pure advection in transport)**

- **Hydrogeological Model:**
  - **Comparison of model results with new field data to reduce non uniqueness**
  - **Transient heads**
  - **Transient plume**
  - **Environmental tracers**
  - **Isotopes information**

Widespread Errors in Modeling

- Wrong conceptual model
- Inappropriate boundary conditions
- Simultaneous calibration of fluxes and conductivities
- Variation of too many parameters ("over fitting")
- Inappropriate discretization in transport models
- Inappropriate comparison of model results with observed data
- No sensitivity analysis of results

Never Forget:

- A model is not reality
- A good model includes important features of reality
- A model does not replace data acquisition
- A good modeler explores the uncertainty of her / his predictions
- What we really want are robust decisions
- Do not overstretch a model

Recommended Literature

Recommended Literature

ANDERSON, M.P., WOESSNER, W.W. (1992): Applied Groundwater Modelling. - 381 S.; San Diego (Academic Press).

DE MARSILY, G. (1986): Quantitative hydrogeology - Groundwater hydrology for engineers. - 440 S.; Orlando, San Diego, New York (Academic Press).

DOMENICO, P.A., SCHWARZ, F.W. (1997): Physical and Chemical Hydrogeology. - 506 S.; New York (Wiley & Sons).

FH-DGG [FACHSEKTION HYDROGEOLOGIE DER DEUTSCHEN GEOLOGISCHEN GESELLSCHAFT] (1999): Hydrogeologische Modelle: Ein Leitfaden für Auftraggeber, Ingenieurbüros und Fachbehörden. - Schriftenreihe der Deutschen Geologischen Gesellschaft, **10**, 36 S.; Hannover.

KINZELBACH, W., RAUSCH, R. (1995): Grundwassermodellierung: Eine Einführung mit Übungen. – 283 S.; Berlin, Stuttgart (Borntraeger).

KINZELBACH, W., VOSS, A., RAUSCH, R., SAUTY, J.-P., CHIANG, W.-H., CORDES, C., FANG, S.Z. (1996): Altlastenhandbuch des Landes Niedersachsen, Materialienband Berechnungsverfahren und Modelle. – Hrsg.: NLfB, 216 S.; Berlin, Heidelberg, New York (Springer).

RAUSCH, R., SCHÄFER, W., WAGNER, C. (2002): Einführung in die Transportmodellierung im Grundwasser. – 193 S.; Berlin, Stuttgart (Borntraeger).

RAUSCH, R., SCHÄFER, W., THERRIEN, R., WAGNER, C. (2005): Solute Transport Modelling – An Introduction to Models and Solution Strategies. – 205 p., 66 fig., 11 tab.; Berlin, Stuttgart (Gebr. Borntraeger).

