

# Groundwater modelling

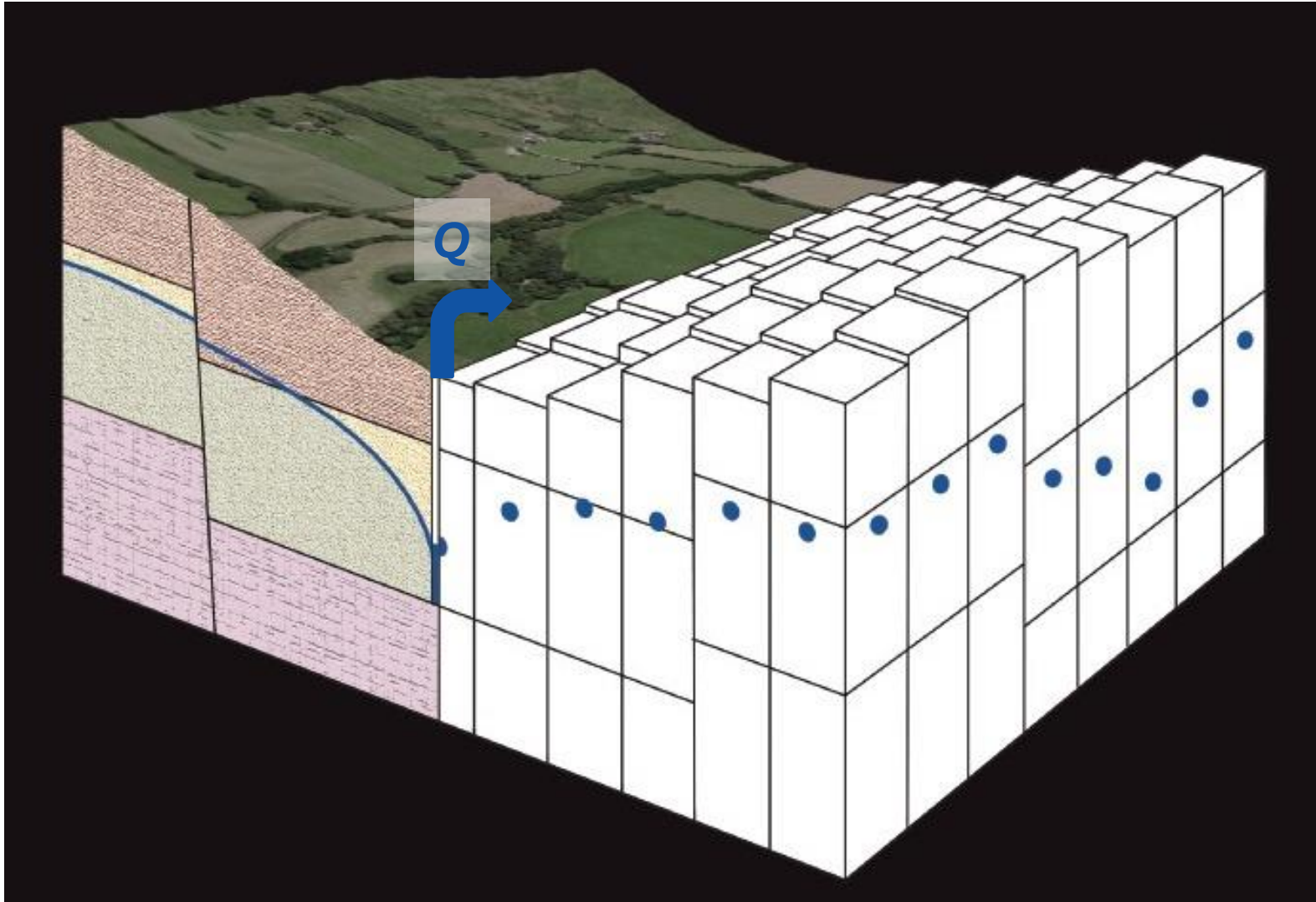
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**for ENV 504: Remediation of Soils and Groundwater (Prof. Rizlan Bernier-Latmani)**

# 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 a 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 analogously to dissolved substances)
- **Multiphase flow and transport** (unsaturated zone)
- **Other coupled models** including density-dependent flow, thermo-hydro-mechanical coupling

# Basic Principles for Modeling

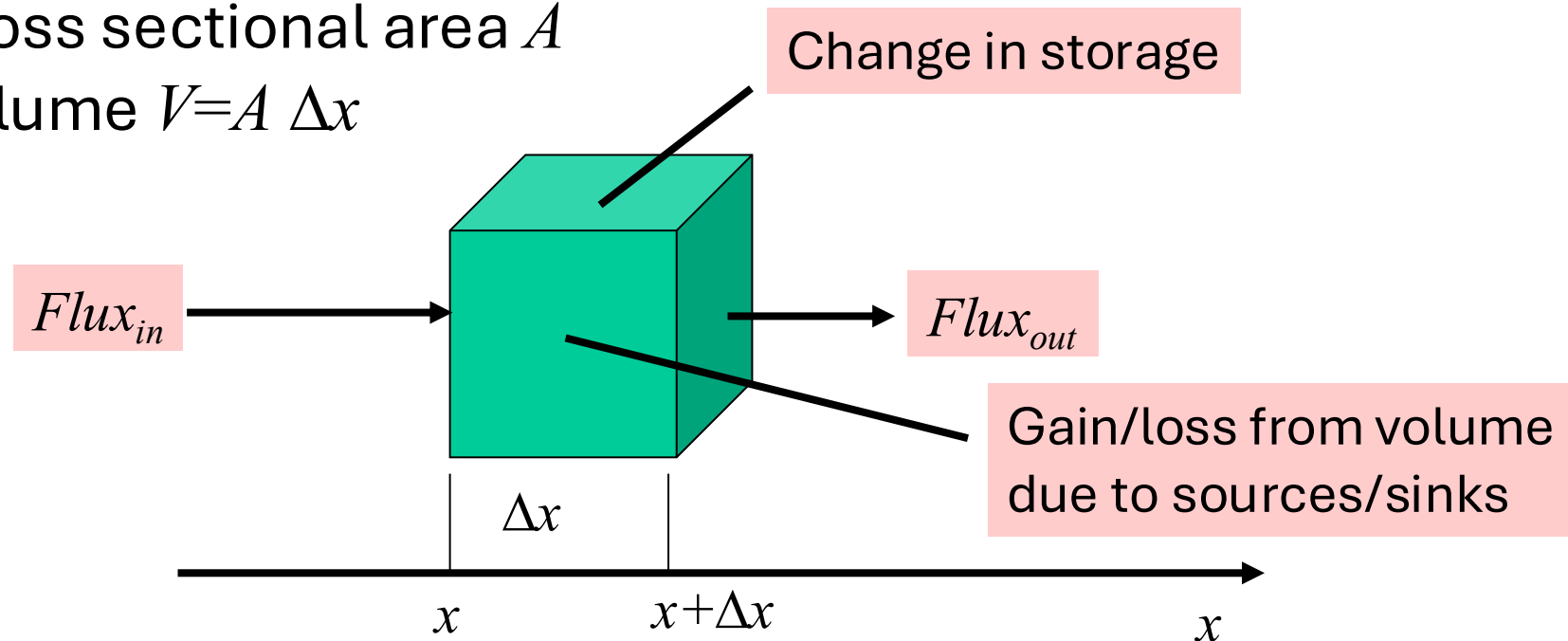
- **Starting from first principles:**
  - Conservation of mass (or volume if density is constant)
  - Conservation of dissolved mass
- **General approach based on the following quantities:**
  - **Extensive quantity**  $\Phi$  (volume, mass)
  - **Intensive quantity**  $\xi$  = extensive quantity per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

