ETH zürich

Groundwater modelling

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for ENV 504: Remediation of Soils and Groundwater (Prof. Rizlan Bernier-Latmani)

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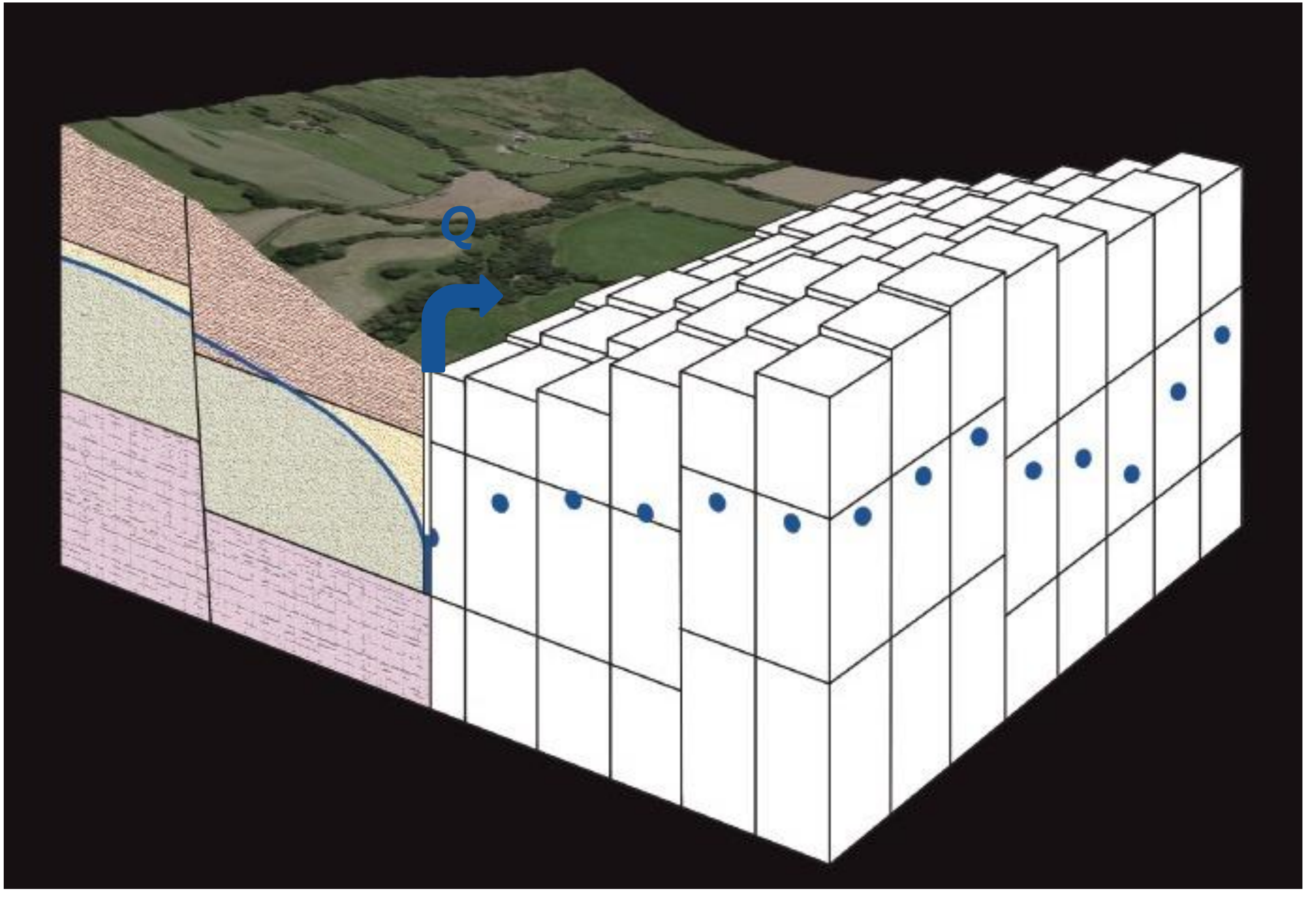
Groundwater model



Shepley, M.G., Whiteman, M.I., Hulme, P.J. and Grout, M.W., 2012. Introduction: groundwater resources modelling: a case study from the UK. *Geological Society, London, Special Publications*, *364*(1), pp.1-6.

Why do we need models?

- Relative **inaccessibility** of aquifers
- **Scarce data** in the subsurface requires conceptual model for analysis
- **Complexity of nature** requires simplification
- **Slowness of processes** (contaminant transport, climate change) requires predictive capability
- Large effort in interpretation (for models) justified by **high cost of data**

Where are groundwater models required?

- For improved **understanding of the functioning** of aquifers (e.g. determination of aquifer parameters)
- For **prediction of water flow and/or transport** (e.g. contaminants, both conservative and reactive)
- For **design of measures of aquifer management** (e.g. contaminant remediation, pumping site)
- For **risk analysis** (e.g. contamination, sustainable water management)

Examples for groundwater models

- **Installation of new well fields**
  - Sustainability? Environmental impacts? Effects on water quality?
- **Groundwater protection zones**
  - Size and shape of well catchments, travel times
- **Design of remediation measures**
  - Feasibility, optimization of costs
- **Risk analysis of waste repositories**

