



Research Group: Geo- and Environment sciences · Hydrogeochemistry

Water-nexus modelling and Modelling of MAR schemes

I. Mathematical background

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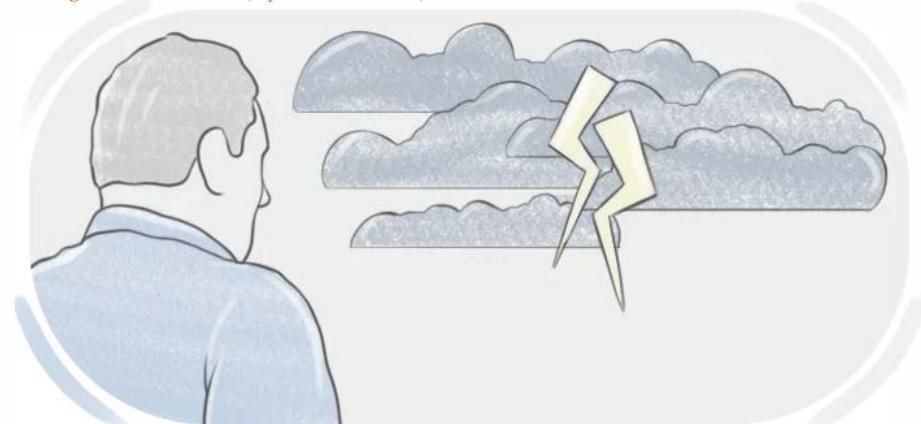


Motivation - Why Model?

- ▶ For **Predictions** (mostly forward)
- ▶ For better **Planning**
- ▶ Optimum output (Economy)

Groundwater is a fundamental resources -
proper **planning** and **Optimum** use is
essential

Image Source: LanGeek.co (<https://shorturl.at/TaOtP>)



The sky is dark.
Is it going to rain?

How to know if it will „very likely“ rain?

MODEL IT!

Contents

1. Mathematical aspects: Theory and methods (This Session)¹
2. Numerical modelling: MODFLOW-ModeMuse (Second Session)
3. Modelling MAR scenarios (The Last Session)

The materials for the second and last sessions can be found at [Here](#)

Please **download** the `*.exe` files and install in your (**Windows**) system

¹ Contents are based on the interactive GW teaching book developed at TU Dresden [Here](#)

Darcy Law: The starting point

$$Q \propto \frac{A \Delta h}{x}$$

with : Q [LT^{-3}] = water discharge

A [L^2] = Area

Δh [L] = hydraulic head difference

x [L] = distance

Generalized 1D Darcy's Law

$$\frac{Q}{A} = q = -K \frac{dh}{dx}$$

with: q [L] = specific discharge

K [LT^{-1}] = Hydraulic Conductivity

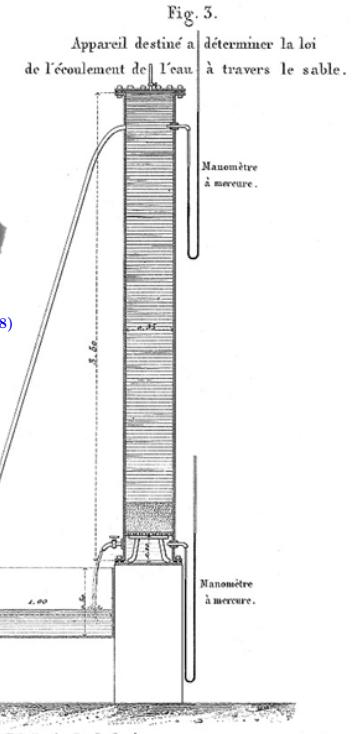
minus (-): flow towards low head

K characterizes domain physical properties and $\frac{dh}{dx} = I[-]$, also called head gradient, is actually an energy gradient

