Groundwater flow and transport modeling

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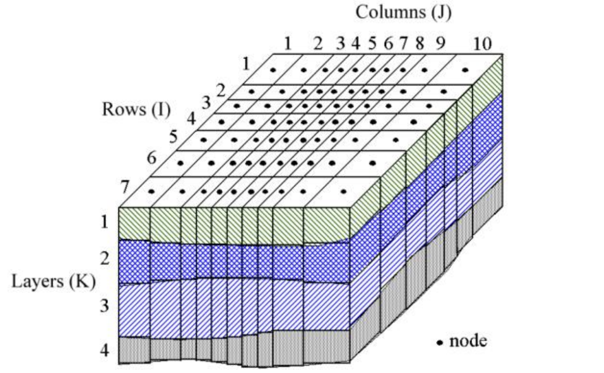
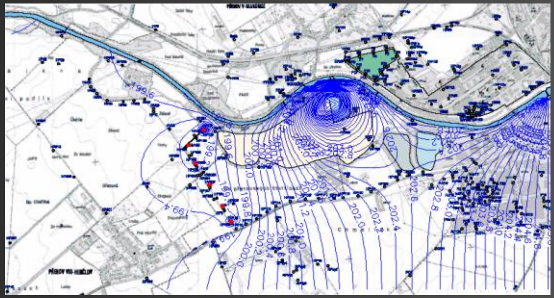
Content of the workshop

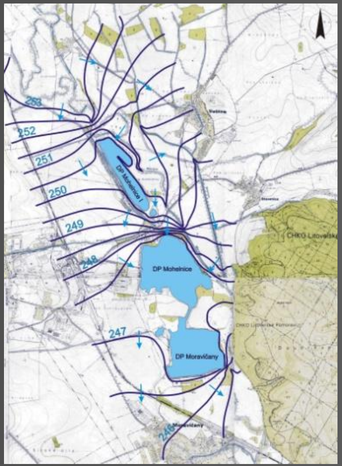
Introduction to ground-water modeling

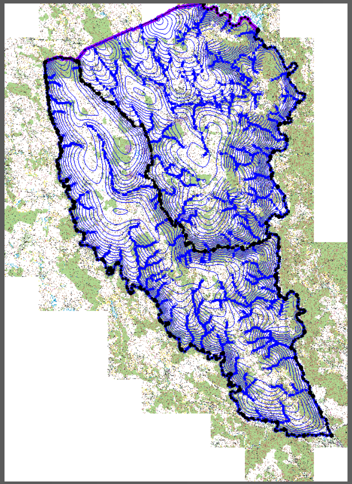
$$\frac{\partial}{\partial x}\left(K_{xx}\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_{yy}\frac{\partial h}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_{zz}\frac{\partial h}{\partial z}\right)-W=S_s\frac{\partial h}{\partial t}$$



Modeling case studies







Aim of the lectures + workshop

- Introduction to basic principles of gorundwater flow modeling
- Overview of important input data
- Set-up of model geometry nad boundary conditions
- Model calibration and verification
- Practical using of Processing Modflow – PMWIN

What is a model?

- Model is any device representing a field situation
- Model types: physical (sand tanks), analogous (electric field) and mathematical (governing equation)

Mathematical model: can be solved analytically and numerically

Analytical model is too simplistic

Mathematical model is easy applicable and allows to solve more complex flow problems

Why model?

- **Prediction**:
most groundwater modeling efforts - predicting the consequences of a proposed action

- **Interpretation**:
insight into the controlling parameters in a site-specific setting, framework for formulating ideas about system dynamics

- **Generic geologic settings**: helpful in formulating regional regulatory quidelines and screening tool to identify regions suitable for some proposed action

Numerical model is a set of equations that describes the physical and/or chemical processes occurring in a system.

Groundwater flow: determination of filtration velocity vector *q* (flow direction and velocity) and hydraulic head *h* in modeled area

Solute transport: flow velocities

Components of numerical model:

Darcy's low + **Law of mass balance** = **Groundwater flow equation**

Groundwater flow equation

Darcy's law

$$Q = -kA\frac{h_1 - h_2}{L}$$

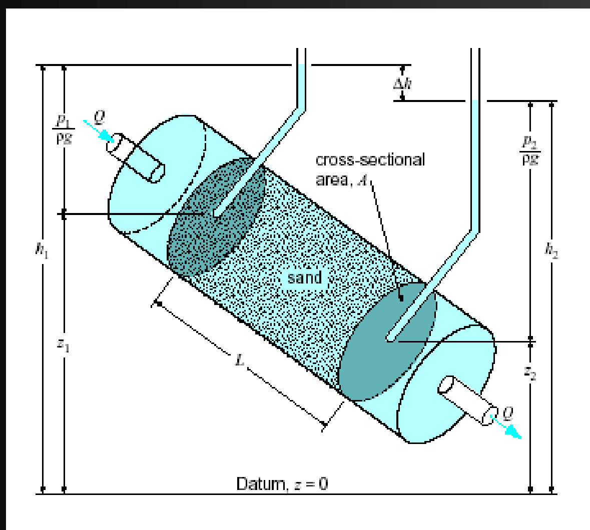
Negative sign because fluids flows from high pressure to low pressure, If the change in pressure is negative (where $h_1 > h_2$) then the flow will be in the positive x direction

$$q = -k\frac{h_1 - h_2}{L}$$

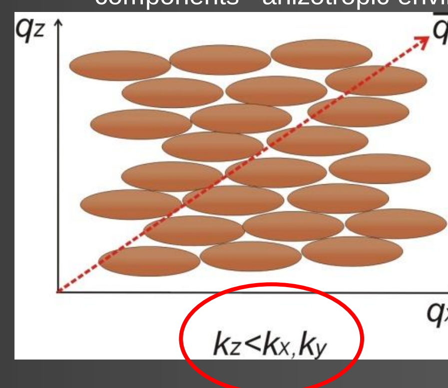
Divided by flow cross-sectional area A

$$q = -k.gradh$$

Hydraulic head *h* is a scalar (1 component)



Specific discharge *q* is a vector (3 components - anizotropic environment)



$$q_x = k_x \frac{\partial h}{\partial x}$$
$$q_y = k_y \frac{\partial h}{\partial y}$$
$$q_z = k_z \frac{\partial h}{\partial z}$$

3D Vector form of Darcy law

$$q = \kappa \nabla h$$

Hydraulic gradient at anisostropic media

Hydraulic conductivity *k* is a Tensor (9 components in anisotropic media)

$$\kappa = \kappa(x,y,z) = \begin{bmatrix} k_{xx} & k_{xy} & k_{xz} \\ k_{xy} & k_{yy} & k_{yz} \\ k_{xz} & k_{yz} & k_{zz} \end{bmatrix}$$

Itemized form of hydraulic conductivity tensor

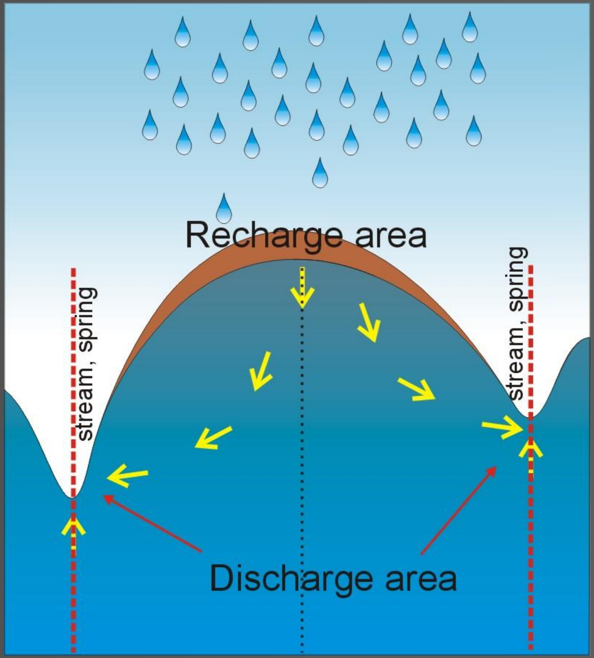
$$q_x = k_{xx}\frac{\partial h}{\partial x} + k_{xy}\frac{\partial h}{\partial y} + k_{xz}\frac{\partial h}{\partial z},$$
$$q_y = k_{xy}\frac{\partial h}{\partial x} + k_{yy}\frac{\partial h}{\partial y} + k_{yz}\frac{\partial h}{\partial z},$$
$$q_z = k_{xz}\frac{\partial h}{\partial x} + k_{yz}\frac{\partial h}{\partial y} + k_{zz}\frac{\partial h}{\partial z}.$$