Types of groundwater models

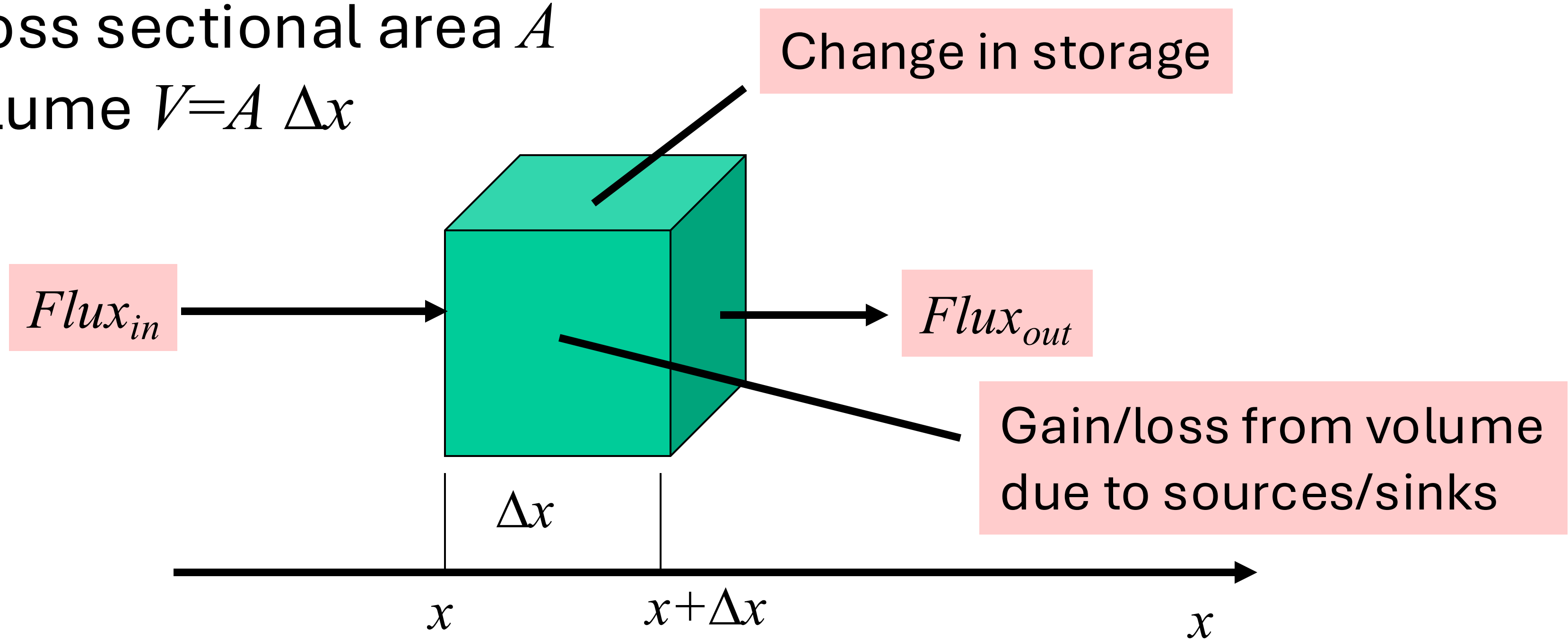
- **Flow models** (saturated flow)
- **Solute transport models** (non-reactive, dissolved substances)
- **Reactive transport models** (simple to complex multi-component reactive transport)
- **Heat transport models** (heat behaves analogous to dissolved substances)
- **Multiphase flow and transport** (unsaturated zone)
- **Other coupled models** including density dependent flow, thermo-hydro-mechanical coupling

Basic Principles for Modeling

- **Starting from first principles:**
  - Conservation of mass (or volume if density is constant)
  - Conservation of dissolved mass
- **General approach based on the following quantities:**
  - **Extensive quantity** Φ (volume, mass)
  - **Intensive quantity** ξ = extensive quantity per unit volume (porosity, concentration)
  - **Flux** $\boldsymbol{j}$ (of volume, mass) (quantity per unit area and time)
  - **Source-sink distribution** σ (volume per geometric unit volume and unit time, mass per unit water volume and unit time)

Basic principle in 1D

For time interval $[t, t+\Delta t]$
Cross sectional area A
Volume $V=A\ \Delta x$



Conservation law in words:

$$(Flux_{in} - Flux_{out}) \cdot A \cdot \Delta t + Source \cdot V \cdot \Delta t = Storage$$

Basic principle in 1D

$$\left[j(x) - j(x+\Delta x) \right] A \Delta t \;+\; \sigma V \Delta t \;=\; \Phi(t+\Delta t) - \Phi(t)$$

Division by $(\Delta t,\ V = \Delta x\ A)$ yields:

$$\frac{j(x) - j(x+\Delta x)}{\Delta x} + \sigma = \frac{\xi(t+\Delta t) - \xi(t)}{\Delta t}$$

In the limit: $\Delta t \rightarrow 0,\ \Delta x \rightarrow 0$:

$$-\frac{\partial j}{\partial x} + \sigma = \frac{\partial \xi}{\partial t}$$

Basic principle in 3D

Balance equation:

$$-\frac{\partial j_x}{\partial x}-\frac{\partial j_y}{\partial y}-\frac{\partial j_z}{\partial z}+\sigma=\frac{\partial \xi}{\partial t}$$