K and I deserves a further attention



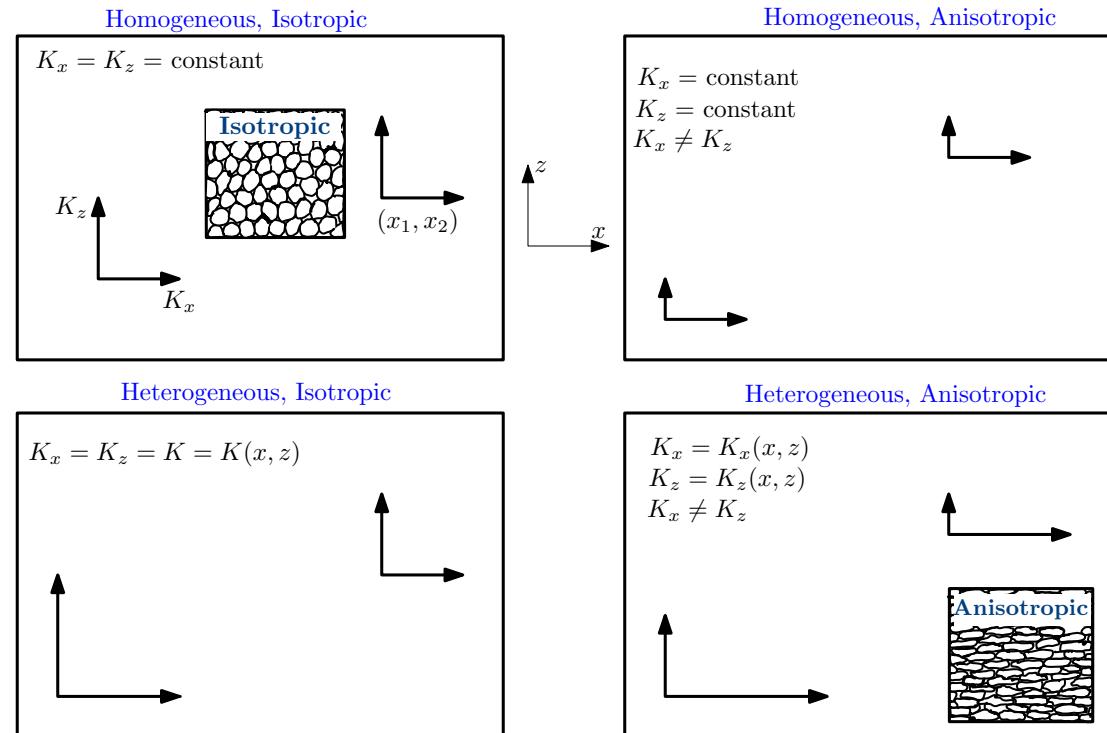
Henry Darcy (1803 - 1858)



Source: <https://doi.org/10.1029/2001WR000727>

The Conductivity (K)

- ▶ **K** is a **composite property** of porous media and fluid
- ▶ Groundwater (GW) **normally** has uniform fluid properties
- ▶ Porous media is **generally** very heterogeneous.
- ▶ **Primarily**, GW problem is homogeneity - heterogeneity and isotropic - anisotropic pairs or any of their combination



The hydraulic head gradient ($I = \frac{dh}{dx}$)

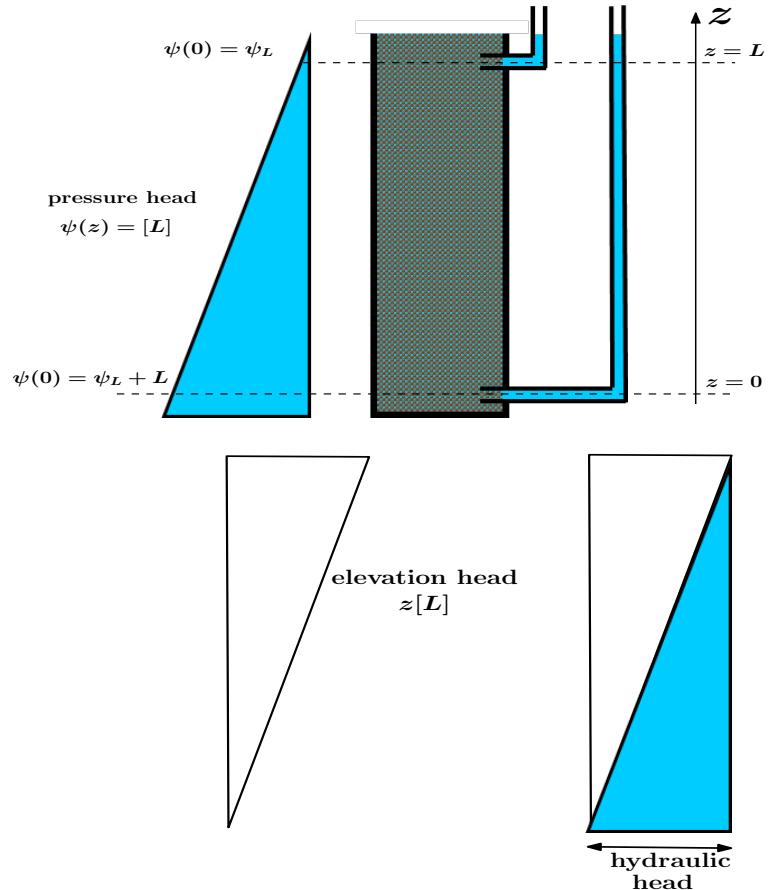
- ▶ h , also called **piezometric head**, sums the energy available for the GW flow.
- ▶ Only considered are **Potential** (pressure) and **Elevation** energy.
- ▶ Thus:

with:

$$h = z + \frac{p}{\rho g}$$

p [$M L^{-1} T^{-2}$]: *Pressure*
 ρ [ML^{-3}]: *density*
 g [LT^{-2}]: *gravity*

- ▶ GW flows only when $\Delta h \neq 0$
- ▶ Flow direction: higher to lower head



Other important aquifer quantities

- ▶ **Specific Storage (S_s) [L⁻¹]** quantifies water storage capacity of an Aquifer from:

$$S_s = \frac{\Delta V_w}{V_T \cdot \Delta \psi}$$

with:

ΔV_w [L³]: changed Water volume

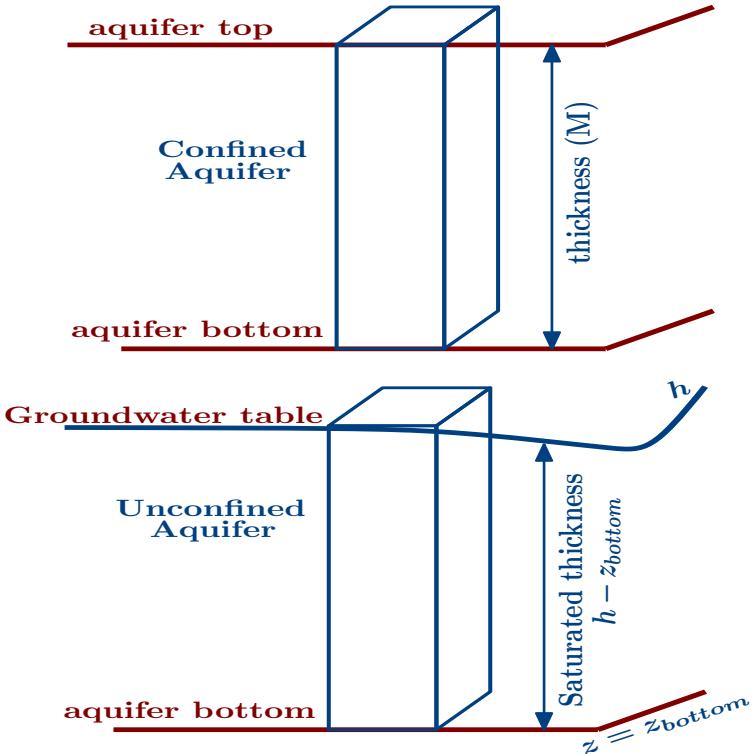
$\Delta \psi$ [L]: change in Hydrostatic pressure head

V_T [L³]: Total aquifer volume

- ▶ **Confined Aquifer** - Aquifer bounded in both end:

$S = S_s \cdot M$, with Storativity (S) [-] and Aquifer thickness (M)[L]

- ▶ **Unconfined Aquifer** - Aquifer top is groundwater table: $S = \eta_e$ with effective porosity (η_e)[-]