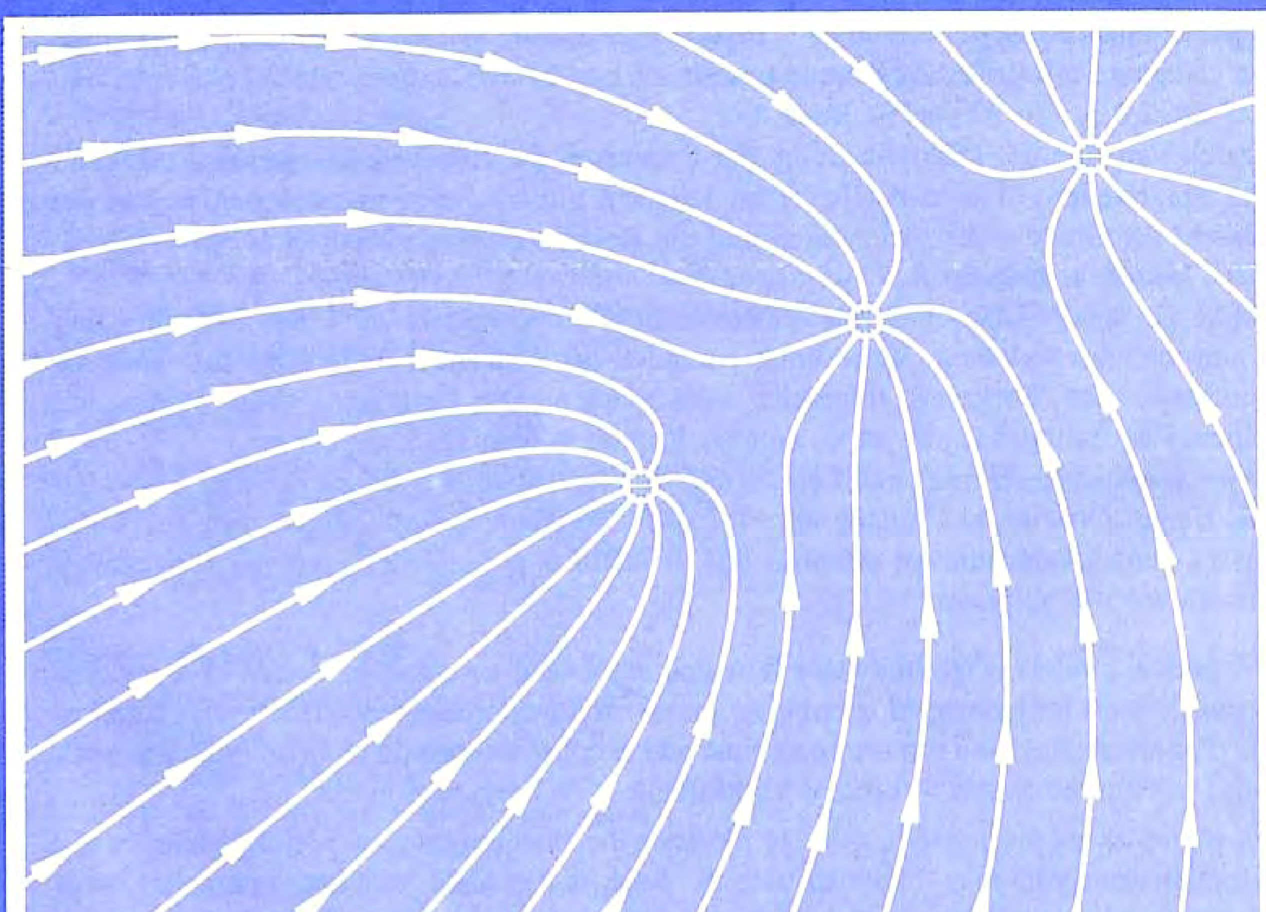
SPITZ, K., MORENO, J. (1996): A Practical Guide to Groundwater and Solute Transport Modeling. - 461 S.; New York (John Wiley & Sons, Inc.).

Annex

Grundwasser-modellierung

Eine Einführung mit Übungen

W. Kinzelbach und R. Rausch



Gebrüder Borntraeger Berlin · Stuttgart

Grundwassermodellierung

Eine Einführung mit Übungen mit 2 Disketten

Von W. KINZELBACH, Heidelberg und DR. RAUSCH, Stuttgart

VIII, 284 Seiten, m. 223 Abb. u. 15 Tab. sowie 2 Disketten. 17 x 24 cm. 1995.
ISBN 3-443-01032-6

Numerische Modelle für Strömungs- und Transportvorgänge im Grundwasser sind zu einem unverzichtbaren Werkzeug von Hydrogeologen, Bauingenieuren und Umweltwissenschaftlern geworden. Durch die rasche Entwicklung der Computertechnologie ist es heute möglich, auch sehr komplexe Fragestellungen mit dem PC zu bearbeiten.

Das Buch wendet sich an alle, die die Grundprinzipien der Grundwassermodellierung kennenlernen und praktische Erfahrungen damit sammeln möchten. Die hier geschilderten Methoden sind in zahlreichen Lehrgängen über Grundwassermodellierung erprobt worden, die beide Autoren seit vielen Jahren regelmäßig abhalten. Das Buch eignet sich daher sowohl als einführendes Lehrbuch als auch zum Selbststudium.

Ausgehend von den theoretischen Grundlagen werden 27 Beispiele ausführlich besprochen und gelöst, die neben den wichtigsten Techniken der Modellierung auch grundlegende Phänomene der Grundwasserhydraulik erklären. Mit der dem Buch auf Disketten beigefügten Software ASM können Leserinnen und Leser alle Beispiele auf einem PC (ab MS-DOS 3.3, 286 AT) selbst lösen.

Durch Variation der Diskretisierung, der Parameter, der Randbedingungen und eventuell der Fragestellungen wird der Leser im Umgang mit Modellen vertraut werden und ein Gefühl für Grundwasserströmungen und die Reaktionen eines Modells auf unterschiedliche Eingaben gewinnen.