or

$$-\nabla\cdot\mathbf{j}+\sigma=\frac{\partial \xi}{\partial t}$$

$\nabla\cdot(\mathbf{j})$: Divergence of flux vector $\mathbf{j}$

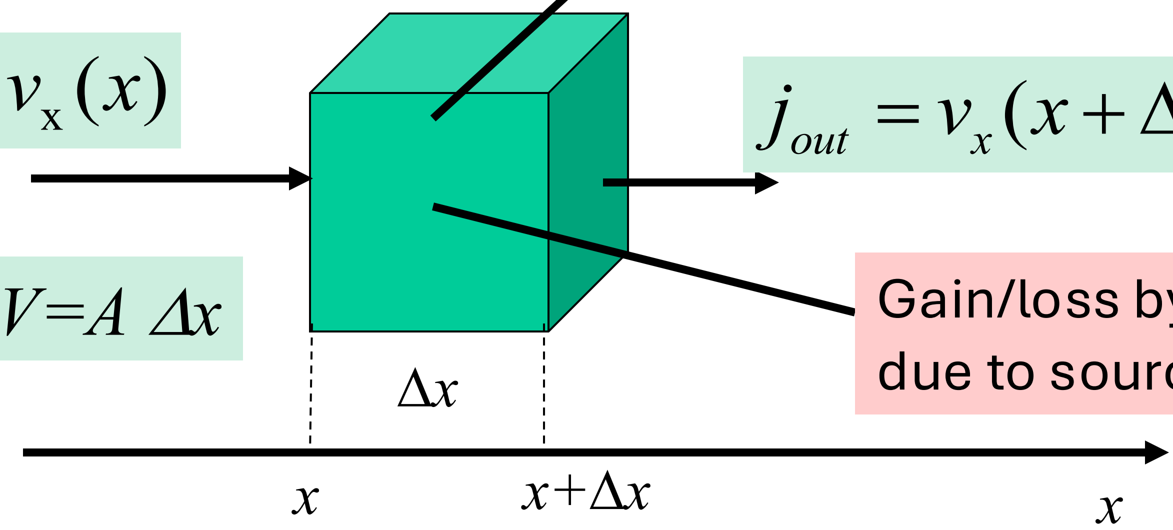
Water balance in 1D

For compressible water

Time interval $[t, t+\Delta t]$

Change in storage of water can be seen as a change in intensive quantity (= porosity)

$$j_{in} = v_x(x)$$



$$j_{out} = v_x(x+\Delta x)$$

$V = A\ \Delta x$

Gain/loss by volume due to sources/sinks w

Conservation equation for water volume:

$$\left[v_x(x) - v_x(x+\Delta x)\right] A\ \Delta t + w\ V\ \Delta t = V_{water}(t+\Delta t) - V_{water}(t)$$

Water balance in 1D

Division by $(\Delta t,\ V = \Delta x\ A)$ yields:

$$-\frac{v_x(x+\Delta x)-v_x(x)}{\Delta x}+w=\frac{\Delta V_{water}/V}{\Delta t}=\frac{\Delta n}{\Delta t}$$

In the limit:

$$-\frac{\partial v_x}{\partial x}+w=\frac{\partial n}{\partial h}\frac{\partial h}{\partial t}$$

$$(V_{water}/V=n)$$

Using the definition of **specific storage** S_0 [L^{-1}]
and **Darcy's law** with hydraulic conductivity

$$\frac{\partial n}{\partial h}=S_0$$

and

$$v_x=-K\frac{\partial h}{\partial x}$$

$$\Longrightarrow$$

$$\frac{\partial}{\partial x}\left(K\frac{\partial h}{\partial x}\right)+w=S_0\frac{\partial h}{\partial t}$$

Generalization to 3D

$$-\frac{\partial v_x}{\partial x}-\frac{\partial v_y}{\partial y}-\frac{\partial v_z}{\partial z}+w=S_0\frac{\partial h}{\partial t}$$

with $\mathbf{v} = -\mathbf{K}\nabla h$ and $\frac{\partial v_x}{\partial x}+\frac{\partial v_y}{\partial y}+\frac{\partial v_z}{\partial z}=\nabla\cdot\mathbf{v}$

$$\nabla\cdot\left(\mathbf{K}\nabla h\right)+w=S_0\frac{\partial h}{\partial t}$$

+ Initial condition
+ Boundary conditions

Multitude of aquifers through distribution of $\mathbf{K}$, S_0 and w and of initial and boundary conditions

In practical applications: often 2D and 2.5D models

2D confined aquifer: by integration over z-coordinate

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

with $T = K \cdot (Top\text{-}Bottom = thickness)$
$S = S_0 \cdot (Top\text{-}Bottom = thickness)$

2D unconfined aquifer: by integration over z-coordinate

$$\nabla \cdot (K \cdot (h - Bottom) \nabla h) + w = S \frac{\partial h}{\partial t}$$

with $S \cong n_e$ = drainable porosity

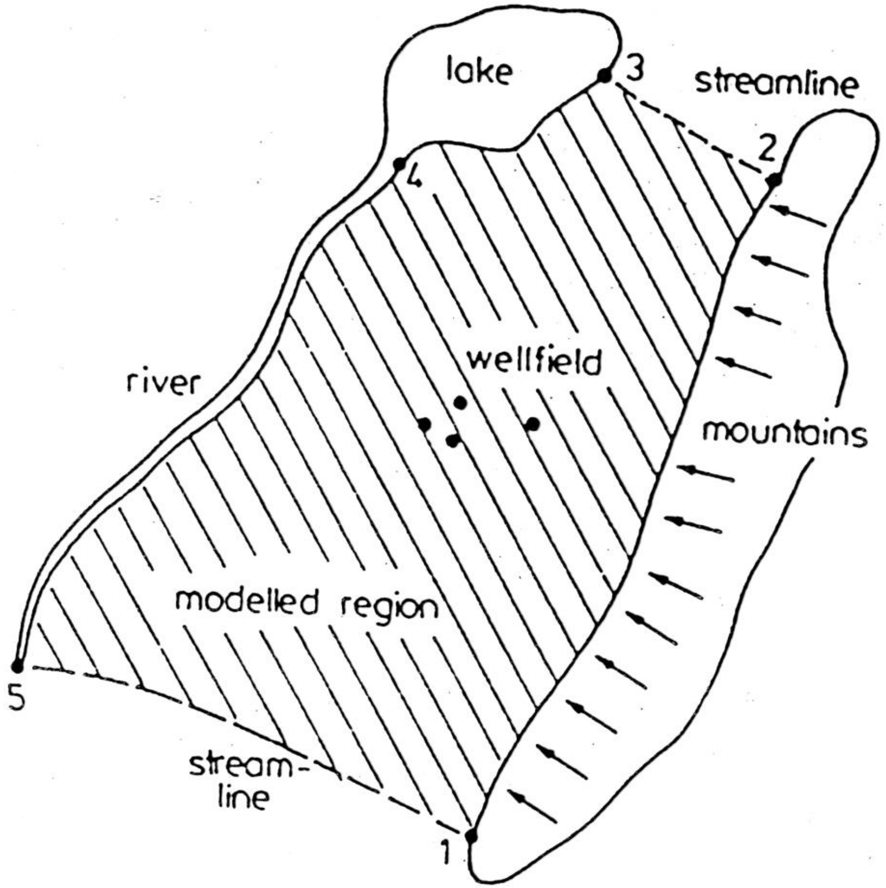
2.5D by vertical coupling of 2D layers through leakage-term