GW flow is normally a 2D problem due a small thickness compared to length/width

Darcy's law in 2D and 3D

- ▶ K and h are space-dimension dependent
- ▶ They appear in the Darcy's law
- ▶ Thus in 3D, h is a **column vector**:

$$\text{grad } h = \nabla h = \begin{bmatrix} \frac{dh}{dx} \\ \frac{dh}{dy} \\ \frac{dh}{dz} \end{bmatrix}$$

- ▶ For 2D, the third dimension can be omitted
- ▶ The Darcy's law in 3D is:

$$q = -K \cdot \nabla h$$

▶ K tensors:

3D and **anisotropic & heterogeneous**:

$$\begin{bmatrix} K_{xx} & K_{xy} & K_{xz} \\ K_{yx} & K_{yy} & K_{yz} \\ K_{zx} & K_{zy} & K_{zz} \end{bmatrix}$$

Principal axis aligned to the domain:

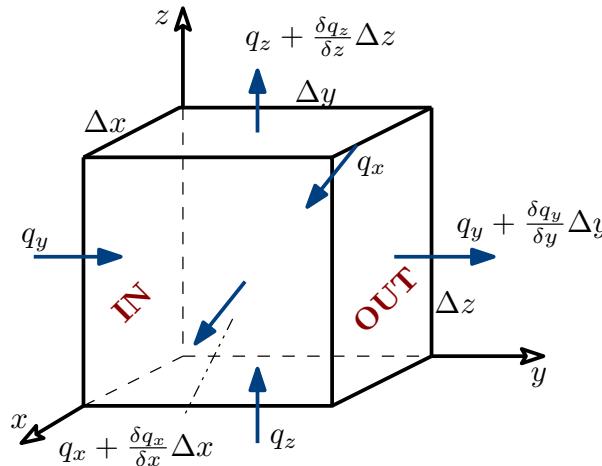
$$\begin{bmatrix} K_{xx} & 0 & 0 \\ 0 & K_{yy} & 0 \\ 0 & 0 & K_{zz} \end{bmatrix}$$

- ▶ Other simplified form of K can be obtained
- ▶ The most **general** Darcy's law:

$$q = \begin{bmatrix} K_{xx} & K_{xy} & K_{xz} \\ K_{yx} & K_{yy} & K_{yz} \\ K_{zx} & K_{zy} & K_{zz} \end{bmatrix} \cdot \begin{bmatrix} \frac{dh}{dx} \\ \frac{dh}{dy} \\ \frac{dh}{dz} \end{bmatrix}$$

Groundwater flow system equations

- ▶ Consider a unit volume ($\Delta x, \Delta y, \Delta z$)



- ▶ **Mass (water) and budget (storage)** and applying **Darcy's law** generates the Groundwater flow equation

- ▶ 3D Transient, Homogeneous and Isotropic

$$S_s \frac{\partial h}{\partial t} = \frac{\partial}{\partial x} \left(K \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left(K \frac{\partial h}{\partial y} \right) + \frac{\partial}{\partial z} \left(K \frac{\partial h}{\partial z} \right)$$

- ▶ 3D Transient, Homogeneous and Anisotropic with Source/Sink (N) [T^{-1}]

$$S_s \frac{\partial h}{\partial t} = \frac{\partial}{\partial x} \left(K_x \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left(K_y \frac{\partial h}{\partial y} \right) + \frac{\partial}{\partial z} \left(K_z \frac{\partial h}{\partial z} \right) + N$$

- ▶ 3D Steady-State, Homogeneous and Isotropic

$$\frac{\partial}{\partial x} \left(K_x \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left(K_y \frac{\partial h}{\partial y} \right) + \frac{\partial}{\partial z} \left(K_z \frac{\partial h}{\partial z} \right) = 0$$

Special groundwater flow system equations

► The Laplace equation:

$$\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2} + \frac{\partial^2 h}{\partial z^2} = 0$$

- 3D, Steady-state, homogeneous, isotropic, and confined aquifer **without** source/sink

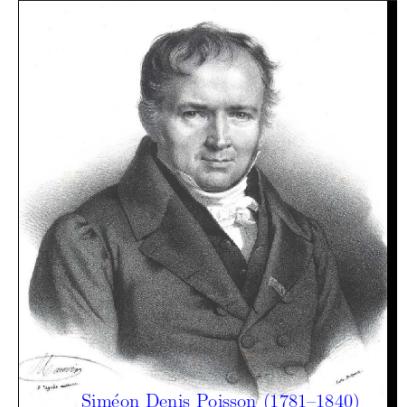


Pierre-Simon Laplace (1749 - 1827)