Groundwater flow equation

Law of Mass Balance = water balance equation

<u>Steady State</u> Water Balance Equation

Inflow = Outflow

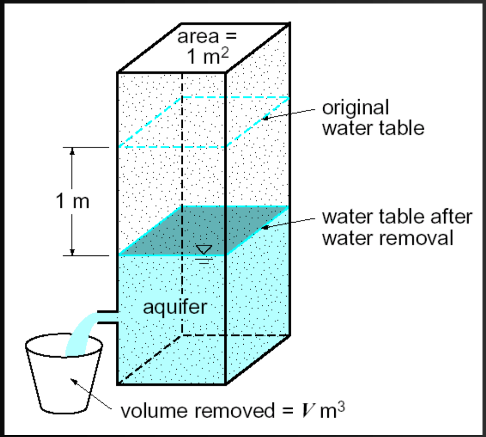


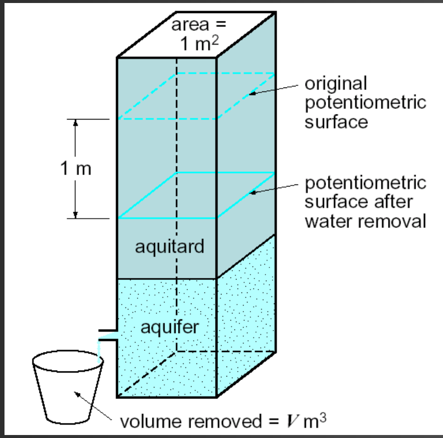
<u>Transient</u> Water Balance Equation

Outflow - Inflow = Change in Storage

Specific yield = S_y

Storativity = S





Specific discharge *q* at anizotropic environment with flow of compressible fluid, Transient regime

$$\frac{\partial(q_x\rho)}{\partial x}+\frac{\partial(q_y\rho)}{\partial y}+\frac{\partial(q_z\rho)}{\partial z}=-S\rho\frac{\partial h}{\partial t}+W\rho$$

Enters or leaves of groundwater

$$\nabla(q\rho)=-S\rho\frac{\partial h}{\partial t}+W\rho$$

Diveregence – scalar product of Hamilton operator and vector field (d**ivergence** is a vector operator that measures the magnitude of a vector field's source or sink at a given point, in terms of a signed scalar)

Groundwater flow equation

Darcy's law + **Law of mass balance** = **Groundwater flow equation**

$$q = \kappa \nabla h \quad + \quad \nabla(q\rho) = -S\rho\frac{\partial h}{\partial t} + W\rho \quad = \quad \nabla(\kappa \nabla h \rho) = -S\rho\frac{\partial h}{\partial t} + W\rho$$

Equation of transient flow of compressible fluid in anisotropic and compressible environment

Simplification of Groundwater flow equation based on assumptions that:

- Tensor *κ* replaced by one-directional hydraulic conductivity *k*
- Water density *ρ* is constant and thus can be released
- Very often is possible to release transient term $S\rho\frac{\partial h}{\partial t}$
- Sometimes may be *z* direction neglected

Groundwater flow equation

Transient flow

Incompressible fluid in anisotropic incompressible medium

3D $$\frac{\partial}{\partial x}\left(k_{xx}\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(k_{yy}\frac{\partial h}{\partial y}\right)+\frac{\partial}{\partial z}\left(k_{zz}\frac{\partial h}{\partial z}\right)=-S_s\frac{\partial h}{\partial t}+W$$

2D $$\frac{\partial}{\partial x}\left(k_{xx}b\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(k_{yy}b\frac{\partial h}{\partial y}\right)=-S_s\frac{\partial h}{\partial t}+W$$

Incompressible fluid in isotropic incompressible medium

3D $$\left(\frac{\partial^2 h}{\partial x^2}+\frac{\partial^2 h}{\partial y^2}+\frac{\partial^2 h}{\partial z^2}\right)k=-S_s\frac{\partial h}{\partial t}+W$$

2D $$\left(\frac{\partial}{\partial x}\left(b\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(b\frac{\partial h}{\partial y}\right)\right)k=-S_s\frac{\partial h}{\partial t}+W$$

Steady state flow

Incompressible fluid in anisotropic incompressible medium

3D $$\frac{\partial}{\partial x}\left(k_{xx}\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(k_{yy}\frac{\partial h}{\partial y}\right)+\frac{\partial}{\partial z}\left(k_{zz}\frac{\partial h}{\partial z}\right)=W$$

2D $$\left(\frac{\partial}{\partial x}\left(k_{xx}b\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(k_{yy}b\frac{\partial h}{\partial y}\right)\right)k=W$$

Incompressible fluid in isotropic incompressible medium

3D $$\left(\frac{\partial^2 h}{\partial x^2}+\frac{\partial^2 h}{\partial y^2}+\frac{\partial^2 h}{\partial z^2}\right)k=W$$

2D $$\left(\frac{\partial}{\partial x}\left(b\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(b\frac{\partial h}{\partial y}\right)\right)k=W$$

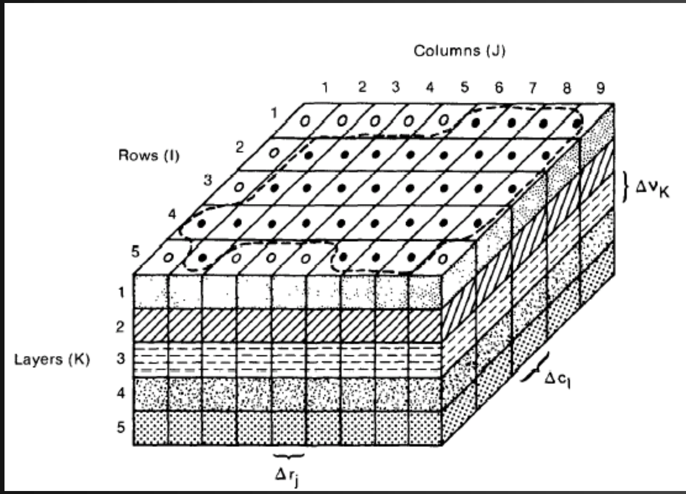
If W=0 → Laplace equation

Finite difference method

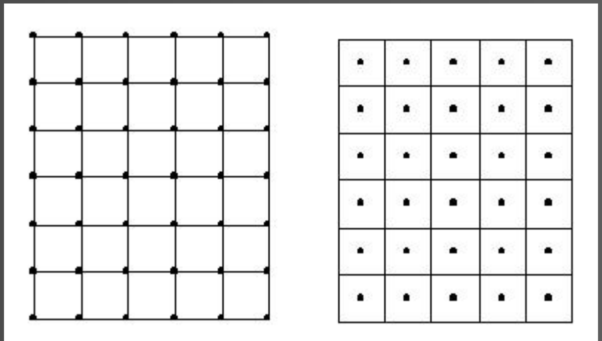
If is Analytical solution difficult – approximation by numerical methods

The finite differences method (FDM)