$$q = \omega_{i-1} \cdot (h_{layer\ i} - h_{layer\ i-1}) + \omega_i \cdot (h_{layer\ i} - h_{layer\ i+1})$$

with $\omega = \frac{K_{vert}}{\Delta z}$

Boundary conditions for flow

- **1st type BC**: h on boundary specified (water level-*Dirichlet*)
- **2nd type BC**: $\partial h / \partial n$ given on boundary (water flow-*Neumann*)
- **3rd type BC**: $\alpha \cdot h + \beta \cdot \partial h / \partial n$ given on boundary (*Cauchy*)
- **Further**:
  - Free surface: $p=0$
  - Evaporation boundary
  - Moving boundary (free surface)



Practical rules for boundary conditions of flow models

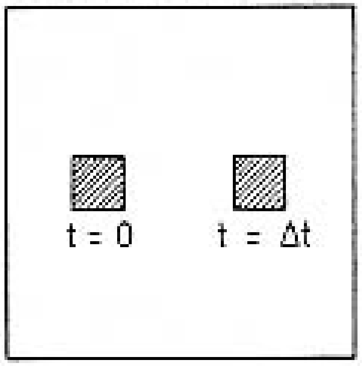
- **Use natural hydrogeological boundaries** (*e.g.*, rivers, water divides, aquifer limits)
- **Use as few fixed head boundaries as possible** (at least one is necessary in a steady state model)
- **At upstream boundaries use fixed flux boundary**. At downstream boundaries use fixed head boundary.
- **Use third type boundary conditions for distant fixed heads**.
- **Streamlines are boundaries of the second type** (no flow perpendicular to streamline)

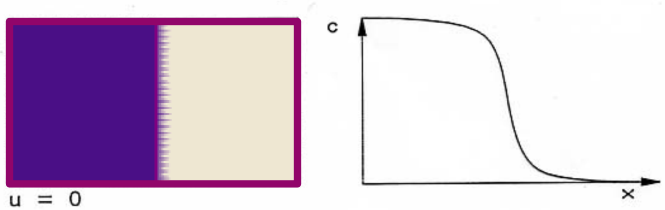
And now the same for transport of a solute

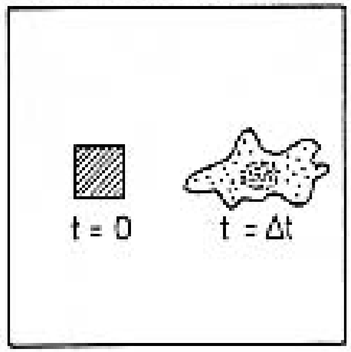
- The flux is more complicated.
- It is composed of:
  - Advective flux $\mathbf{j}_{adv} = \mathbf{v}\, c$
  - Diffusive flux $\mathbf{j}_{diff} = -n_e D_m \nabla c$
  - Dispersive flux $\mathbf{j}_{disp} = -n_e \mathbf{D} \nabla c$

  $\mathbf{v}$ is specific flux (Darcy velocity)

- Total flux: $\mathbf{j}_{tot} = \mathbf{j}_{adv} + \mathbf{j}_{diff} + \mathbf{j}_{disp}$

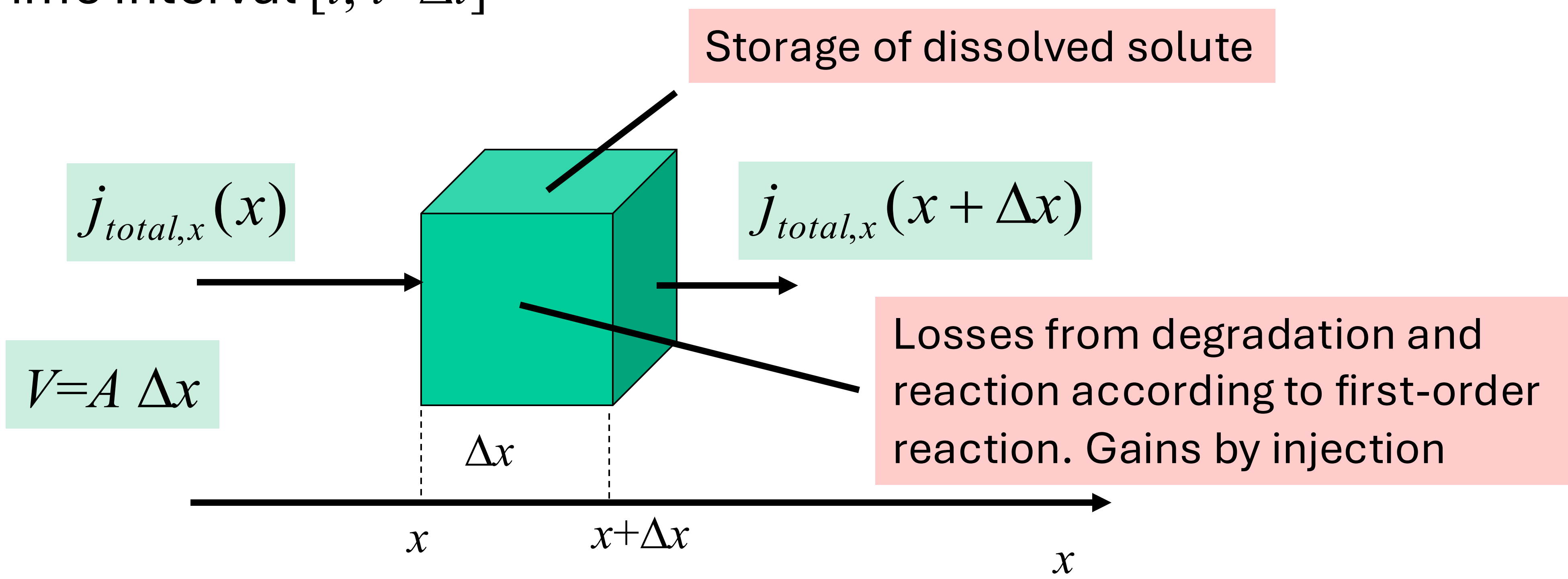






Mass balance in 1D

Time interval $[t, t{+}\Delta t]$



Conservation equation for dissolved

$$\left(j_{total,x}(x) - j_{total,x}(x+\Delta x)\right) \cdot A \cdot \Delta t - \lambda \cdot c \cdot n_e \cdot V \cdot \Delta t + w \cdot c_{in} \cdot V \cdot \Delta t = \left(m(t+\Delta t) - m(t)\right)$$