► The Poisson equation:

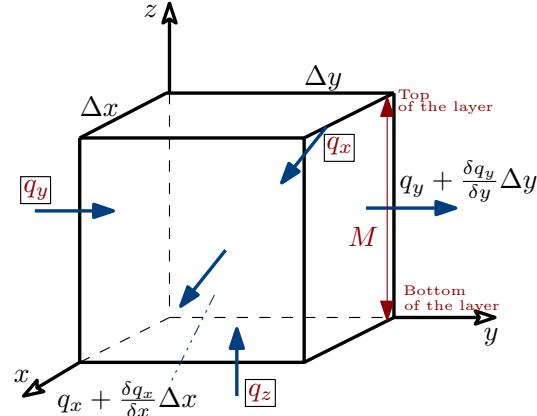
$$\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2} + \frac{\partial^2 h}{\partial z^2} = -\frac{N}{K}$$

- 3D, steady-state, homogeneous, isotropic and confined aquifer **with** source/sink (N)



Siméon Denis Poisson (1781–1840)

Special groundwater flow system equations: The 2D cases



- ▶ Vertical GW flow to layering are negligible,
i.e., $q_x, q_y \gg q_z$
- ▶ Therefore, GW flow problems are often considered as **2D** problems

- ▶ Transmissivity (T) [$L^2 T^{-1}$] is then used to **sum the vertical flow component**:

$$T = K \cdot M$$

with: M [L] Aquifer thickness
 K [$L T^{-1}$] Hyd. conductivity

- ▶ Thus, for **anisotropic aquifers**:

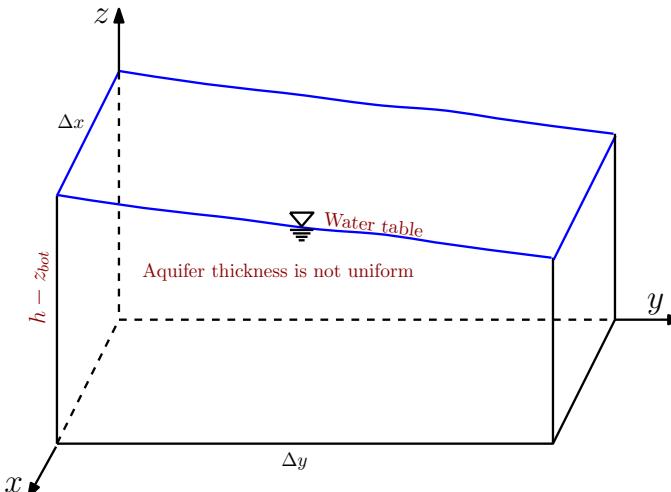
$$T_x = K_x \cdot M \quad \text{and} \quad T_y = K_y \cdot M$$

- ▶ for horizontally **Isotropic** confined aquifers:

$$T = K \cdot M$$

The special 2D flow equations: Unconfined aquifers

- ▶ Aquifer thickness is a variable



- ▶ Thus:

$$T_x = K_x \cdot (h - Z_{bot})$$

$$T_y = K_y \cdot (h - Z_{bot})$$

- ▶ The 2D GW flow equation for **unconfined** and **anisotropic** with **source/sink** is:

$$S \frac{\partial h}{\partial t} = \frac{\partial}{\partial x} \left(T_x \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left(T_y \frac{\partial h}{\partial y} \right) + N$$

with Storativity (S) [-]

- ▶ Same equation is for the **confined** case with T calculated as in the previous slide
- ▶ This equation is also called the **Boussinesq equation**



Joseph Valentin Boussinesq (1842 – 1929)



Complete formulation of Groundwater flow equation

Step I: Specify the geometric properties of the region of interest (dimension, shape...)

Step II: Characterize aquifer - K , S_s , S or T , by considering heterogeneity and Anisotropy

Step III: Select the appropriate flow equation, and provide additional data (e.g., wells, river)

Step IV: Specify the initial condition(IC):

- A. head value at time $t = 0$
- B. Not required for steady-state problems.