ASM ist ein vollständiges zweidimensionales Grundwassermodell für Strömung und Transport, das weltweite Verbreitung gefunden hat und unabhängig vom Text auch als professionelles Werkzeug eingesetzt werden kann. Die Programmdokumentation mit einem Einführungsbeispiel ist als eigenes Kapitel in dem Buch enthalten.

Wir wünschen Leserinnen und Lesern, daß sie beim eigenen Arbeiten mit dem Computer die Hemmschwelle im Umgang mit Modellen überwinden, die Möglichkeiten des Werkzeugs ohne Überschätzung erfahren und schließlich genausoviel Spaß am Modellieren finden wie die Verfasser.

Numerical models of groundwater flow and associated transport processes have become valuable tools for hydrogeologists, civil ans environmental engineers. However, numerical models are abstract and require some time and exercise to become familiar with. The book aims to help the reader to become comfortable with numerical modelling.

27 examples are discussed in detail to illustrate the most important modelling methods and groundwater hydraulics. Included with the book is the ASM-program, a complete, two-dimensional groundwater model, with which the reader can solve all the examples. The program has been used worldwide and allows variation of parameters encountered in groundwater modelling (minimum requirement 286 processor, MS-DOS 3.3).

Interessenten: Das Buch bietet Geologen und Hydrogeologen, Bauingenieuren und Umweltwissenschaftlern eine ausgezeichnete, praxisnahe Einführung in die Grundwassermodellierung.

Inhalt

7 Nachtrag zu weiteren Modellierungstechniken

W.-H. Chiang • W. Kinzelbach • R. Rausch

Aquifer Simulation Model for WINdows

Groundwater flow and transport modeling, an integrated program

Gebrüder Borntraeger Berlin • Stuttgart

Aquifer Simulation Model for WINdows

Groundwater flow and transport modeling, an integrated program

by Dr. W.-H. Chiang, Hamburg,
Prof. Dr. W. Kinzelbach, Inst. f. Hydromechanik und Wasserwirtschaft, ETH Zürich and Dr. R. Rausch, Landesamt für Geologie, Rohstoffe und Bergbau Baden-Württemberg, Stuttgart

1998. V, 137 pages, 115 figures, 2 tables, 1 CD-ROM. 17 x 24 cm.
ISBN 3-443-01039-3

Aquifer Simulation Model for Windows (ASMWIN) implements a complete two-dimensional groundwater flow and transport model. This new model is a strongly enhanced Windows-version of ASM 5.0, which runs under MS-DOS (Kinzelbach & Rausch, 1995). ASMWIN comes with a professional graphical user-interface, a finite-difference flow model, a tool for the automatic calibration of a flow model, a particle tracking model, a random walk transport model, a finite-difference transport model and several other useful modeling tools.

The graphical user-interface allows you to create and simulate models with ease and fun. It can handle models with up to 150 x 150 cells and 1000 time periods (pumping intervals). ASMWIN can create contour maps or solid fill plots of input data and simulation results. Solid fill can utilize the full range of RGB colors to fill cells with different values. Contours can be added to these plots. Report-quality graphics may be saved to a wide variety of file formats, including SURFER, DXF, HPGL and BMP (Windows Bitmap).

The discretized flow equations are solved by the preconditioned conjugate gradient (PCG) method (module ASMSIM1) with the choice of diagonal and Cholesky preconditioning. For steady state flow fields, an automatic model calibration procedure using the Marquardt-Levenberg algorithm is available in the module ASMOPTI.

The particle tracking module ASMPATH offers several velocity interpolation methods and uses Euler-Integration to compute flow paths and travel times. ASMPATH allows you to perform particle tracking with just a few mouse clicks. Both forward and backward particle tracking schemes are feasible for steady-state and transient flow fields. ASMPATH calculates and shows pathlines or flowlines and travel time marks simultaneously. It provides various on-screen graphical options including head contours, drawdown contours, and velocity vectors.

Two transport simulation modules are available. The first uses a finite-difference scheme (Module ASMT2SIM) while the second uses a random-walk method based on Ito-Fokker-Planck theory (Module ASMWALK).

The modeling tools include a **Result Extractor,** a **Field Interpolator,** a **Field Generator,** a **Water Budget Calculator** and a **Graph Viewer.**

The **Result Extractor** allows the user to extract simulation results from any period to a spread sheet. You can then view the results or save them in ASCII or SURFER-compatible data files. Simulation results include hydraulic heads, drawdowns, Darcy velocities, leakage terms and concentrations.