Mass balance in 1D

Division by $(\Delta t,\ V = \Delta x\ A)$ yields:

$$-\frac{j_{total,x}(x+\Delta x) - j_{total,x}(x)}{\Delta x} - \lambda n_e c + w c_{in} = \frac{\left(V_{water} \cdot c(t+\Delta t) - V_{water} \cdot c(t)\right)/V}{\Delta t}$$

In the limit: $$-\frac{\partial j_{total,x}}{\partial x} - \lambda n_e c + w c_{in} = \frac{\partial (n_e c)}{\partial t}$$

Substitute of expression into fluxes:

$$-\frac{\partial (v_x c)}{\partial x} + \frac{\partial}{\partial x}(n_e \cdot (D_m + D_L)\frac{\partial c}{\partial x}) - \lambda n_e c + w c_{in} = \frac{\partial (n_e c)}{\partial t}$$

For constant effective porosity n_e and pore velocity $u = v/n_e$:

$$-\frac{\partial (u_x c)}{\partial x} + \frac{\partial}{\partial x}\left((D_m + D_L)\frac{\partial c}{\partial x}\right) - \lambda c + \frac{w c_{in}}{n_e} = \frac{\partial c}{\partial t}$$

Mass balance: Generalization to 3D

With $$\frac{\partial(u_x c)}{\partial x}+\frac{\partial(u_y c)}{\partial y}+\frac{\partial(u_z c)}{\partial z}=\nabla\cdot(\mathbf{u}c)$$

and

$$\mathbf{j}_{diff}+\mathbf{j}_{disp}=-(D_m+\mathbf{D})\nabla c$$

$$\mathbf{D}=\begin{bmatrix} D_L & 0 & 0 \\ 0 & D_T & 0 \\ 0 & 0 & D_T \end{bmatrix}$$

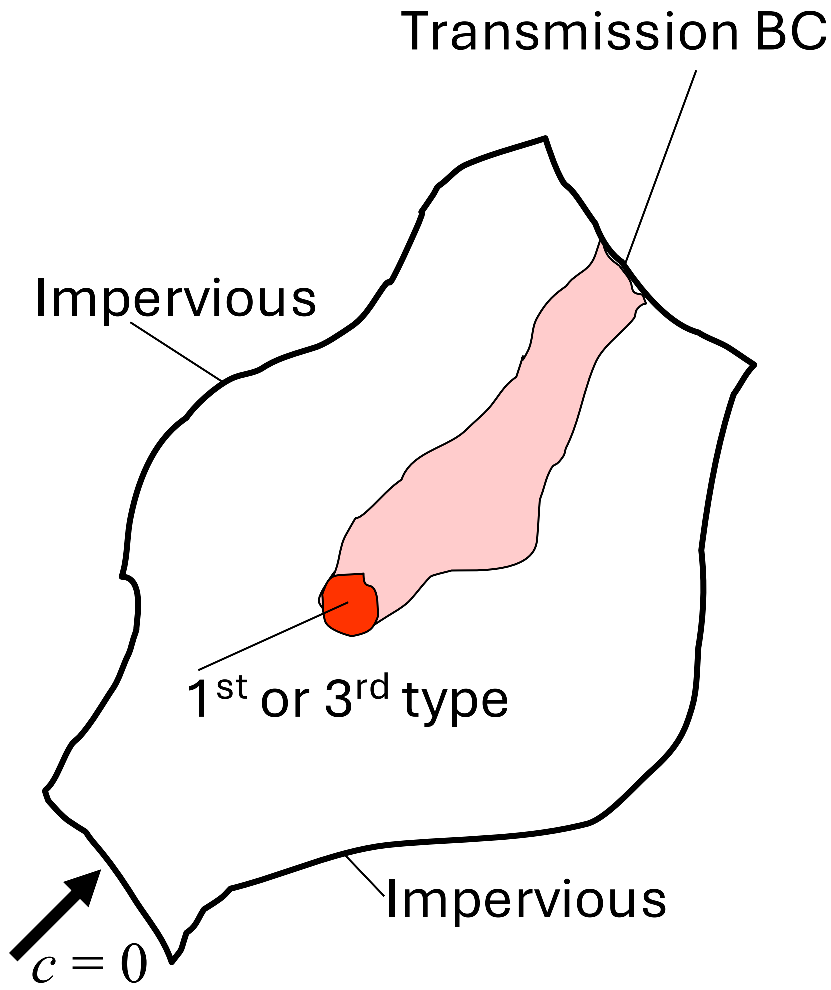
In a system, in which $\mathbf{u}$ is parallel to x-axis!

$$-\nabla\cdot(\mathbf{u}\,c)+\nabla\cdot\left(\left(D_m+\mathbf{D}\right)\nabla c\right)-\lambda\,c+\frac{w\,c_{in}}{n_e}=\frac{\partial c}{\partial t}$$