- Problem is solved by difference equations, which are discretized by nodes in grid
- Derivation is in nodes of grid replaced by differences – linear combination of functional value (hydraulic heads, flow rates) in surrounding nodes
- System of linear algebraic equations with unknown values of differences in nodes
- System of equations is solved in district Ω bounded by boundary conditions



Mesh centered cell-centered



Finite difference method

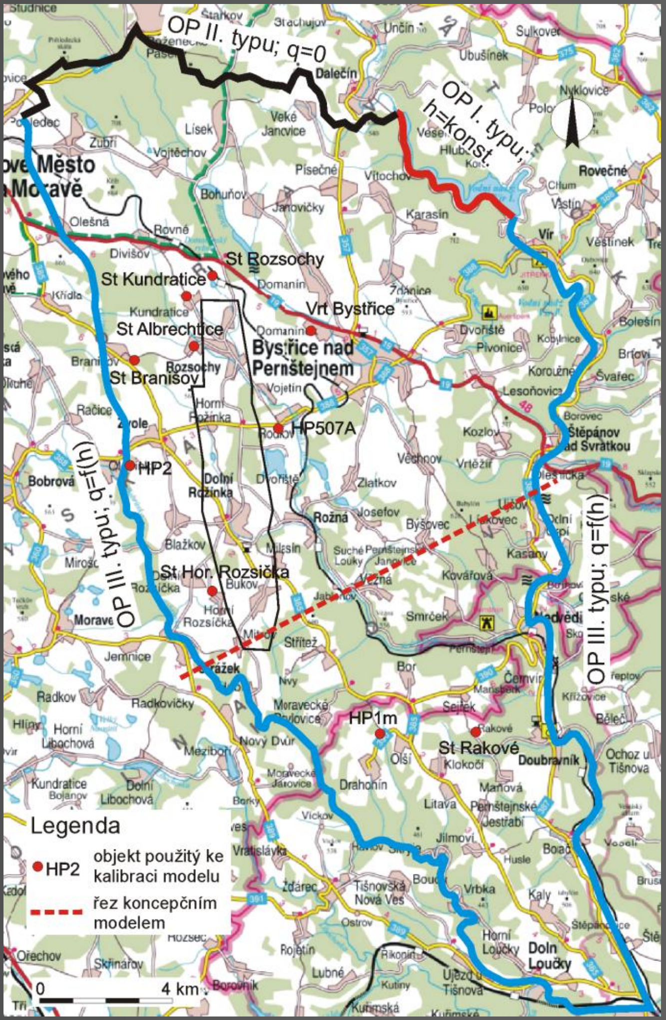
Boundary Conditions

- **<u>Dirichlet boundary condition</u>** (boundary condition of 1. type): it specifies the values of solution on the boundary of the domain, specified head *h=k*

- **<u>Neumann boundary condition</u>**: it specifies the flow rate values on the boundary of the domain, specified flow, mostly *q=0* (boundary condition of 2. type)

- **<u>Cauchy boundary condition</u>**: flow rate is dependent on hydraulic head on boundary, head dependent flow *h=f(h)*
- (boundary condition of 3. type)

- **<u>Initial conditions</u>**: in case of transient flow - hydraulic heads in time=0



Groundwater flow equation + boundary conditions = **numerical groundwater flow model**

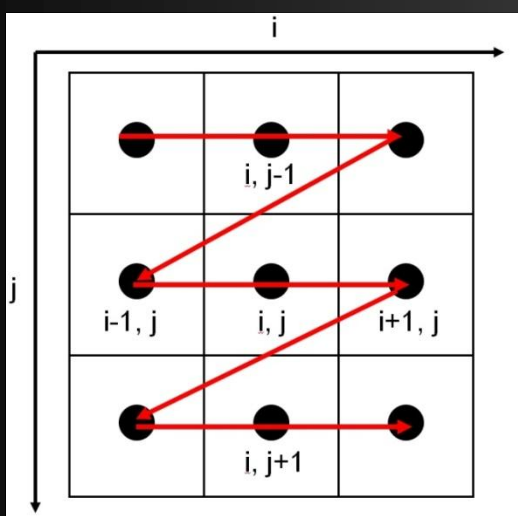
Finite difference method

Numerical methods - **iteration**:

Problem is solved by **repeating a process** with the aim of approaching a desired goal. Each repettion is called an iteration and the result of one iteration is used as the starting point for the next iteration.

- The iteration process starts from intial estimation h^0 (or measured).
- Calculation process proceeds for example In Gauss-Seidel interation from upper left corner to right and from up to down.
- In every node $x_{i,j}$ is calculated new value $h^m_{i,j}$ according to values in adjacent nodes
- New values are also calculated both new $h^m_{i,j}$ and old $h^{m-1}_{i,j}$ values in adjacent nodes
- Iterations proceed until reaching of Convergence criteria ε (i. e. required accuracy) $\left\| h^m - h^{m+1} \right\| < \varepsilon$

2-D



Cell *i j k* and indices for the six adjacent cells

Gauss-Seidel Iteration

$$h_{i,j}{}^{m} = \frac{h_{i+1,j}{}^{m} + h_{i-1,j}{}^{m} + h_{i,j+1}{}^{m} + h_{i,j-1}{}^{m}}{4}$$

initial guesses *m*

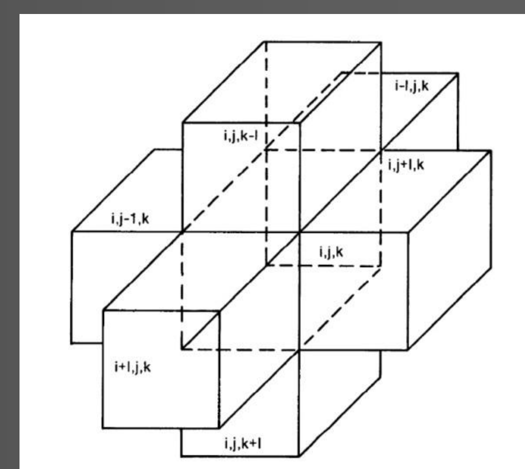
$$h_{i,j}{}^{m+1} = \frac{h_{i+1,j}{}^{m} + h_{i-1,j}{}^{m+1} + h_{i,j+1}{}^{m} + h_{i,j-1}{}^{m+1}}{4}$$

initial guesses *m*
and next step *m+1*

$$\left\| h^m - h^{m+1} \right\| < \varepsilon$$

Iteration reached Convergence criteria

3-D



Numerical methods – **iteration**:

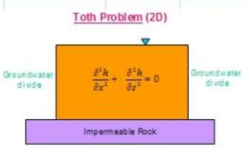
Example of spreadsheet modeling

100	100.4	100.8
100.6398	100.785247	101.04
100.9887	=(A10+B9+C10+B11)/4	
101.1923	101.2395055	101.366
101.3013	101.3386139	101.443

	A	B	C
7	h (L)		
8	100	100.4	100.8
9	=(2*B9+A8+A10)/4		101.016
10	100.938	101.0121718	101.185
11	101.1243	101.17354	101.302
12	101.3013	101.3386139	101.443
13	101.3359	101.3703955	101.468

	A	B	C
7	h (L)		
8	100	100.4	100.8
9	100.6398	100.785247	101.0398
10	100.9887	101.0613861	101.2321
11	101.1923	101.2395055	101.3658
12	101.3013	101.3386138	101.4432
13	101.3359	101.3703954	101.4685
14			
15	K		
16	30	30	30
17			
18	Q(L3/L/T)		
19	-9.5970	-11.5574	-7.1940
20	-5.2336	-8.2842	-5.7684
21	-3.0533	=B$16*(B10-B11)	
22	-1.6361	-2.9733	-2.3237
23	-0.5179	-0.4767	-0.3791