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

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

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

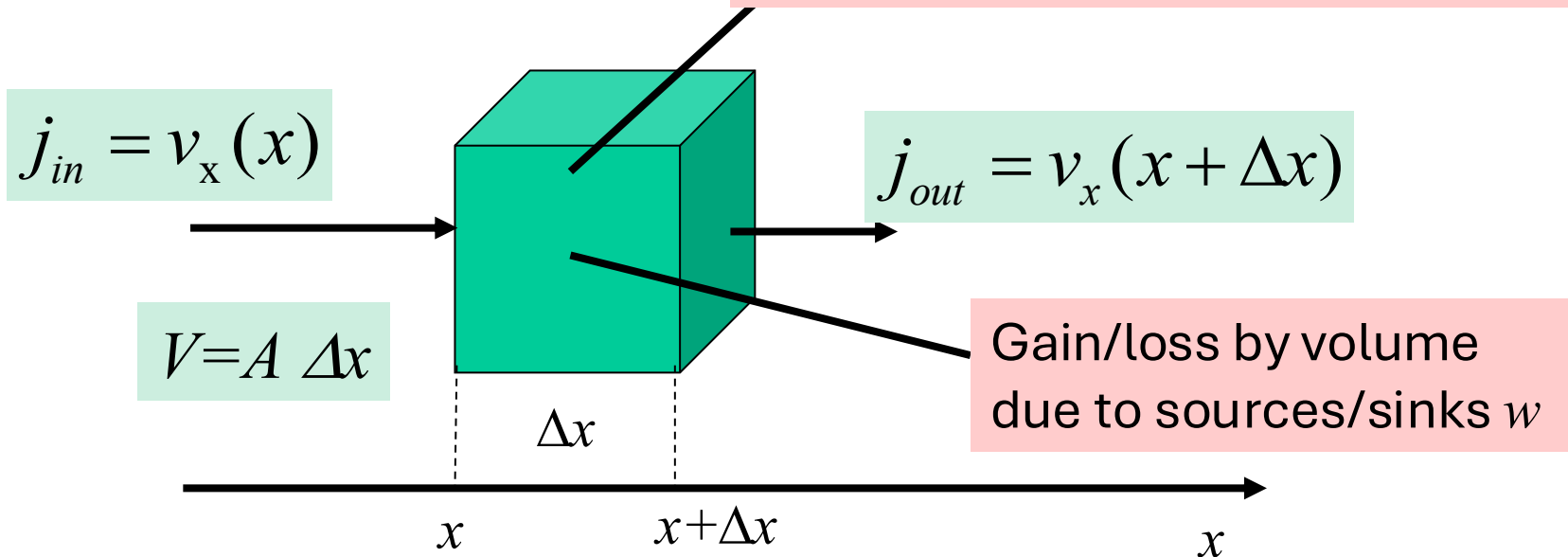
$\nabla \cdot (\mathbf{j})$  : Divergence of flux vector  $\mathbf{j}$

# 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)



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:

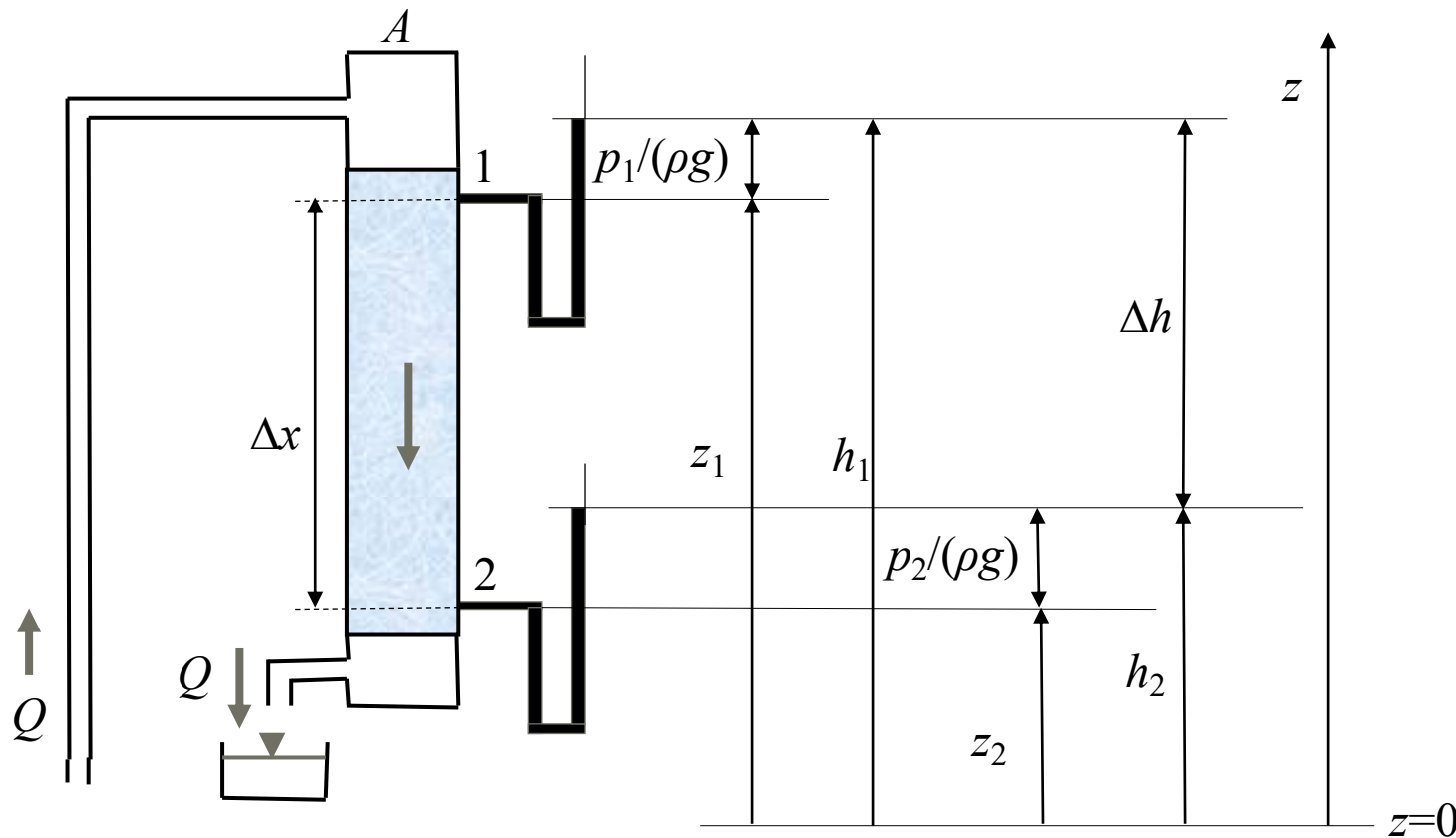
$$-\frac{v_x(x + \Delta x) - v_x(x)}{\Delta x} + w = \frac{\Delta V_{water} / V}{\Delta t} = \frac{\Delta n}{\Delta t}$$

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<sup>-1</sup>]  
and **Darcy's law** with hydraulic conductivity

$$\frac{\partial n}{\partial h} = S_0 \quad \text{and} \quad v_x = -K \frac{\partial h}{\partial x} \quad \Rightarrow \quad \frac{\partial}{\partial x} \left( K \frac{\partial h}{\partial x} \right) + w = S_0 \frac{\partial h}{\partial t}$$

# Darcy's law – Hydraulic conductivity



$$v_x = \frac{Q}{A} = -K \frac{\Delta h}{\Delta x}$$

# Darcy's law – Hydraulic conductivity

- $K$  is mainly dependent on particle size and distribution, as well as porosity (and fluid properties)
- $K$  has the dimension of velocity (but it is not!)
- Pore water velocity

$$u = \frac{v_x}{n}$$

| Material      | $K$ [m/s]            |
|---------------|----------------------|
| Coarse gravel | $1 - 10^{-2}$        |
| Sandy gravel  | $10^{-2} - 10^{-5}$  |
| Sand          | $10^{-2} - 10^{-7}$  |
| Silt          | $10^{-5} - 10^{-9}$  |
| Clay          | $10^{-9} - 10^{-12}$ |