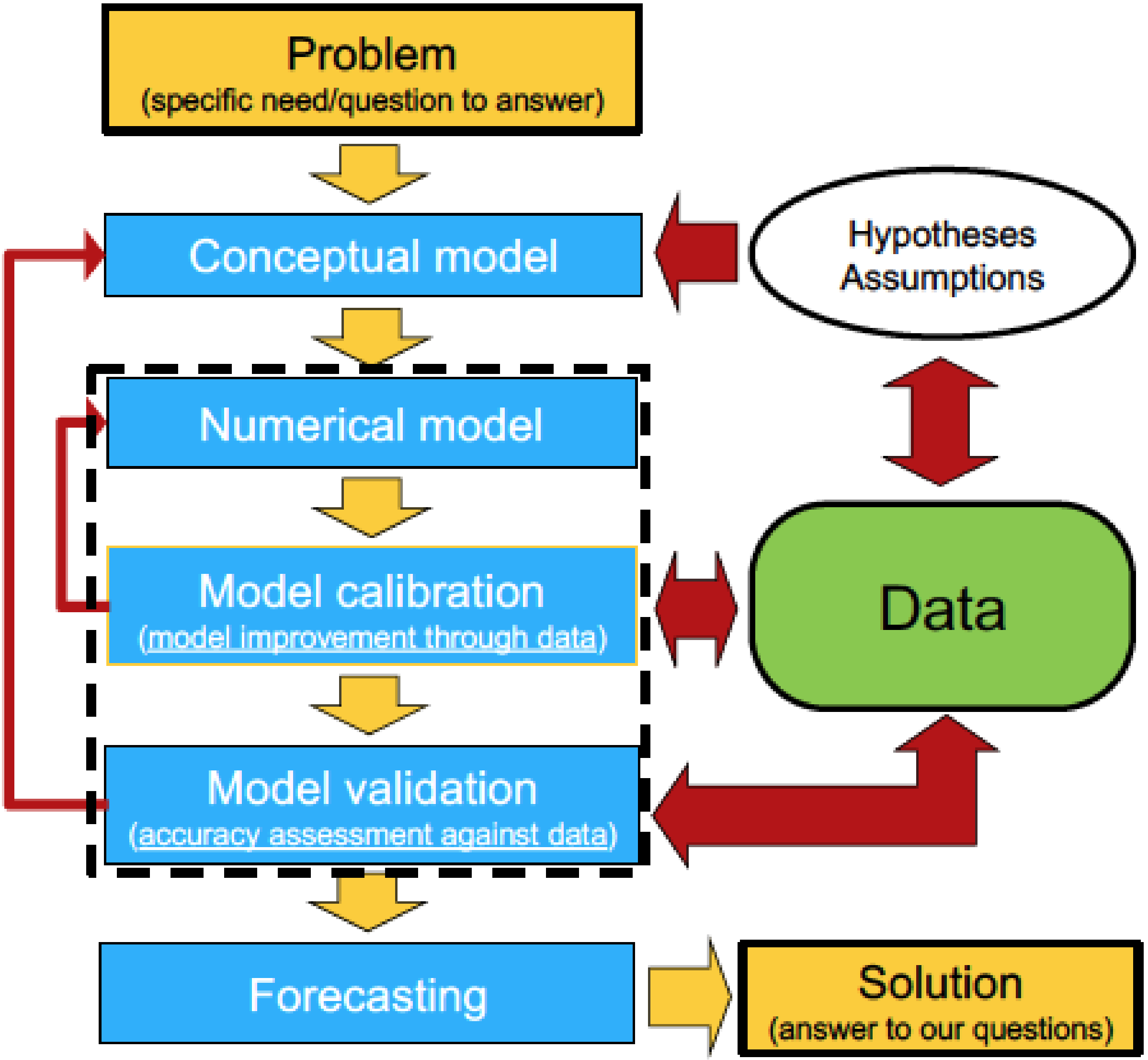
Again: Initial condition + Boundary conditions

Boundary conditions for transport problems

- **1st type BC**: Concentration c prescribed on the boundary. This determines the advective flux.
- **2nd type BC**: Derivative $\partial c / \partial n$ prescribed on boundary. This determines the diffusive-dispersive flux. **Only used to make a no-flow boundary impervious for diffusion/dispersion**.
- **3rd type BC**: $\alpha \cdot c + \beta \cdot \partial c / \partial n$ prescribed on the boundary. This determines the total mass flux.
- **Transmission BC**: $\partial^2 c / \partial n^2 = 0$ along boundary to keep the concentration gradient constant (implementation: $\mathbf{D} = 0$ on boundary cell).