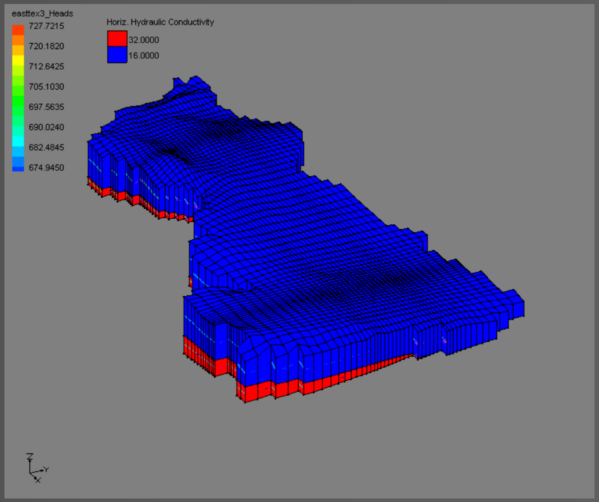
	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P
1	2-D															
2	Cross-section, unconfined aquifer															
3	Numerical - discrete solution															
4	Solution by Gauss-Seidl iteration															
5	Mesh-centered grid															
6																
7	h (L)															
8	100	100.4	100.8	101.2	101.6	102	102.4	102.8	103.2	103.6	104				konstantní hladina	
9	100.6398	100.785247	101.0398	101.3419	101.6663	102	102.3337	102.65813	102.9602	103.2148	103.3602			q=0	modelovaná oblast	q=0
10	100.9887	101.0613861	101.2321	101.4614	101.7234	102	102.2766	102.53861	102.7679	102.9386	103.0113				q=0	
11	101.1923	101.2395055	101.3658	101.5482	101.7658	102	102.2342	102.45178	102.6342	102.7605	102.8077					
12	101.3013	101.3386138	101.4432	101.6	101.7914	102	102.2086	102.4	102.5568	102.6614	102.6987					
13	101.3359	101.3703954	101.4685	101.6171	101.8	101.9999999	102.2	102.38288	102.5315	102.6296	102.6641					
14																
15	K															
16	30	30	30	30	30	30	30	30	30	30	30					
17																
18	Q(L3/L/T)															
19	-9.5970	-11.5574	-7.1940	-4.2562	-1.9893	0.0000	1.9893	4.2562	7.1940	11.5574	9.5970	v okrajových podmínkch q = 0 je přítok poloviční, proto /2				
20	-5.2336	-8.2842	-5.7684	-3.5854	-1.7116	0.0000	1.7116	3.5854	5.7684	8.2842	5.2336					
21	-3.0533	-5.3436	-4.0102	-2.6052	-1.2718	0.0000	1.2718	2.6052	4.0102	5.3436	3.0533					
22	-1.6361	-2.9733	-2.3237	-1.5533	-0.7705	0.0000	0.7705	1.5533	2.3237	2.9733	1.6361					
23	-0.5179	-0.4767	-0.3791	-0.2568	-0.1284	0.0000	0.1284	0.2568	0.3791	0.4767	0.5179					
24																
25																
26	R Total	D Total		Error												
27	-3.46E+01	3.46E+01		5.65E-06												
28						MESH CENTERED										
29						slope										



Basic principles of numerical modeling

Governing groundwater flow equation – transient prediction of hydraulic head in 3-D domain for an anizothropy hydraulic conducticity field

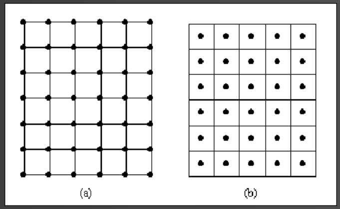
$$\frac{\partial}{\partial x}\left(K_{xx}\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_{yy}\frac{\partial h}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_{zz}\frac{\partial h}{\partial z}\right)-W=S_s\frac{\partial h}{\partial t}$$



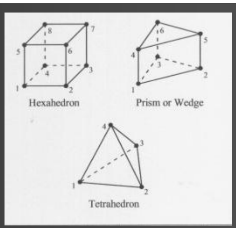
Kxx, Kyy, Kzz = hydraulic conductivity
Ss = specific storage
W = flux term (sources or sinks)
h = hydraulic head
x, y, z = space coordinates
t = time

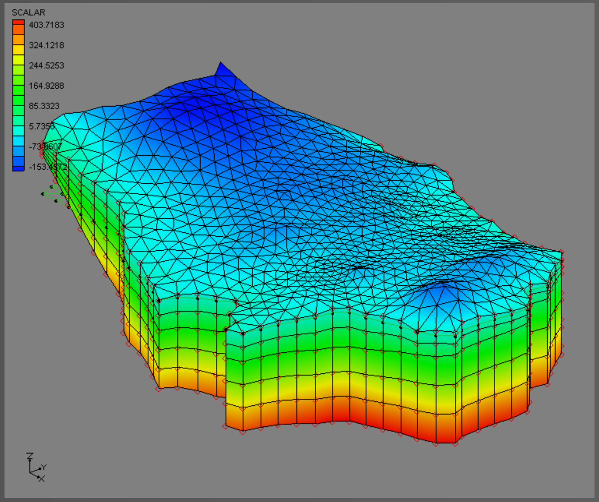
Governing flow equation is replaced by algebraic equations written and solved for aech node of subdivided modeled region:

Finite differences:
Rectangular grid – cells
mesh-centered, block-centered



Finite elements:
Triangular elements – more accurate diskretization

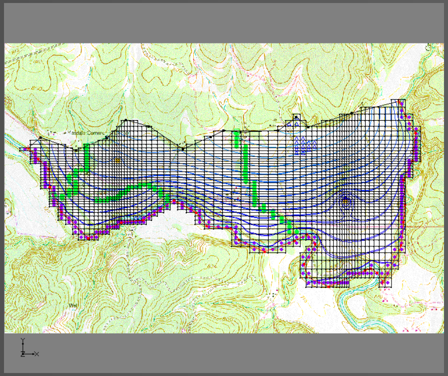




Numerical model conception

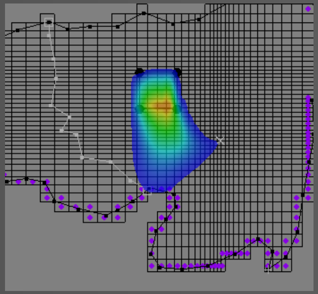
Varies approach to model:

- determinical - detailed knowledge of geology
- stochastic – statistical evaluation



Model aplication:

- conceptual model of groundwater flow – idealized aquifer geometry
- model as predictive tool –calibration, verification

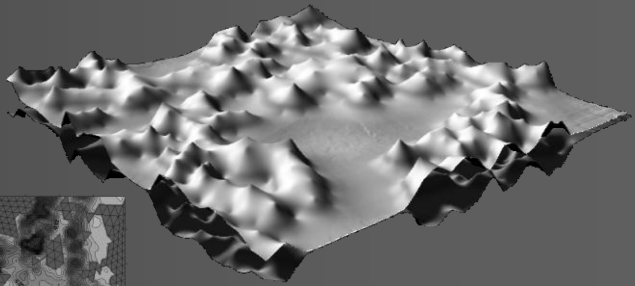


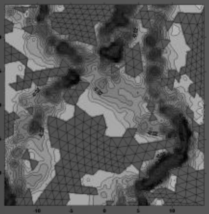
Simulation:

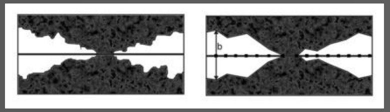
- groundwater flow – steady-state, transient
- transport model – based on ground-water flowing model

Ground-water flow media:

- pore media – the most sophisticated method, less problems with hydraulic anisotropy
- fractured media – difficulties coupled with fractured net estimation