# Darcy's law – Hydraulic conductivity

## Permeability

The hydraulic conductivity  $K$  can be separated into a fluid-dependent share and a component depending only on the pore geometry:

$$K = \kappa \frac{g}{\nu}$$

- $\kappa$  : permeability of the porous medium [ $L^2$ ],  
i.e., also a tensor of 2<sup>nd</sup> order
- $\nu$  : kinematic viscosity of the fluid [ $L^2/T$ ]

# Generalization to 3D

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

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

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

+ Initial condition  
+ Boundary conditions

A multitude of aquifers through the 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  $T = K \cdot (\text{Top-Bottom} = \text{thickness})$   
 $S = S_0 \cdot (\text{Top-Bottom} = \text{thickness})$

**2D unconfined** aquifer: by integration over z-coordinate

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

with  $S \cong n_e = \text{drainable porosity}$

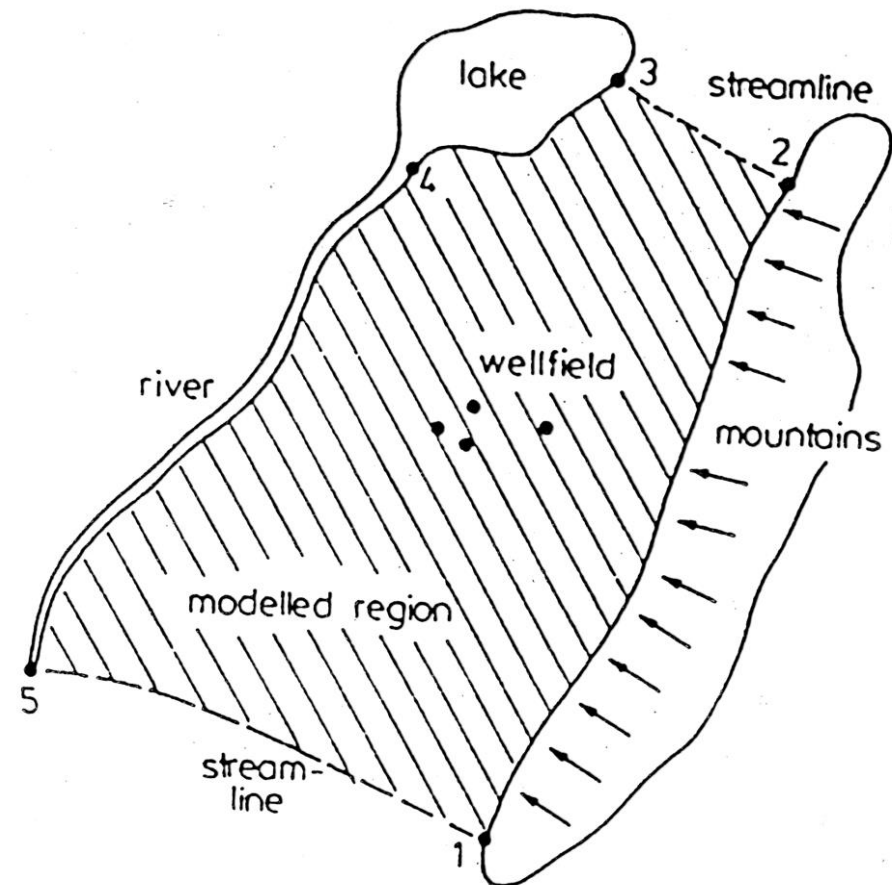
**2.5D** by vertical coupling of 2D layers through leakage-term

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

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

# Boundary conditions for flow

- **1<sup>st</sup> type BC:**  $h$  on boundary specified (water level-*Dirichlet*)
- **2<sup>nd</sup> type BC:**  $\partial h / \partial n$  given on boundary (water flow-*Neumann*)
- **3<sup>rd</sup> 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 a fixed-flux boundary.** At downstream boundaries, use a fixed-head boundary.
- **Use third-type boundary conditions for distant fixed heads.**
- **Streamlines are boundaries of the second type** (no flow perpendicular to the 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

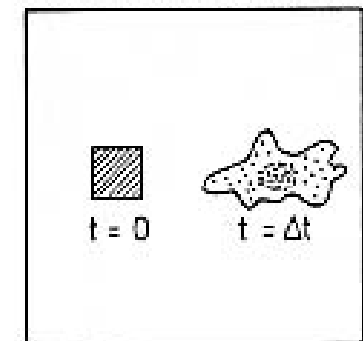
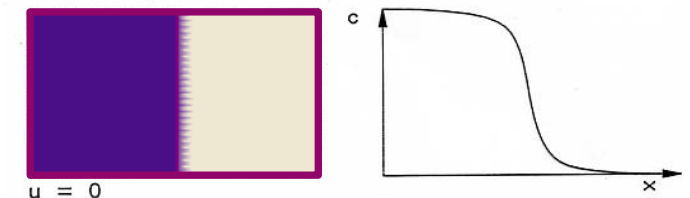
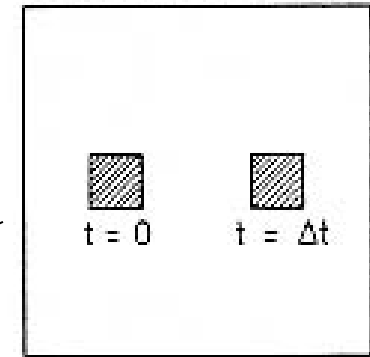
$$\mathbf{j}_{diff} = -n_e D_m \nabla c$$

- Dispersive flux

$$\mathbf{j}_{disp} = -n_e \mathbf{D} \nabla c$$

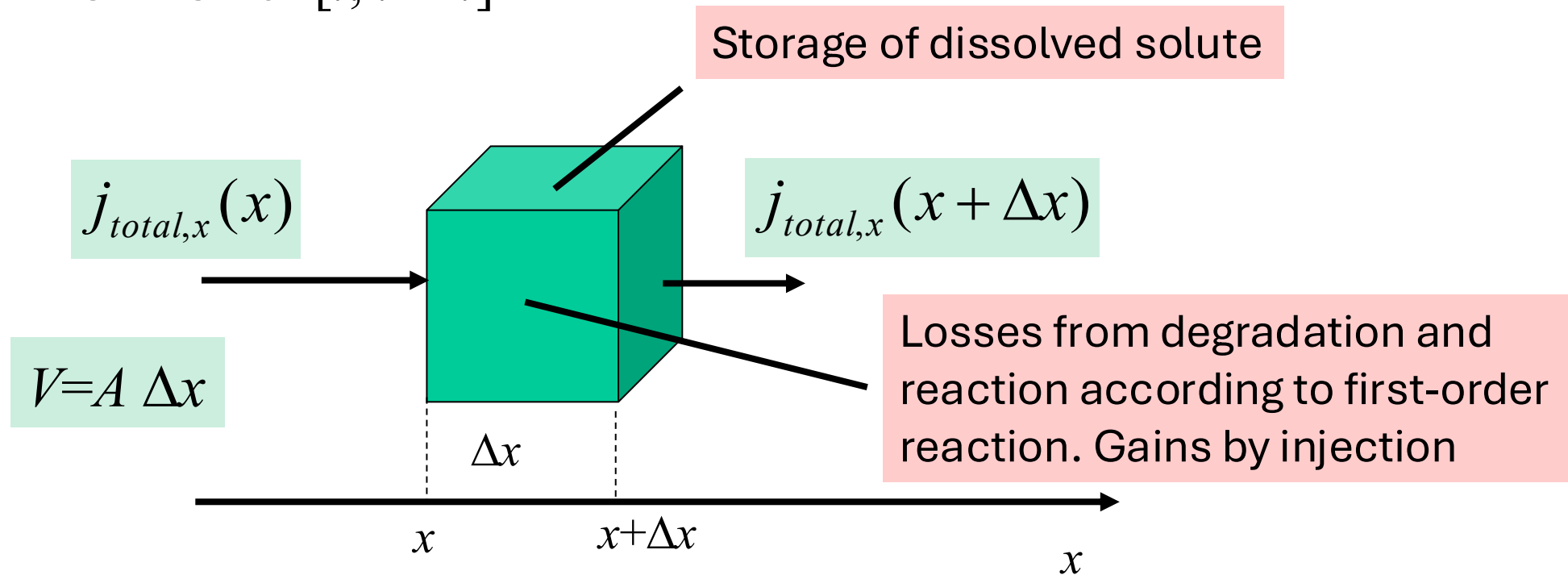
$\mathbf{v}$  is specific flux (Darcy velocity)