Building a groundwater model

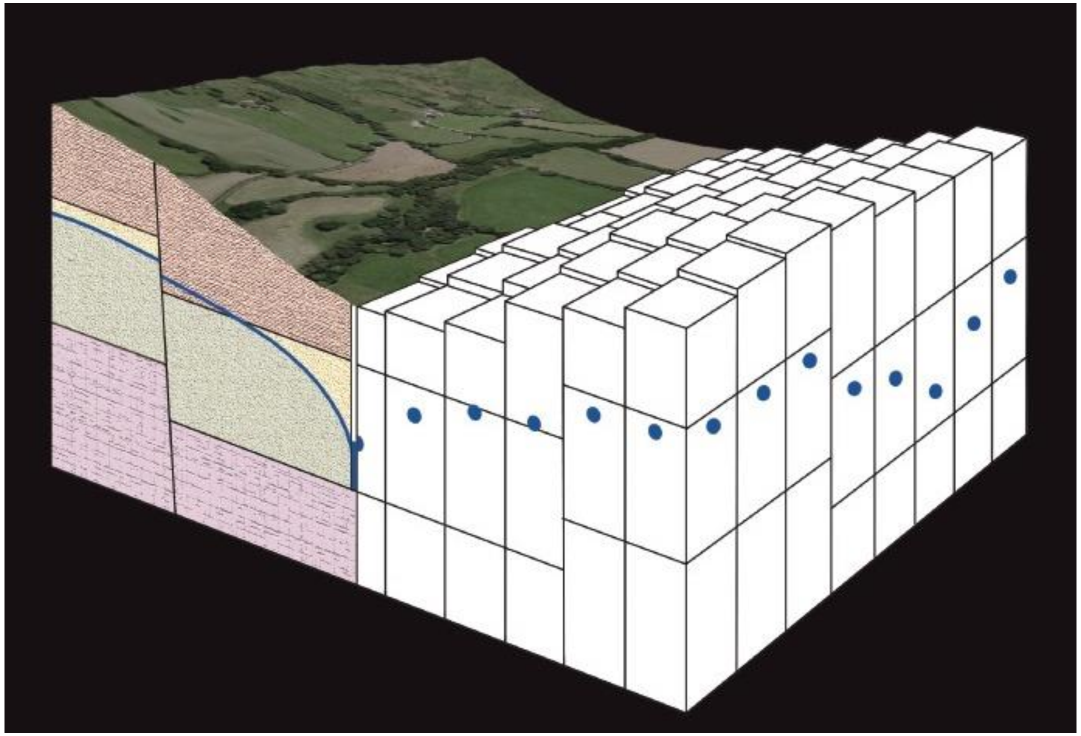


from I. Lunati (Empa)

Where does the data come from?

- Geometry:
  - Top-Bottom: boreholes, geophysics
  - Surface: LIDAR, Synthetic Aperture Radar
- Transmissivity, Storage coefficient:
  - Pumping tests
- Aquifer recharge:
  - Soil water balance, analysis of low water discharge, and environmental tracers
- River water table, riverbed
  - Geodetic surveys
- Pumping rates
  - Recording of waterworks
- Major difficulties (data): inflows across boundaries, leakage factors
  - From model calibration

Groundwater model



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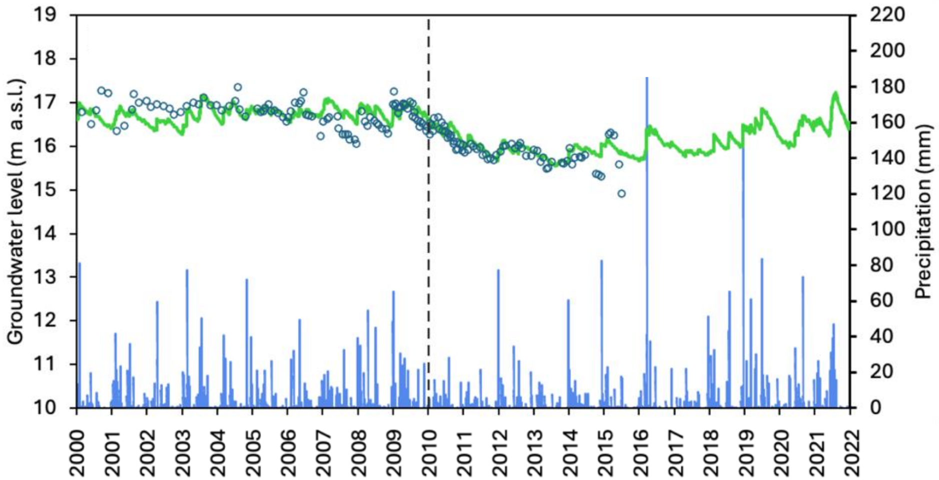
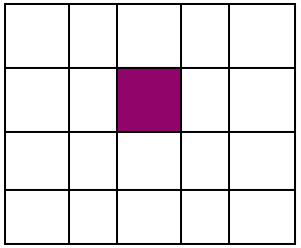
- Ideally, all parameters and boundary conditions are known and can be perfectly parameterized
- Reality: Uncertainty in parameters and boundary conditions, but head values that could be used (calibration)



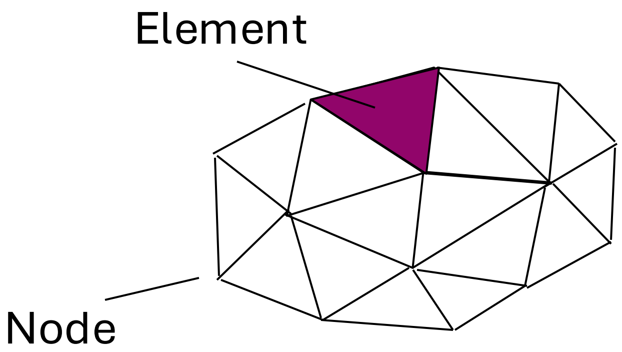
Methods of spatial discretization

Finite Differences
(explained here)



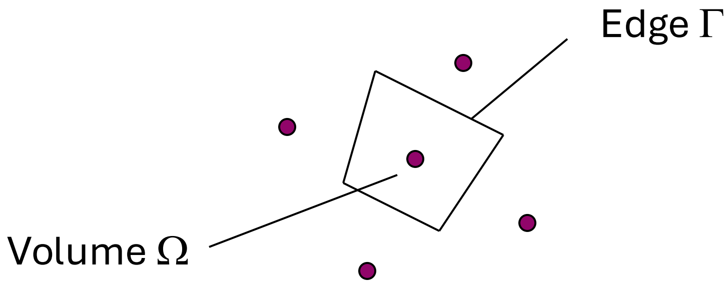
Balance over cells

Finite Elements



Balance over nodal patches

Finite Volumes



Balance over a volume

Methods of spatial discretization

- Formal mathematical approach

  Replacement of the differential equation by the difference quotient

- More illustrative approach:

  Arranging the aquifer in rectangular cells

  Setting up the water balance for each cell

  Expressing water balance in unknown potential heads (Darcy)

  Solving the resulting system of equations

Methods of temporal discretization

To solve the **transient** equation, ***t'*** needs to be defined:

Explicit $t' = t$

Implicit $t' = t+\Delta t$

Crank-Nicolson (implicit) $h(t') = 0.5(h(t+\Delta t)+h(t))$

Each time step is resolved for $h_{ij}(t+\Delta t)$. The solution is used as initial conditions for the next time step.