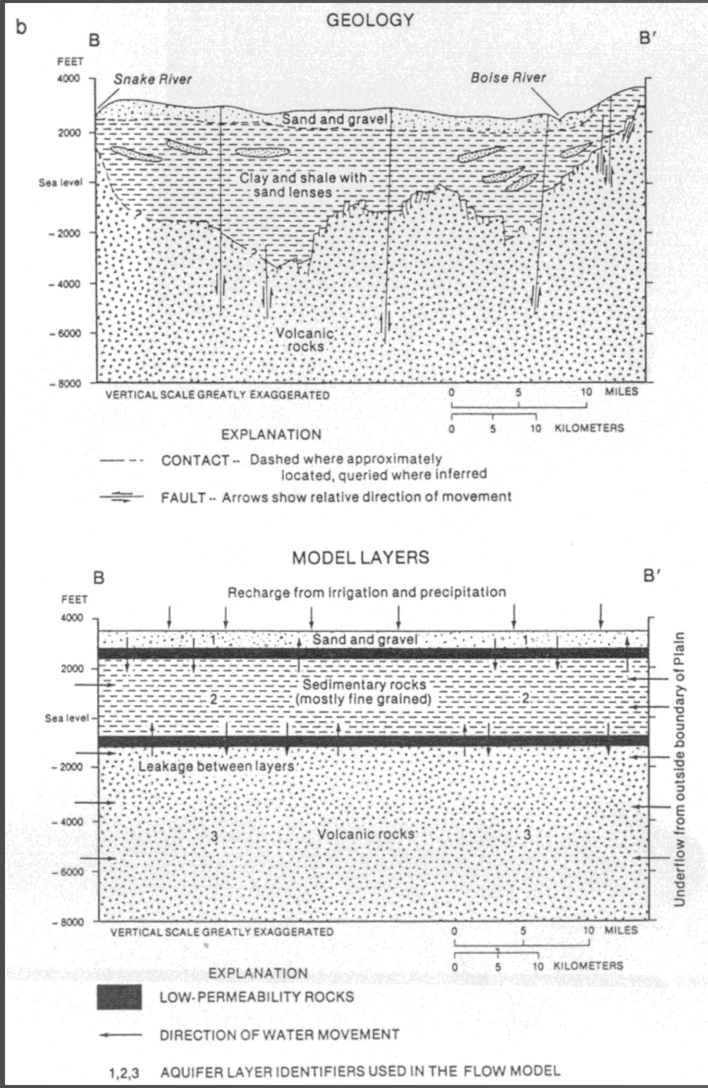


Conceptual model

Conceptual model is a pictoral representation of the gorundwater flow system:

- Block diagram
- Cross section

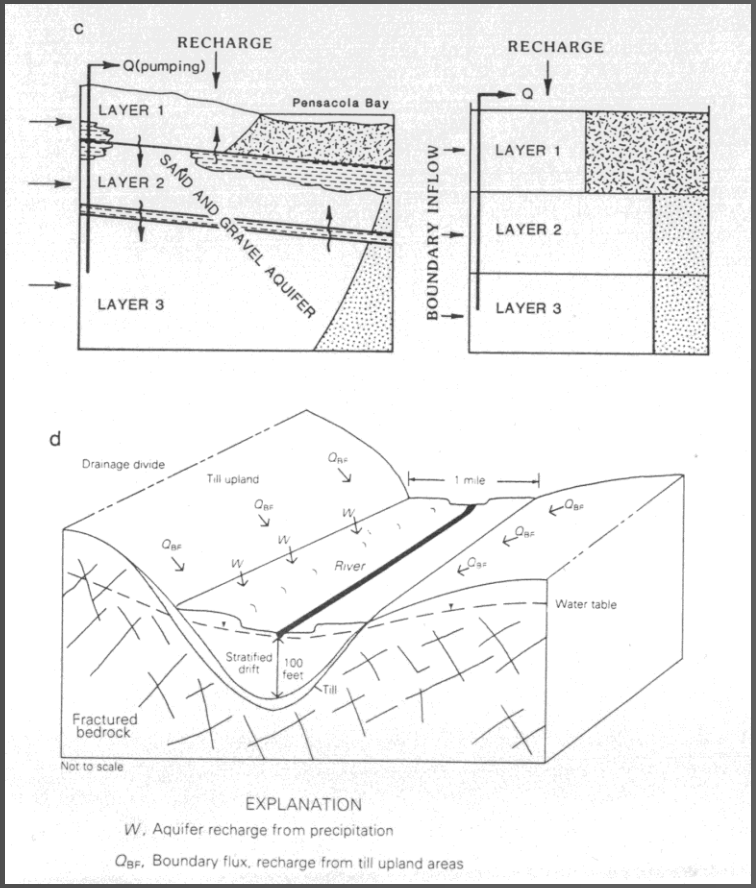
Simplification of the field system, complete reconstrucion is not feasible



Conceptual model

Steps in formulating the conceptual model:

- Define the area of interest – identify the boundaries of the model
- Defining hydostratigraphic units – comprise geologic units of similar hydrogeologic properties (regional x local scale), facies model, structural model
- Prepare a water budget – **sources** of water to the system (recharge: precipitation, overland flow, from surface water bodies), expected flow direction, **outflows** (springflow, baseflow to stream, ET, pumuping)
- Defining the flow system – hydrologic and geochemical information are used to conceptualize the movement of groundwater through system - the location of recharge and discharge areas



Data requirements for a Groundwater Flow Model

Physical framework

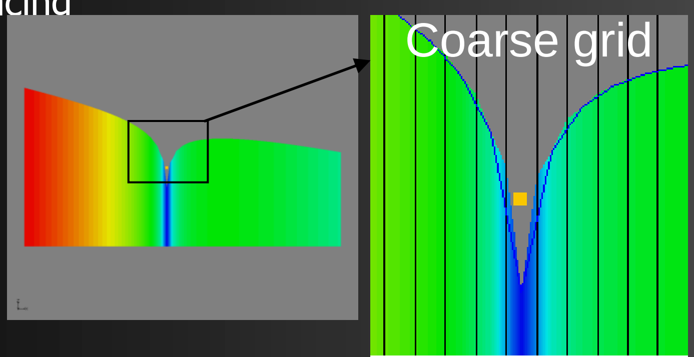
- **Geologic map** and cross sections
- **Topographic map** – surface water bodies and divides
- **Contour maps** – elevation of the base of the aquifers and confining beds
- **Isopach maps** – thickness of aquifer and confining beds
- **Map** – extent and thickness of stream and lake sediments

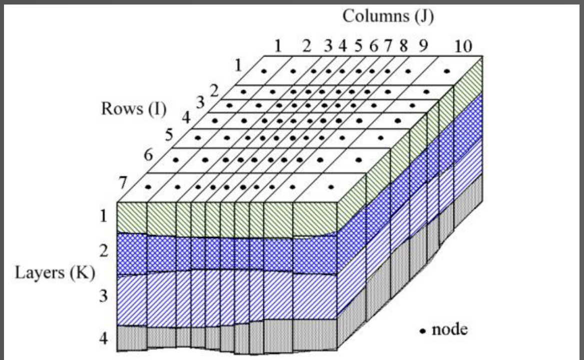
Hydrogeologic framework

- **Water table and potentimetric maps** for all aquifers
- **Hydrographs** of groundwater head and surface water levels and discharge rates
- **Maps and cross sections** – hydraulic conductivity and/or transmissivity distribution
- **Hydraulic conductivity** – distribution for stream and lake sediments
- **Spatial and temporal distribution** of: ET, Groundwater recharge, surface water-groundwater interaction, groundwater pumping and natural groundwater discharge
- **Maps** – morphology, geology, hydrogeology, climatic, landuse, settlement
- **People activity** - pumping or injection wells, build-up area