Step IV: Specify boundary conditions (BC):

- A. BCs have to be given along the complete boundary (also at infinity)
- B. BCs may be time-dependent
- C. There are three major types of BCs (next slide)

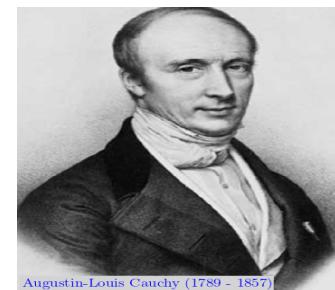
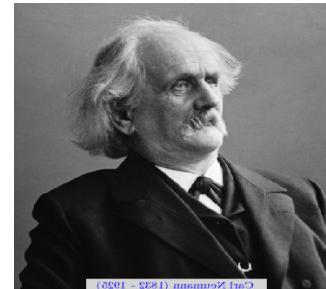
Step V: Select the appropriate Solver

What are the BCs & how they are set?

The 3 Boundary conditions

Dirichlet BC:

- ▶ Also called first type BC
- ▶ The head is specified, e.g., $h = h_0$



Neumann BC:

- ▶ Also called second type BC
- ▶ The head **gradient** is specified, e.g., $\frac{dh}{dx} = h_0$
- ▶ **Special case** - No flow BC: $\frac{dh}{dx} = 0$

Cauchy or Robin BC:

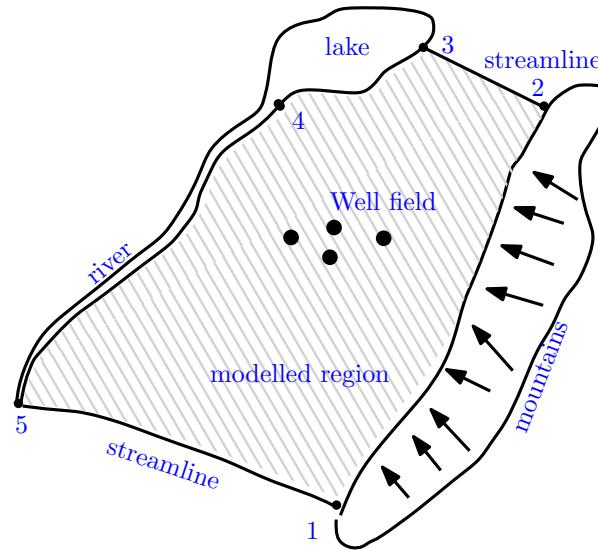
- ▶ Also called Third type or Mixed BC
- ▶ Combines other BCs, e.g., $q = C(h - h_b)$
with Conductance C [LT^{-1}] and external head h_b [L]

Summarizing the mathematical formulation of GW flow problem

Aquifer/Flow property	Mathematical Formulation
Transient	with time derivative
Confined	linear partial differential equation
Anisotropic	$T_x \neq T_y$ or $K_x \neq K_y$ (tensor)
Heterogeneous (inhomogeneous)	coefficients depends on space coordinate(s)
With sources/sinks	inhomogeneous differential equation (contains a term without h)
Fixed-head boundary condition	boundary condition of the first kind (Dirichlet)
Flux BC (e.g.: no flow)	boundary condition of the second kind (Neumann)

Implementing boundary condition to the GW flow problem

- ▶ BCs must be set based on geological and geographical setting.
- ▶ An e.g., GW model domain