The **Water Budget Calculator** not only calculates the budget of user-specified zones but also the exchange of flows between such zones. This facility is very useful in many practical cases. It allows the user to determine the flow through a particular boundary.

The **Field Generator** generates fields with heterogeneously distributed transmissivity or hydraulic conductivity values. It allows the user to statistically simulate effects and influences of unknown small-scale heterogeneities. The **Field Generator** is based on Mejía's (1974) algorithm.

The **Graph Viewer** displays temporal development curves of simulation results including hydraulic heads, drawdowns and concentrations.

Hardware requirements

Personal computer running Microsoft Windows 3.1x/95/98/NT
8 MB of available memory (16 MB or more are recommended)
A CD-ROM drive and a hard disk.
VGA or higher-resolution monitor
Microsoft Mouse or compatible pointing device

Contents

Einführung in die Transportmodellierung im Grundwasser

von R. Rausch, Stuttgart, W. Schäfer, Wiesloch,
Ch. Wagner, Frankfurt/M.

VII, 185 Seiten, 58 Abbildungen, 9 Tabellen, 17 x 24 cm. Fester Einband.
€ 42,— ISBN 3-443-01048-2

Transportmodelle sind mittlerweile ein zentrales Werkzeug bei der Bearbeitung von Fragen zur Grundwassergüte. Das Buch erläutert die hydraulischen, hydrochemischen und numerischen Grundlagen der Transportmodellierung im Grundwasser, wobei der Anwendungsbezug der Modelle im Vordergrund steht.

Nach einem Überblick über verschiedene Transportmechanismen wird die Transportgleichung anschaulich hergeleitet.

Der Schwerpunkt des Buches liegt auf der Herleitung und Beschreibung der aktuellen numerischen Methoden. Behandelt werden explizite und implizite Zeitdiskretisierungen, Finite-Differenzen-, Finite-Elemente- und Finite-Volumen-Verfahren als gitterbasierte Verfahren, und Bahnlinien-, Charakteristiken- und Random-Walk-Methoden als Particle-Tracking-Verfahren. Es werden die Vor- und Nachteile der verschiedenen Verfahren diskutiert und moderne Entwicklungen wie Methoden zur automatischen Gitteradaption vorgestellt.

Ein eigenes Kapitel zu den Lösungsverfahren für lineare und nicht-lineare Gleichungssysteme bietet dem Leser die Möglichkeit, die Funktionsweise der numerischen Verfahren im Detail nachvollziehen zu können und die Besonderheiten der einzelnen Verfahren kennen zu lernen.

Der reaktive Stofftransport wird im letzten Kapitel des Buches behandelt. Dabei werden nicht nur die gängigen einfachen Reaktionsmodelle wie Abbau erster Ordnung und lineare

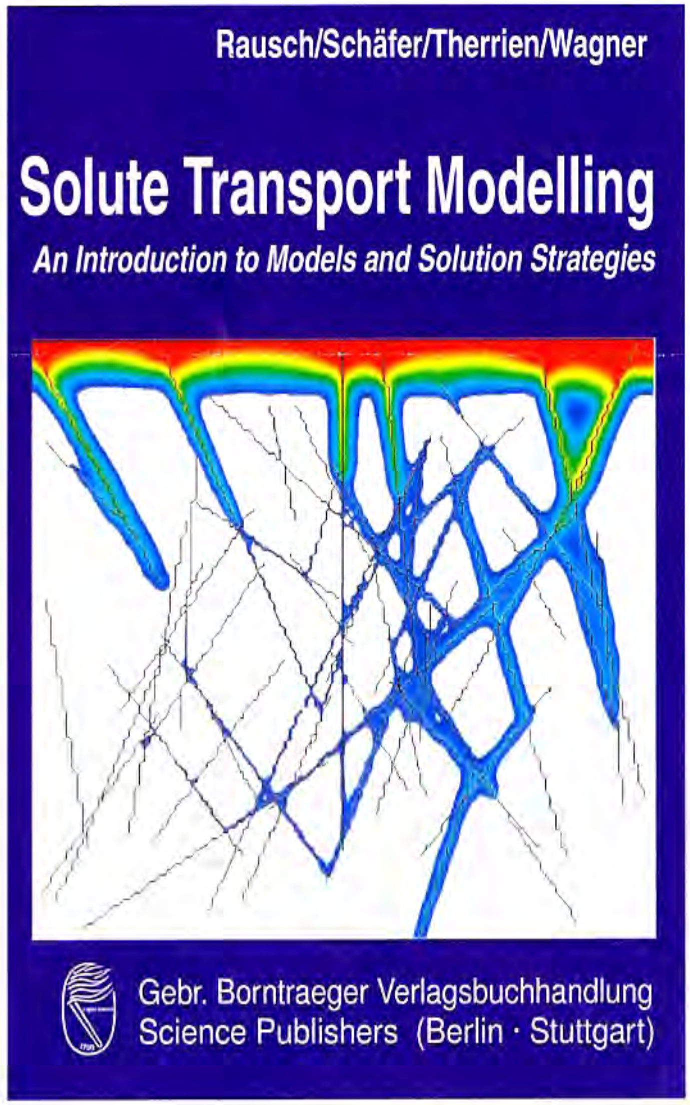
Retardierung besprochen, sondern es werden auch komplexere Ansätze mit Multispezies-Modellen dargestellt. Für den Anwender von Transport-Reaktionsmodellen werden die wichtigsten zur Zeit verfügbaren Computer-Programme in diesem Bereich kurz vorgestellt.
Abgerundet wird das Buch durch ein sehr umfangreiches Verzeichnis weiterführender Literatur und durch ein Schlagwort-Register.
Das Buch ist in erster Linie für den Anwender von Transportmodellen geschrieben und richtet sich an Hydrogeologen, Hydrologen, Geoökologen, Geographen, Bauingenieure, Wasserwirtschaftler, Umweltnaturwissenschaftler und andere Fachleute, die sich mit den unterschiedlichen Aspekten der Grundwasserqualität beschäftigen. Es verzichtet aber nicht darauf, auch die Grundlagen und die Besonderheiten der einzelnen Verfahren und Modellansätze darzustellen. Es ist eine aktuelle und umfassende Einführung in diesen Bereich.