- 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

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

# Mass balance in 1D

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

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

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:

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

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

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

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

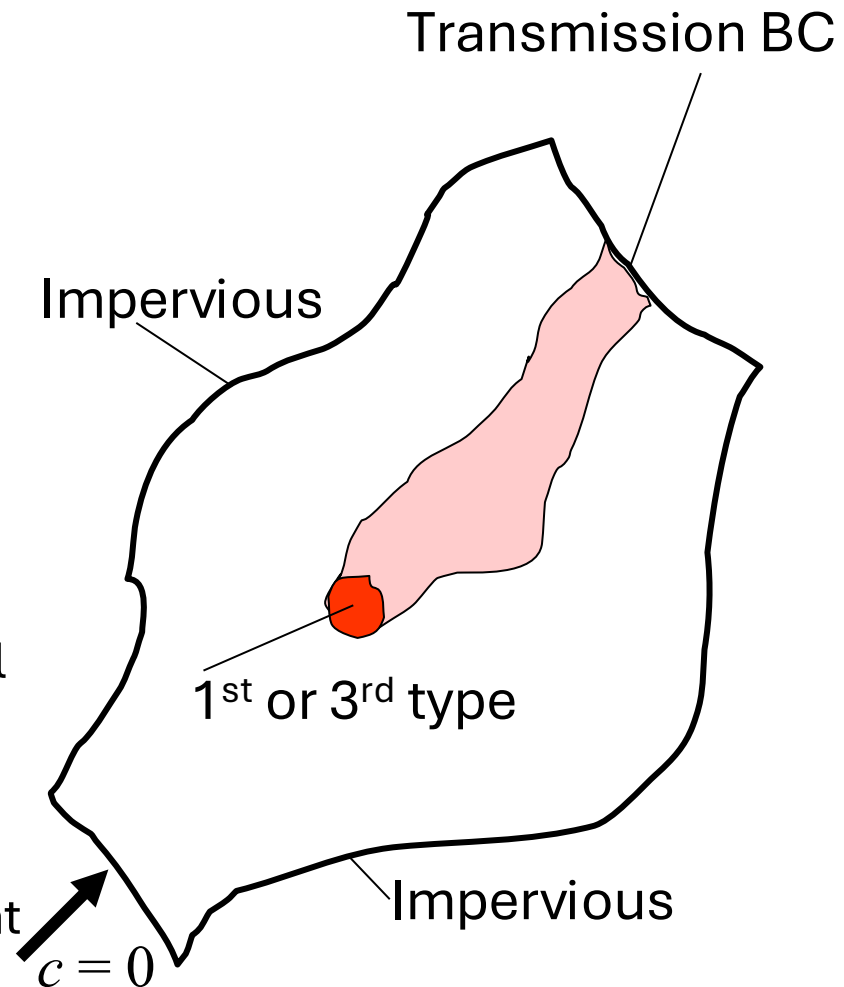
In a system, in which  $\mathbf{u}$  is parallel to  $x$ -axis!

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

Again: Initial condition + Boundary conditions

# Boundary conditions for transport problems

- **1<sup>st</sup> type BC:** Concentration  $c$  is prescribed on the boundary. This determines the advective flux.
- **2<sup>nd</sup> type BC:** Derivative  $\partial c / \partial n$  prescribed on the boundary. This determines the diffusive-dispersive flux. **Only used to make a no-flow boundary impervious to diffusion/dispersion.**
- **3<sup>rd</sup> 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 the boundary to keep the concentration gradient constant (implementation:  $\mathbf{D} = 0$  on boundary cell).

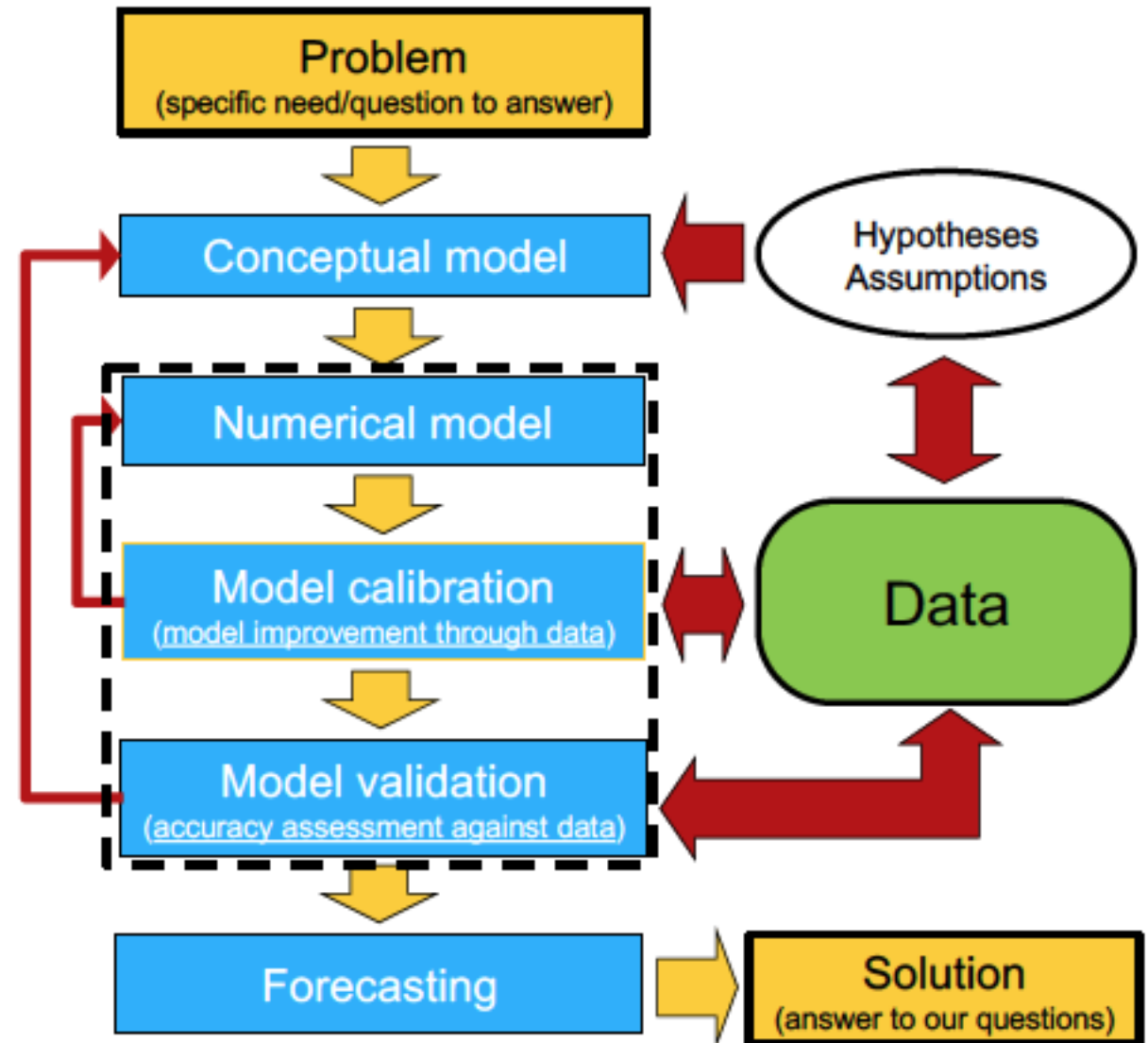


# Building a groundwater model

Good modelling entails a continuous dialogue between model results and experimental data (possibly considering our changing needs in terms of forecasting)