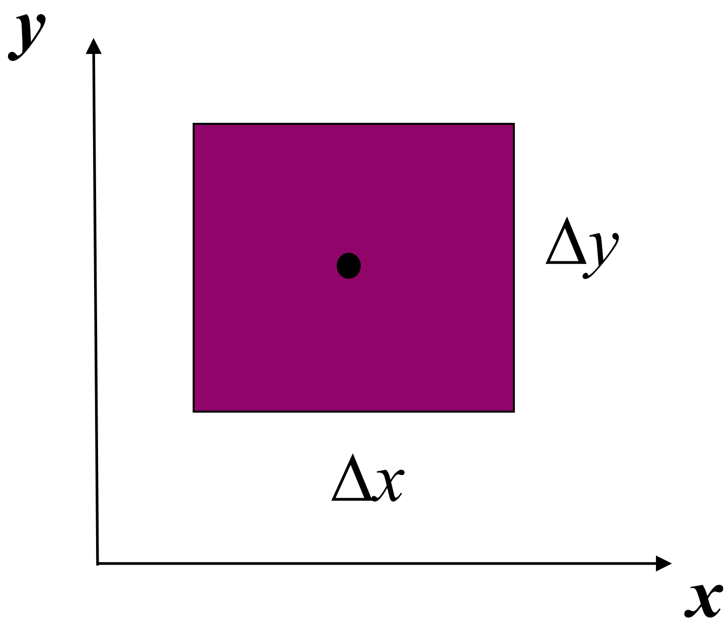
A **steady-state** groundwater model simulates conditions where properties and flows are constant over time (i.e., storage term is equal to zero).

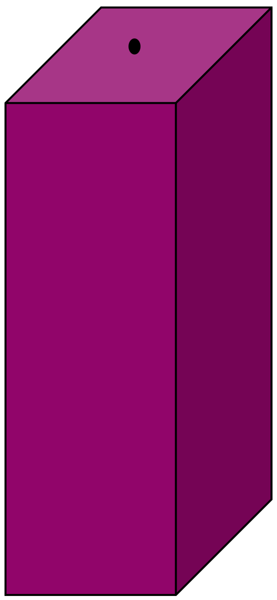
Finite Differences

Example 2D flow

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

Balance at single cells (block-centered method)





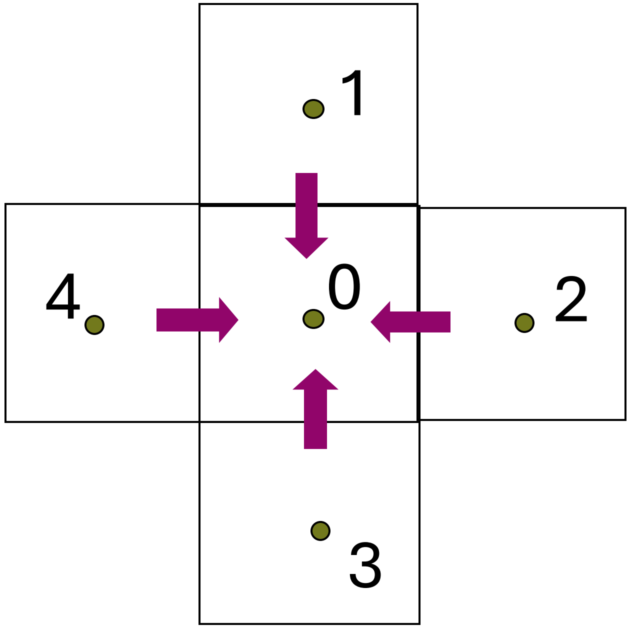
Thickness = Thickness of the aquifer

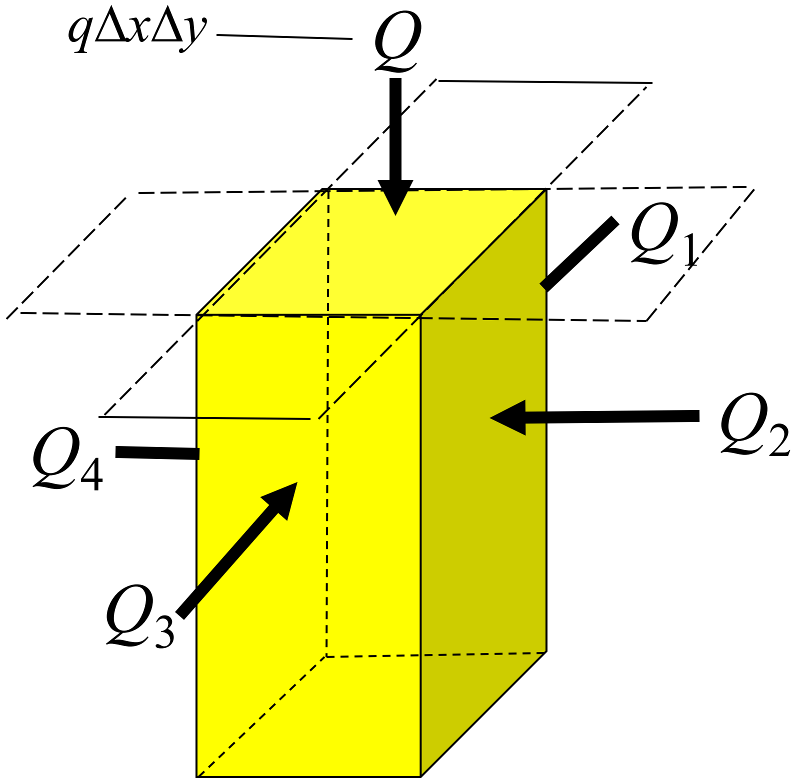
Finite Differences

Flows between cells and neighboring cells

Balance:

$$\Delta t\left(Q_1+Q_2+Q_3+Q_4+Q\right)=\left(h_0(t+\Delta t)-h_0(t)\right)S\Delta x\Delta y$$





Calibration: parameter estimation

Improve the model by comparing it with the data

Adjust unknown model parameters to match observations

- Either steady-state or transient
- It can be done “by hand” or in an automated way