Aus dem Inhalt:

Randolf Rausch, Wolfgang Schäfer, René Therrien and Christian Wagner:

Solute Transport Modelling

An Introduction to Models and Solution Strategies



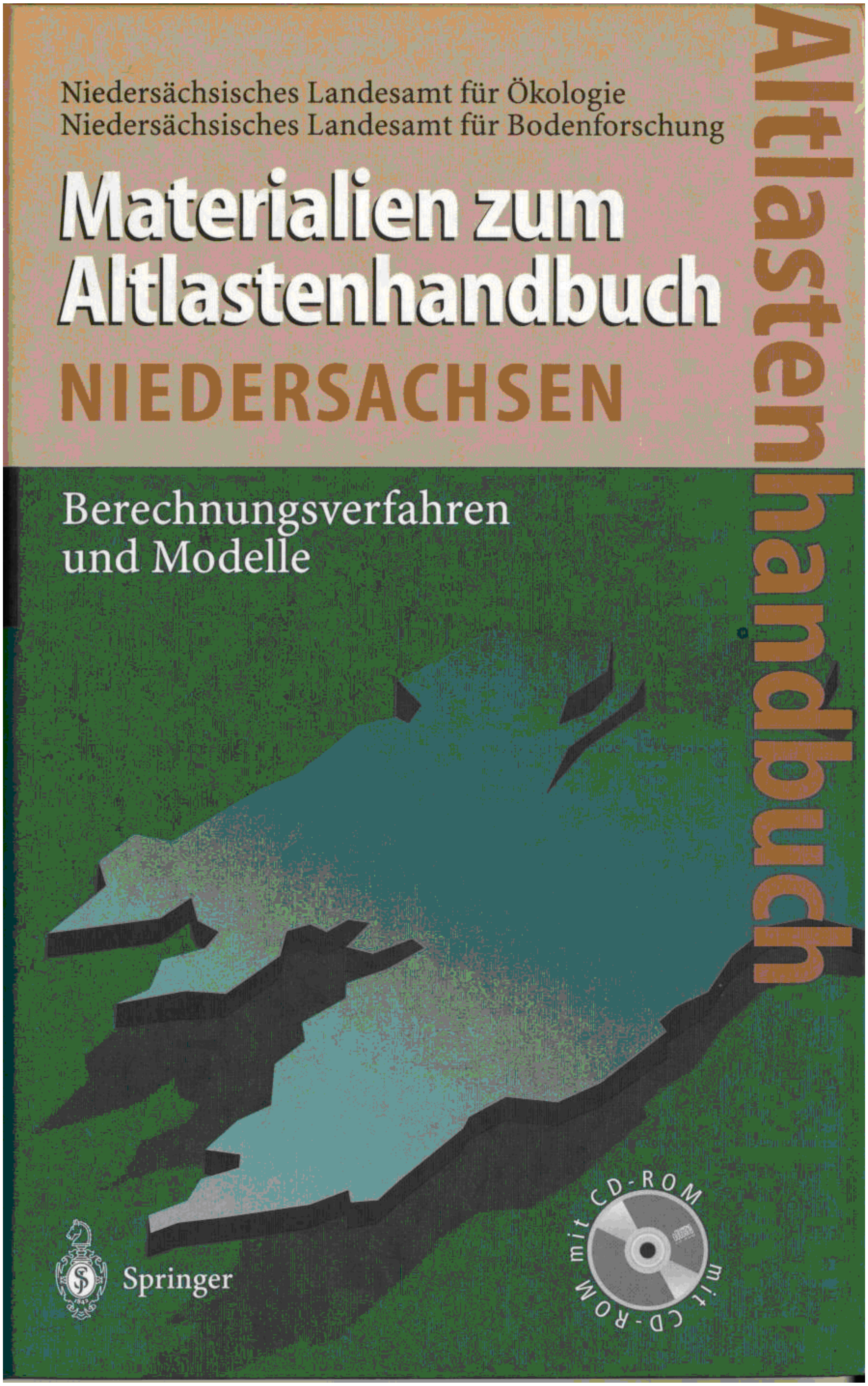
2005. XV, 205 pages, 66 fig., 11 tab., 16x22 cm
ISBN 3-443-01055-5, softcover € 39,80
classroom quantities available.