*“It doesn't matter how beautiful your theory is, it doesn't matter how smart you are. If it doesn't agree with experiment, it's wrong.”*

R. Feynman

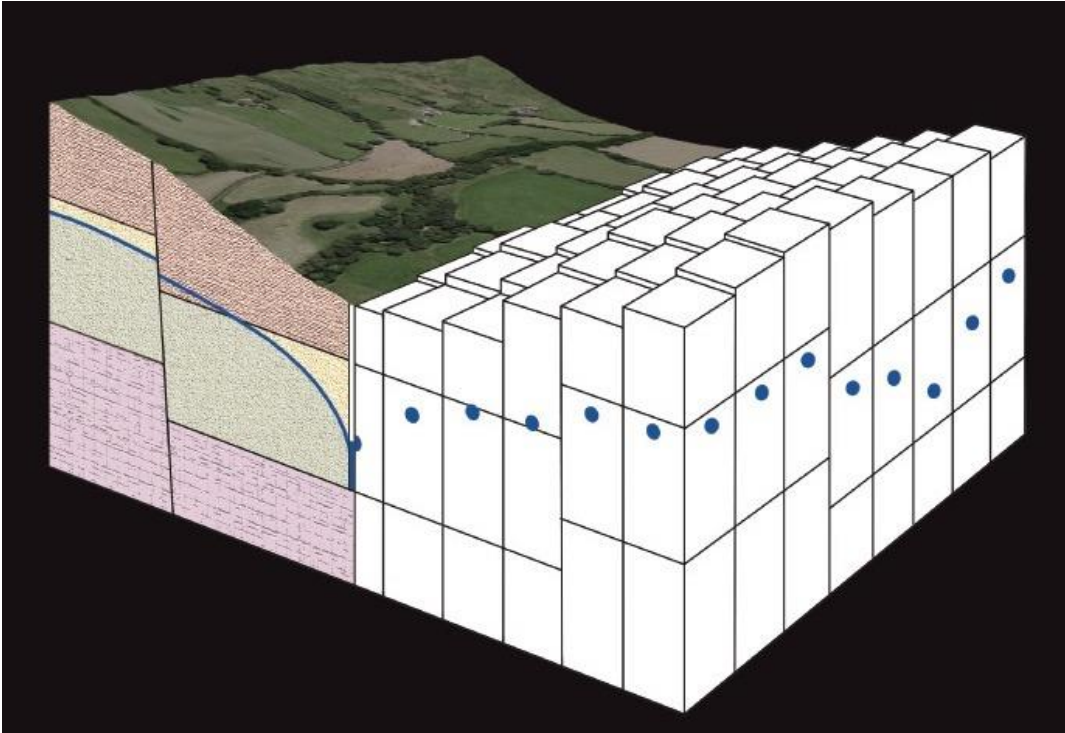


from I. Lunati (Empa)

# Where does the data come from?

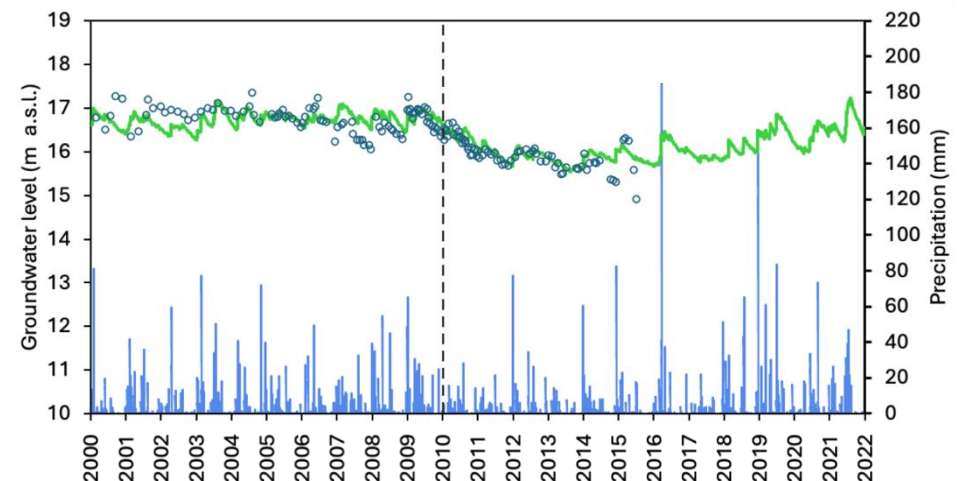
- Geometry:
  - Top-Bottom: boreholes, geophysics
  - Surface: LIDAR, Synthetic Aperture Radar
- Transmissivity, Storage coefficient:
  - Pumping tests
- Aquifer recharge:
  - Soil water balance, analysis of low water discharge, and environmental tracers
- River water table, riverbed
  - Geodetic surveys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

# Groundwater model



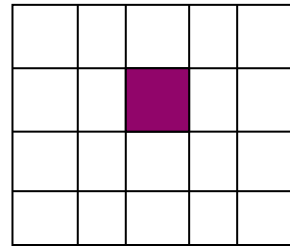
Shepley, M.G., Whiteman, M.I., Hulme, P.J. and Grout, M.W., 2012. Introduction: groundwater resources modelling: a case study from the UK. *Geological Society, London, Special Publications*, 364(1), pp.1-6.

- 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)



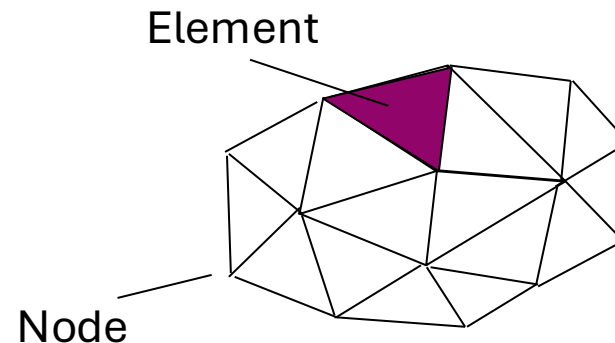
# Methods of spatial discretization

Finite Differences  
(explained here)



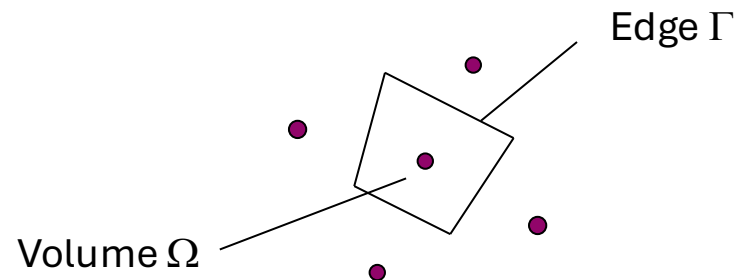
Balance over cells

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.