Hydrogeological model: grid design

- Conceptual model determinates the dimension of the numerical model and the design of the grid
- Grid – continous problem domain si discretized to finite difference blocks – cells
  - Finite difference grids: block centered x mesh-centered
  - Finite elements – more flexibility in designing a grid
- Defining model layers – hydrostratigraphic units (various conditions for groundwater flowing)
- Orienting the grid
  - colinear with the principal direction of the hydraulic conductivity tensor
  - minimalize the number of cells outside the boundaries of the modeled area
  - grid colinear with regional flow direction
- Size of the nodal horizontal and vertical spacing – function of the potentiometric surface and water table curvature, significant gradients requier finer nodal spacing
- Grid refinement (regular and irregular grid) – the rule of thumb is to expand the grid by increasing nodal spacing no more than 1,5 times the previous nodal spacing

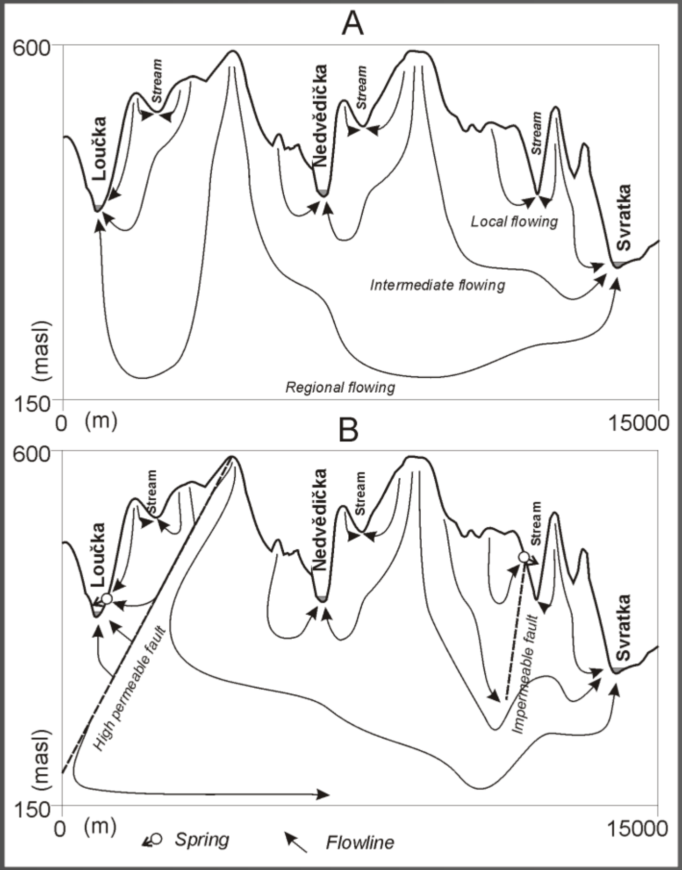




Hydrogeological model: boundaries

Correct selection of boundary condition si a critical step in model design

- Physical boundaries – formed by the physical presence impermeable body of rock (outcrops), river, lake
- Hydraulic boundaries – streamline, groundwater divide
- Internal boundaries – sources and sinks within interior of the grid (river, drain, lake, well etc.)



<u>Hydrogeologic boundary condition:</u>

I. type - specified head boundary, head = constant, often draining stream

II. type - specified flow boundary, q = constant, often inflow - outflow boundary, q = 0, no flow boundary, often groundwater divide, impermeable rock outcrop, impermeable fault

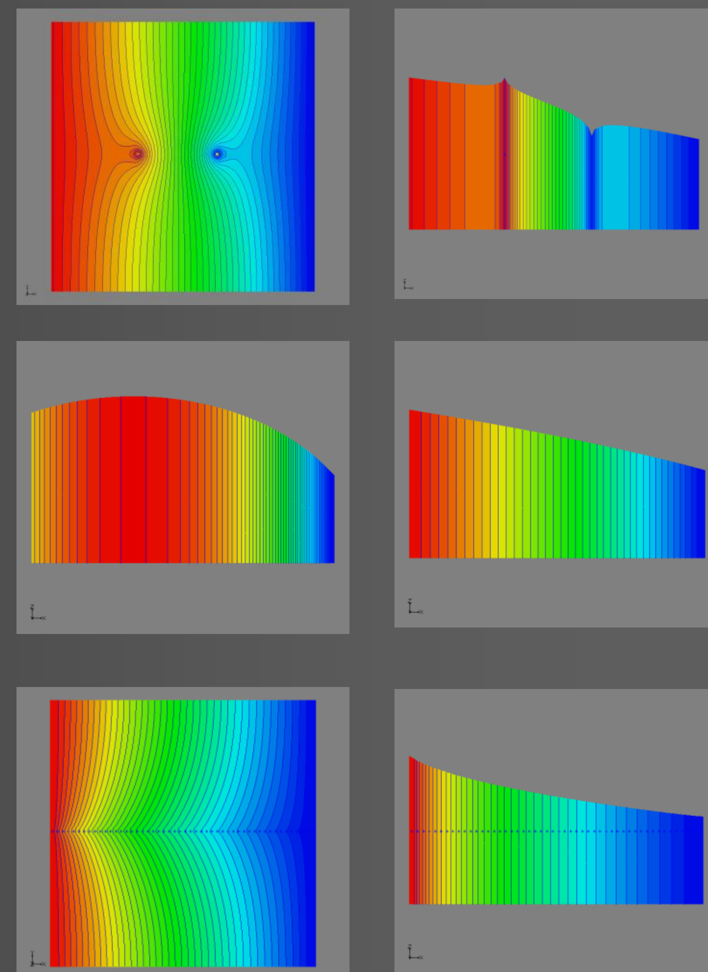
III. type – head dependent flow boundary, q = f (h), mixed function of stream

Hydrogeological model: sources and sinks

Water enters or leaves a model through the boundaries or through sources and sinks

Sources and Sinks

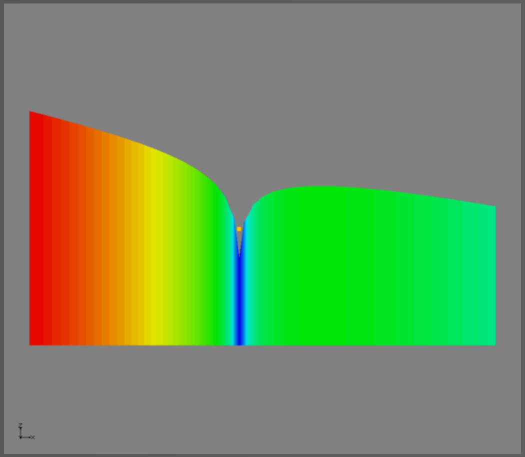
- Injection and pumping wells
- Flux across the water table – recharge x discharge (ET)
- Leakage – movement of water through a layer that has a vertical hydraulic conductivity lower than that of the aquifer. Leakage may enter or leave tle aquifer depending on the relative differences in heads between tle aquifer and the source reservoir – river, lake – III. type



Hydrogeological model: simulation flow type

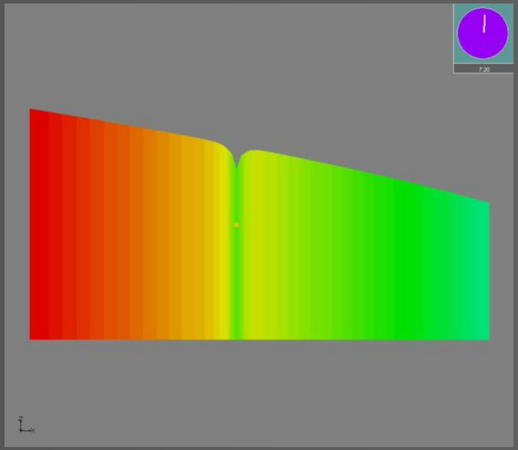
Steady-state flow simulation

- Numerical iterations are calculated until the heads and flow rates are unvarying
- Model calibration