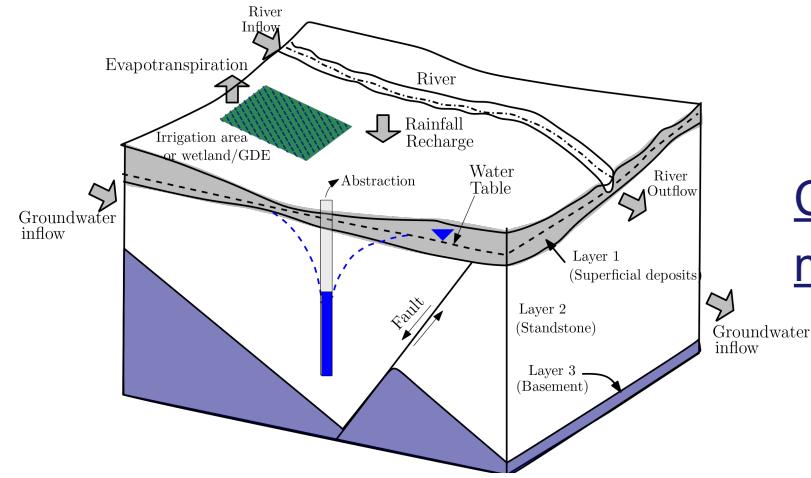


Boundary 1-2: Specified flux (non-zero)
 Boundary 2-3: Specified zero flux
 Boundary 3-4: Specified head
 Boundary 4-5: Semipervious
 Boundary 5-1: Zero flux

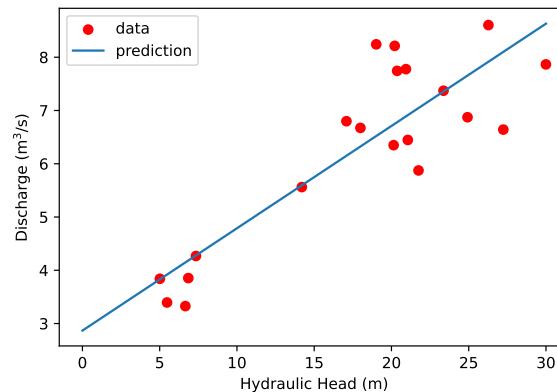
- ▶ A complete GW flow problem: **System equation + fully defined BCs**

Modeling GW flow problems

- ▶ A **Model** is a representation of a **real** or **conceptual** system
- ▶ Model can be:
 - ▶ Conceptual model
(qualitative or graphic representation)
 - ▶ Process-based and empirical models
(data or experiment-based)
 - ▶ Mathematical model
(Conservation laws based)



Conceptual
model



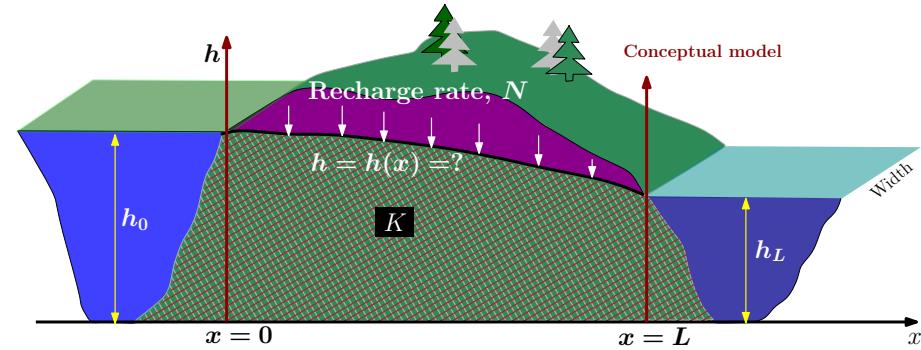
Empirical
model

Solving mathematical models of GW flow problems

- ▶ The mathematical models are generally solved either:
 - ▶ **Analytically** (exact solution), or
 - ▶ **Numerically** (approximate solution)
- ▶ Hybrid methods, e.g., **Analytic Element Method (AEM)**
- ▶ Numerical method is a **universal** one, although not always economical

Analytical Models

- ▶ Can mostly solve **simple** problems, e.g., homogeneous, steady-state



The solution ([Streamlit Web-App](#)):