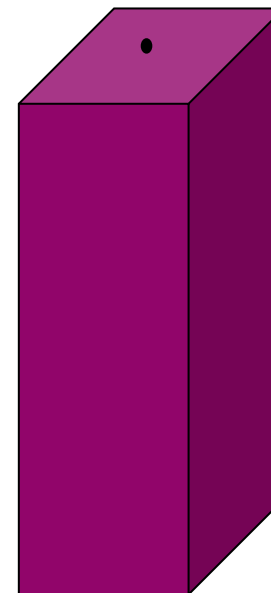
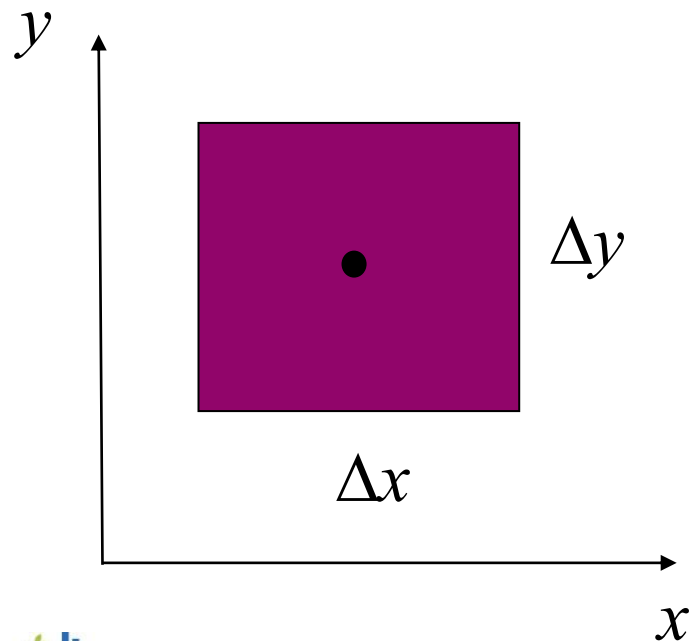
A **steady-state** groundwater model simulates conditions where properties and flows are constant over time (i.e. the storage term is equal to zero).

# Finite Differences

## Example 2D flow

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

Balance at single cells (block-centered method)



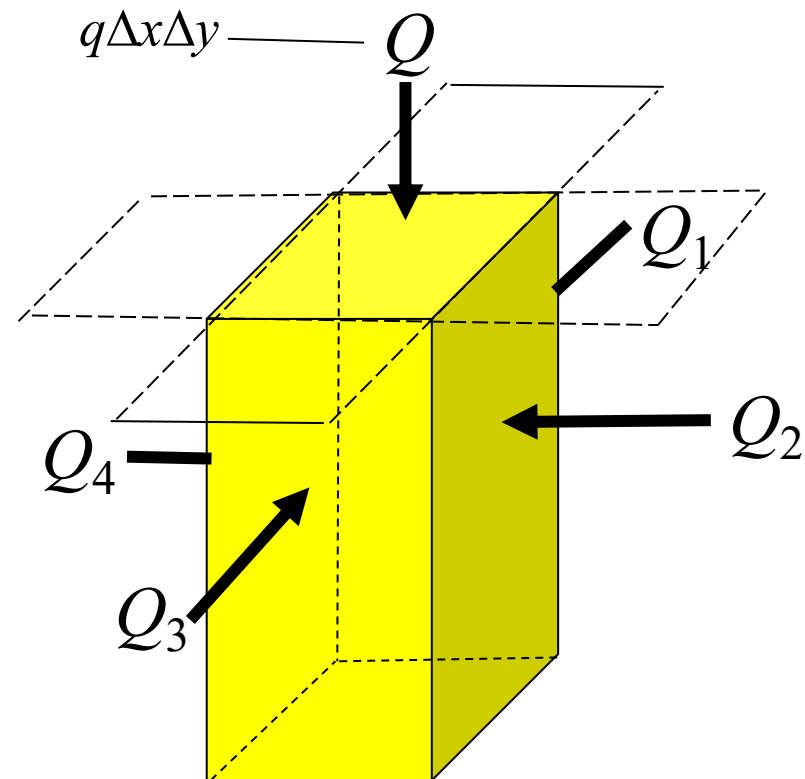
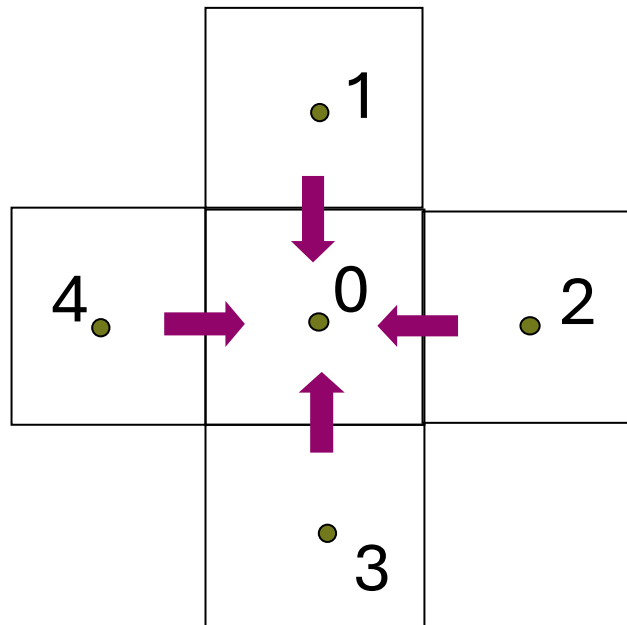
Thickness =  
Thickness of  
the aquifer

# Finite Differences

## Flows between cells and neighboring cells

Balance:

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



# Finite Differences

## Flows between cells and neighboring cells

Balance:

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

With Darcy's law, it follows that:

$$\begin{aligned} Q_1 &= \Delta x T_{10} \frac{h_1(t') - h_0(t')}{\Delta y} & Q_2 &= \Delta y T_{20} \frac{h_2(t') - h_0(t')}{\Delta x} \\ Q_3 &= \Delta x T_{30} \frac{h_3(t') - h_0(t')}{\Delta y} & Q_4 &= \Delta y T_{40} \frac{h_4(t') - h_0(t')}{\Delta x} \end{aligned}$$

$$t' \in [t, t + \Delta t]$$

$T_{ij}$  Transmissivity between nodes  $i$  and  $j$

# Finite Differences

## Flows between cells and neighboring cells

Balance:

$$S_0 \frac{(h_0(t+\Delta t) - h_0(t))}{\Delta t} =$$

$$T_{10} \frac{h_1(t') - h_0(t')}{\Delta y^2} + T_{20} \frac{h_2(t') - h_0(t')}{\Delta x^2} +$$

$$T_{30} \frac{h_3(t') - h_0(t')}{\Delta y^2} + T_{40} \frac{h_4(t') - h_0(t')}{\Delta x^2} + q_0$$

whereby:  $q_0 = Q / (\Delta x \Delta y)$

The equation, in case of **stationarity**, is obtained by setting the storage term to zero.

# Finite Differences

## Averaging of the Transmissivity

The transmissivity between two cells is calculated as the mean of the transmissivities of the single cells

$$T_{ij} = \frac{T_i + T_j}{2}$$

or

$$T_{ij} = \frac{2T_i T_j}{T_i + T_j}$$

- For small differences  $T_i - T_j$ : both means are applicable
- For great differences  $T_i - T_j$ : the harmonic mean is more suitable

The harmonic mean allows the inclusion of impermeable edges: Simply set the outer transmissivity to zero!