Water quality is a serious problem worldwide. Solute transport models have evolved into an essential tool for investigating groundwater quality problems.
This book presents the fundamental hydraulic, hydrochemical and numerical concepts required for the sound and efficient application of solute transport models in groundwater studies.
Advection, dispersion and diffusion, the main physical processes, are first introduced, followed by the derivation of the advection-dispersion equation. A separate chapter is devoted to multispecies reactive transport modelling, presenting both theoretical and simulation examples.
Special methods used to simulated transport in fractured geological material are presented in a newly introduced chapter.

The authors focus on the detailed presentation of numerical methods used in transport models to provide practitioners with a sound theoretical basis for transport model applications. Grid-based methods are presented, including explicit and implicit finite differences, finite elements and finite volume methods. Particle tracking techniques are also covered, among them the method of characteristics and the random-walk techniques.
All of the authors are active in groundwater modelling and involved in numerous projects worldwide.

The volume addresses academics, scientist, engineers, hydrologists and hydrogeologist interested in the use of transport models in hydrogeology, geoecology, hydrology, environmental engineering, hydraulic engineering and water economics.

Table of Contents


Niedersächsisches Landesamt für Ökologie
Niedersächsisches Landesamt für Bodenforschung
Materialien zum Altlastenhandbuch
NIEDERSACHSEN
Berechnungsverfahren und Modelle
Altlastenhandbuch
mit CD-ROM
mit CD-ROM
Springer

Niedersächsisches Landesamt für Ökologie
Niedersächsisches Landesamt für Bodenforschung
als Landesarbeitsgruppe LAA

Altlastenhandbuch des Landes Niedersachsen

Materialienband

Berechnungsverfahren und Modelle

W. Kinzelbach
A. Voss
R. Rausch (Modell PAT, WSG)
J.-P. Sauty (Modell CATTI)
W.H. Chiang, C. Cordes, S.Z. Fang (Modell GFR)

Bearbeitung durch Landesarbeitsgruppe Altlasten:
H. Röhm, Niedersächsisches Landesamt für Bodenforschung
M. Scholtka, Niedersächsisches Landesamt für Ökologie

Mit 164 Abbildungen und 18 Tabellen

Springer

Niedersächsisches Landesamt für Ökologie
Postfach 101062
D-31110 Hildesheim

Wen-Hsing Chiang
Umweltbehörde Hamburg, Amt für Umweltschutz/Geologisches Landesamt
Billstraße 84, D-20539 Hamburg

Wolfgang Kinzelbach
Institut für Umweltphysik, Universität Heidelberg
Im Neuenheimer Feld 366, D-69120 Heidelberg

Randolf Rausch
Heimbergstraße 54
D-70496 Stuttgart

Jean-Pierre Sauty
Bureau de Recherches Géologiques et Minières
B.P. 6009, F-45060 Orléans Cédex

Axel Voss
HPC Harress Pickel Consult GmbH
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