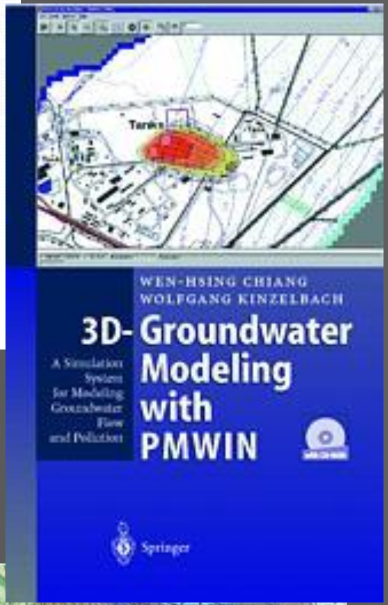


Transient flow simulation

- Time dependent problems – transient variation of water level, flow rates
- Begin with steady-state intial conditions
- More complicated for data manegment:
  1. storage characteristics (storage coeffiecient for confined aquifer and specific yield for unconfined aquifer)
  2. Intial conditions giving the head distributions in the aquifer at the beginning of the simulation must be specified in addition to boundary conditions
  3. The time dimension must be discretized



Hydrogeological model: model execution



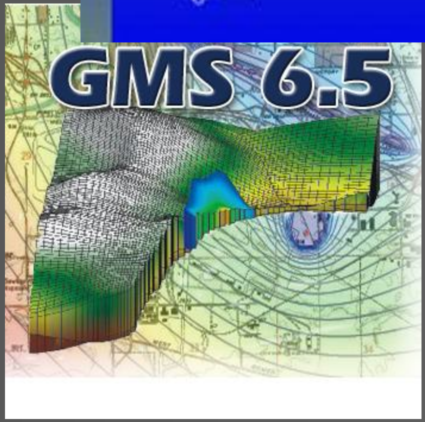
Code selection:

- Finite elements, finite differences
- Saturated, unsaturated flow
- Transport – advective, multiphase
- Heat flow, fluid density

(complex packages – Fefflow, GMS, PMWIN)

Initiating Model Execution:

- Error criterion – nonconvergence (iteration residual error) - inappropriate intial guesses of heads and parameters, poorly discretizated time and space
- Error criterion for heads – convergence criteria
- Error criterion for tha water balance – checking of tle residual error in tle solution allows total simulated inflows and outflows as computed by tle Water Budget



Modeling rules/guidelines

- Boundary conditions always affect a steady state solution.
- Initial conditions should be selected to represent a steady state configuration of heads.
- In general, the accuracy of the numerical solution improves with smaller grid spacing and smaller time step
- A water balance should always be included in the simulation.

Hydrogeological model: calibration process

Calibrated model means that is capable to produce field-measured heads and flows.

Finding of the right parameters (hydraulic conductivity, specific storage), boundary conditions and stresses (recharge):

- First calibration (steady-state flow) and second calibration (transient flow)
- Mean annual water level or seasonal average of heads

Calibration values (Sample Information)

- Heads – errors caused by measure accuracy, scalling effect (average head in well with the long screen, but model require point value), unmodeled heterogeneity, interpolations errors (calibration values do not coincide with nodes)
- Fluxes – baseflow, springflow, infiltration from a losing stream or ET from the water table – usually larger errors than errors asociated with head measurements
- It as advisable to use both heads and fluxes

Hydrogeological model: calibration process

Parameter estimates (Prior information) – used during the calibration process

- Hydraulic conductivity and/or Transmissivity, storage parameters – usually derived from aquifer tests
- Recharge – usually not available information – choose plausible rang of values
- Boundary conditions – uncertainty if do not correspond to the natural physical boundaries of the aquifer, specified head boundary (III. type) will help achieve calibration

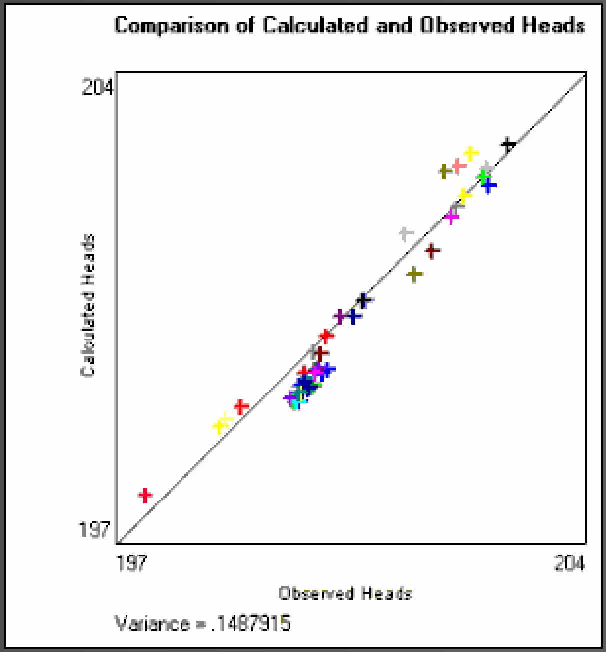
Calibration Techniques

- Manual trial and error adjustment of parameters – parameter values adjusted in sequential model runs to match simulated heads and flows to the calibration targets
- Automated parameter estimation – specially developed codes guarantee the statistically best solution and quantify the uncertainty in parameter estimates

Hydrogeological model: calibration process

Evaluating the Calibration

- Qualitative measure - comparsion between contour maps of measured nad simulated heads
- Quantitative masure – scatter plot of measured against simulated contours



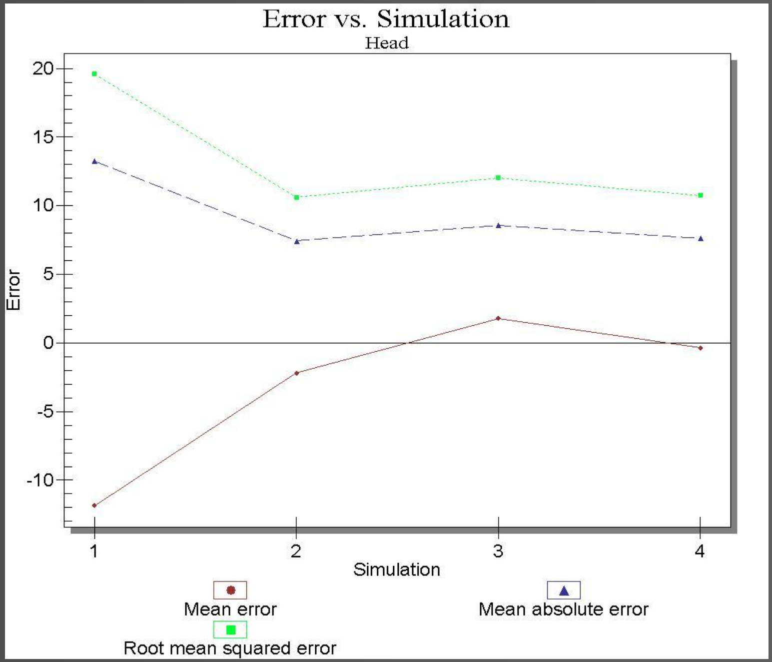
- Deviation of points from the straight line should be randomly distributed
- If a trend is evident, parameter values should be adjusted

Hydrogeological model: calibration process

Expressing the average difference between simulated and measured heads:

1. The mean error (ME) - the mean difference between measured heads (h_m) and simulated heads (h_s)

$$ME = 1/n \sum_{i=1}^{n} (h_m - h_s)_i$$



2. The mean absolute error (MAE) - the mean for the absolute value of tle differences in measured and simulated heads

$$MAE = 1/n \sum_{i=1}^{n} \left| (h_m - h_s)_i \right|$$

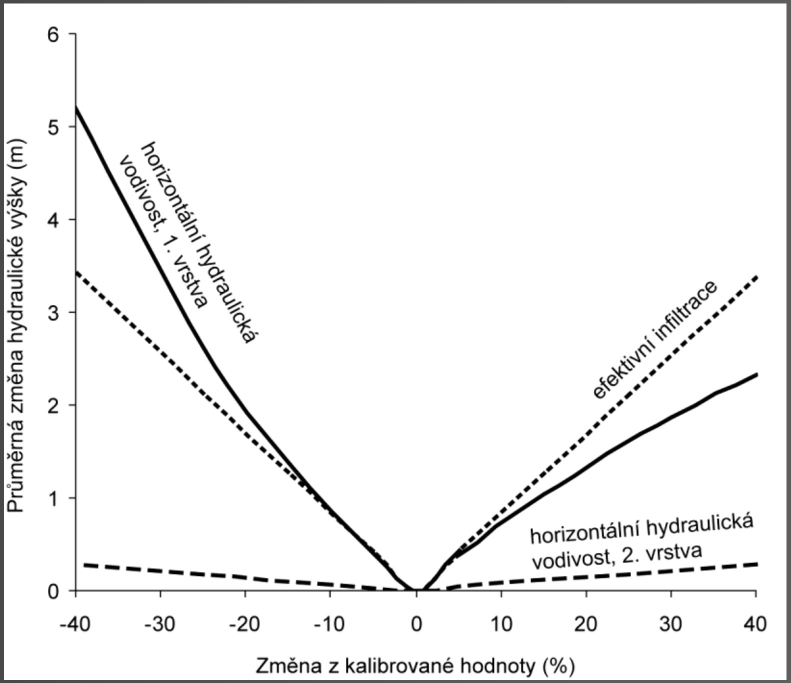
3. The root mean squared (RMS) - error or the standart deviation as the average of the squared differences in measures and simulated heads

$$RMS = \left[1/n \sum_{i=1}^{n} (h_m - h_s)_i^2 \right]^{0,5}$$

Hydrogeological model: sensitivity analysis and model verification

Sensitivitiy analysis - quantify the uncertainity in the calibrated model caused by uncertainity in the estimates of aquifer parameters

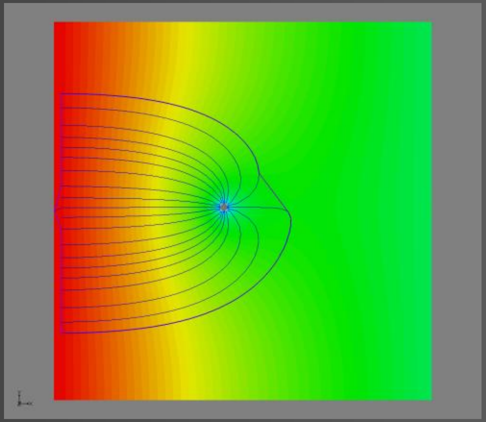
Changing two or more parameters also might be examined to determine the widest range of plausible solutions

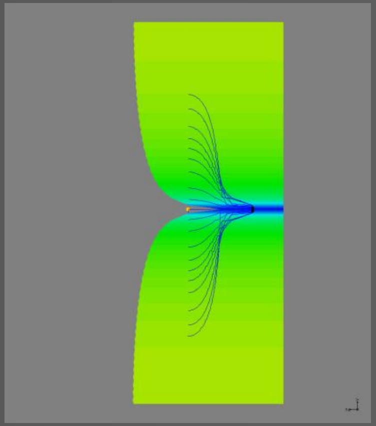


Model verification - help establish greater confidence in the calibration

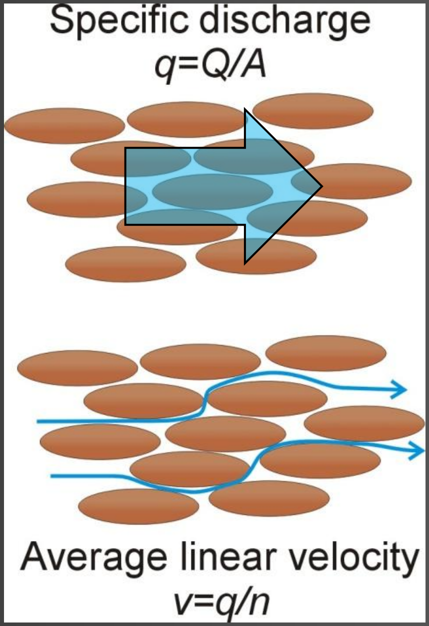
Calibrated values are used to simulate a transient response for which a set of data exists (e.g. Record of groundwater levels in response to drought or long-term pumping)

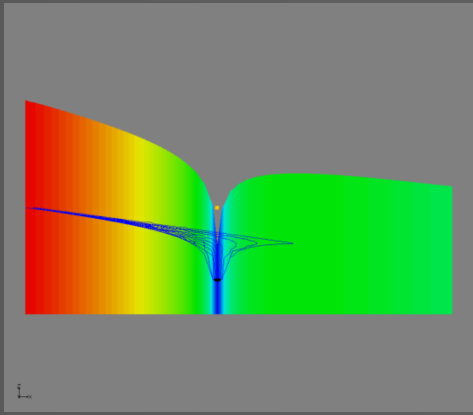
Hydrogeological model: particle tracking of groundwater flow





- Trace of out flow paths or pathlines by tracking the movement of infinitely small imaginary particles placed in the flow field
- Help visualize the flow field and to track contaminant paths
- Detect conceptual errors



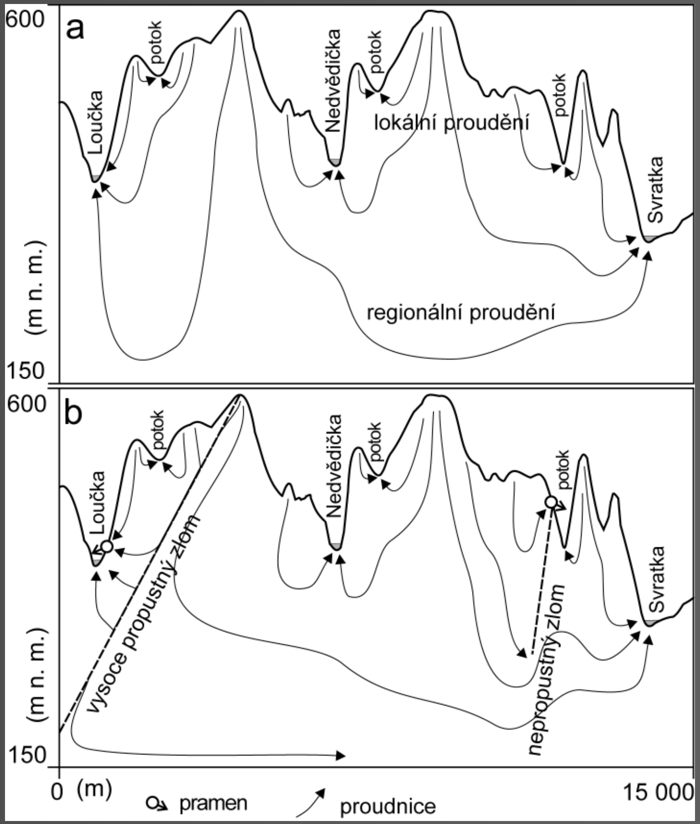


Transport of particles by advection

$$v = -K/n_e (grad\,h)$$

Hydrogeological model: problems

- Unsuitable type of the numerical model – finite elements x differences
- Deficit of important data – heads (lack of the well), flow rates, precipitations (without gauge stations) → poor calibration
- Heterogenity – hydraulic conductivity, character of the heterogenities: linear heterogeneity (fractures) or areal (rock bodies form)
- Drying and wetting of the cells
- Deep flow – recharge, depth of the groundwater circulation – boundary condition



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