# Model calibration and validation

## Model calibration:

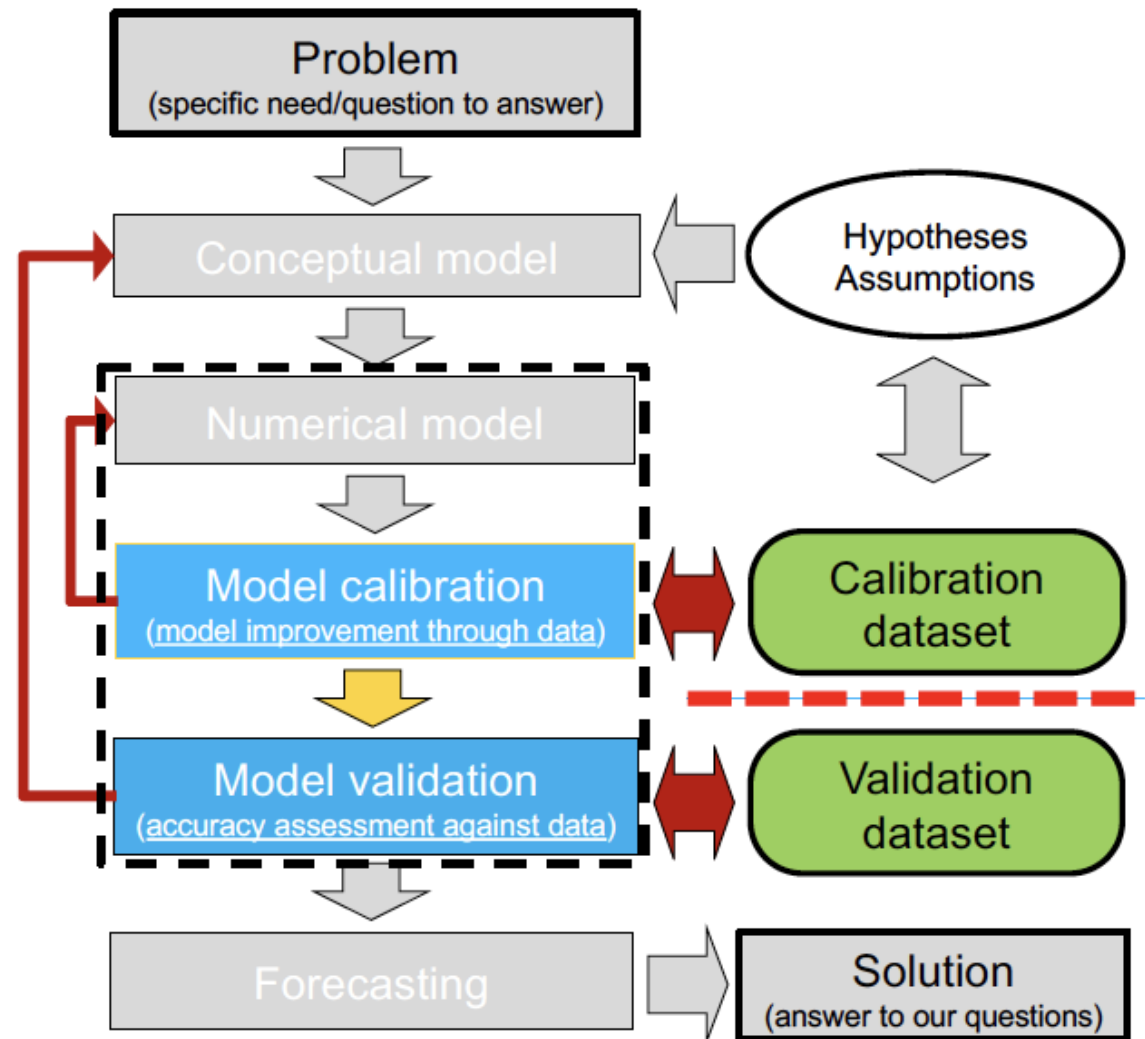
Improves the model by adjusting parameters to fit known data

- Uses a “calibration”(or “training”) dataset
- Modifies parameters

## Model validation:

Assesses predictive capability and accuracy against unseen data.

- Uses independent data, a “validation” dataset
- Fixed parameters



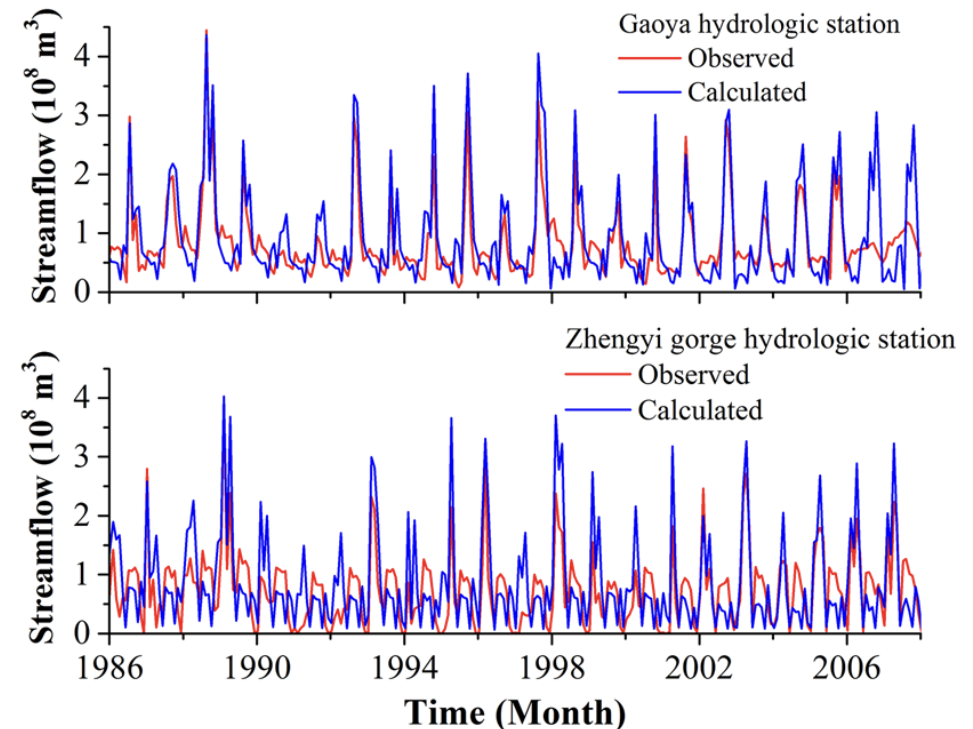
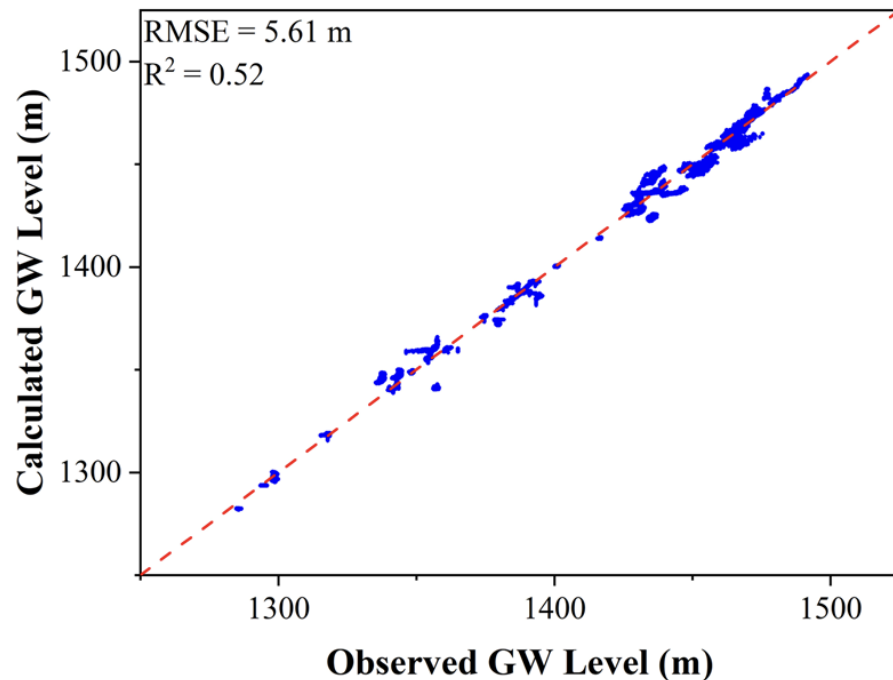
from I. Lunati (Empa)

# Calibration: parameter estimation

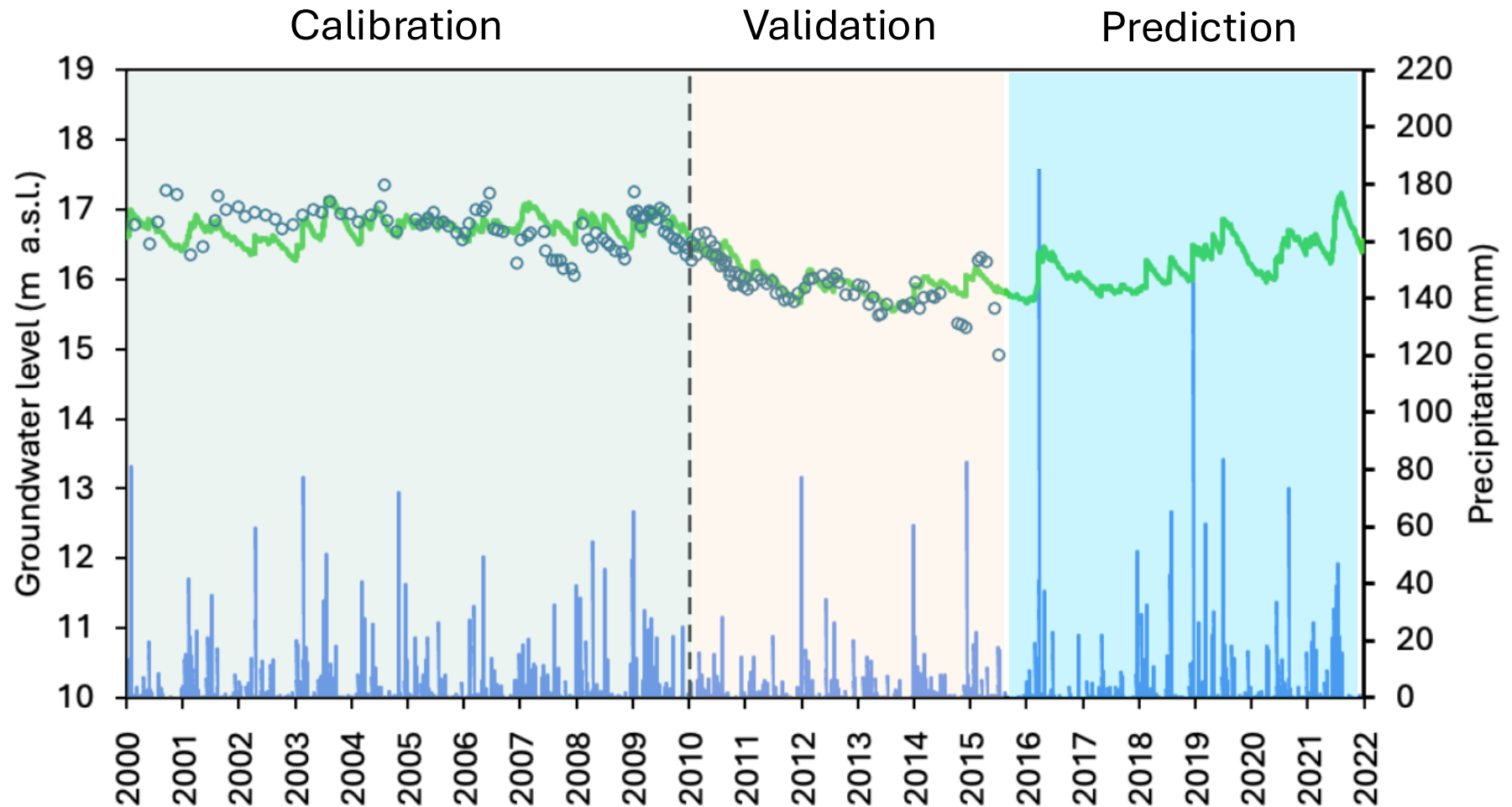
Improve the model parameters by comparing them with the data

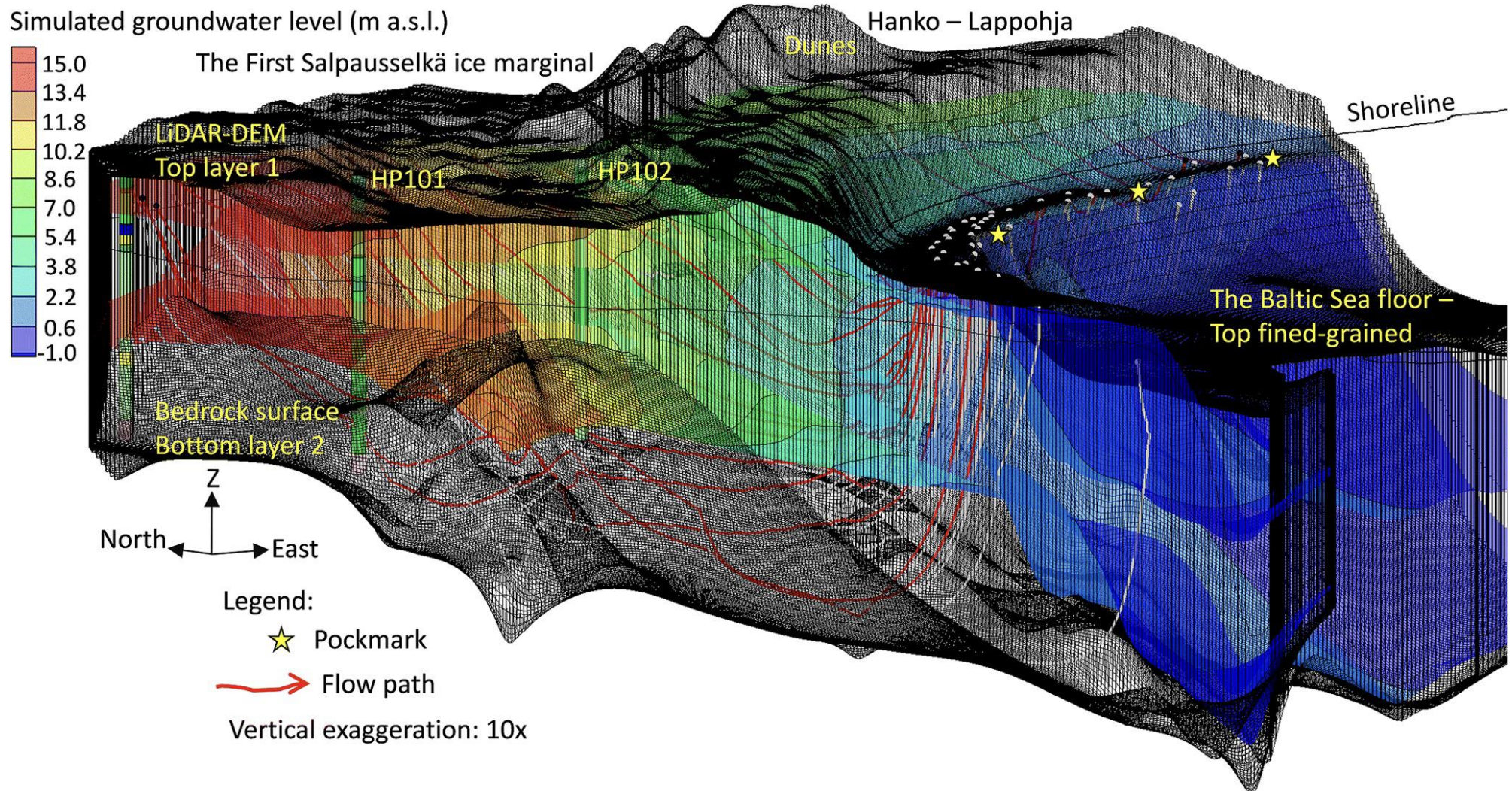
Adjust unknown model parameters to match observations

- **Steady-state** data for conductivity/transmissivity
- **Transient** data required for storativity
- It can be done “by hand” or in an automated way



# Validation and prediction





from Luoma et al. *Hydrogeol. J.* (2021)