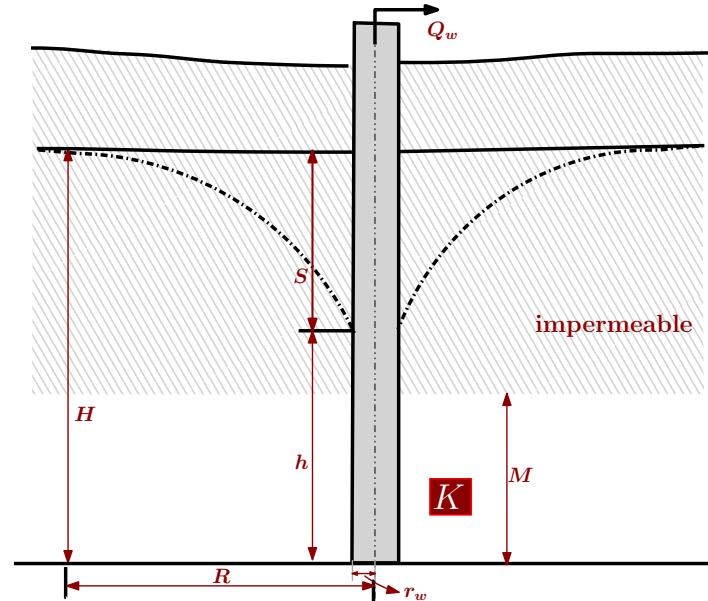
$$h(x) = \sqrt{h_0^2 - (h_0^2 - h_L^2) \cdot \frac{x}{L} + \frac{N}{K} \cdot x \cdot (L - x)}$$

Analytical (Thiem) solution for steadily operating Well

- ▶ For wells in **Confined** Aquifer:
 - ▶ In **Homogeneous** and **Isotropic** aquifer
 - ▶ Operating at **Steady-State** condition
 - ▶ For a **Fully Penetrating** well
 - ▶ GW flow is **Horizontal** and **Radial**
- ▶ Thiem (1906) Solution:

$$Q_w = \frac{2\pi M K (H-h)}{2.3 \log(R/r_w)}$$

with: Well radius r_w [L], Confined thickness M [L], well discharge(Q_w) [$L^3 T^{-1}$], water level in aquifer at rest H [L], water level in the well h [L], drawdown $S = H - h$ [L]



what is

Radius of Influence (R) [L]?

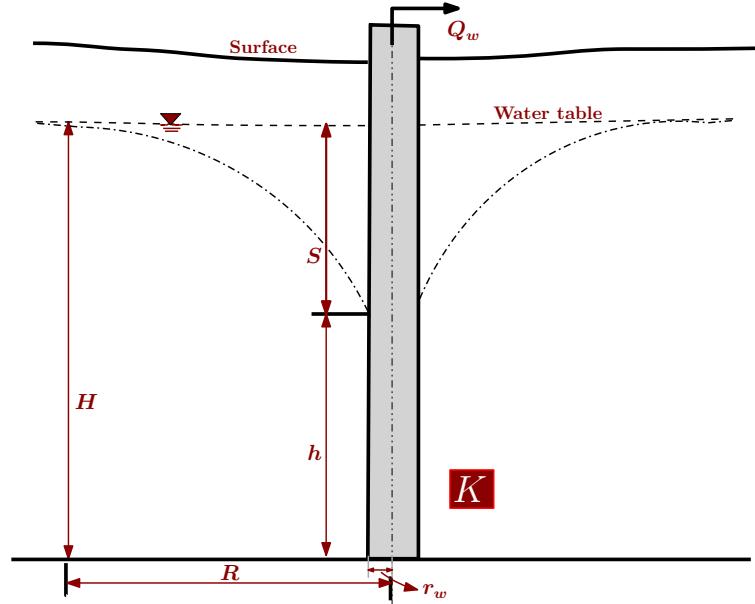
Analytical (Thiem) solution for steadily operating Well

- ▶ For a well in an **Unconfined** Aquifer
- ▶ Other assumptions as in the **confined** case

$$Q_w = \frac{\pi \cdot K \cdot (H^2 - h^2)}{2.3 \log(R/r_w)}$$

- ▶ R is obtained from Empirical formula (e.g.,):

Source	Formula
Kyrieleis and Sichardt (1930)	$R = 3000 \cdot s \sqrt{K}$
Arvin and Numerov (1953)	$R = 1.9 \sqrt{(H \cdot K \cdot t/s)}$ with pumping time (t) [T]



How about transient wells?

Analytical (Theis) solution for transiently operating wells

- ▶ Theis (1935) requires:
 - ▶ $r_w \gg R$ in **Confined** aquifer
 - ▶ Others as is in (Thiem 1906) solution
- ▶ Theis (1935) Solution:

$$s(r, t) = \frac{Q}{4\pi T} \cdot W(u)$$

where r [L] is distance from well to the observation well

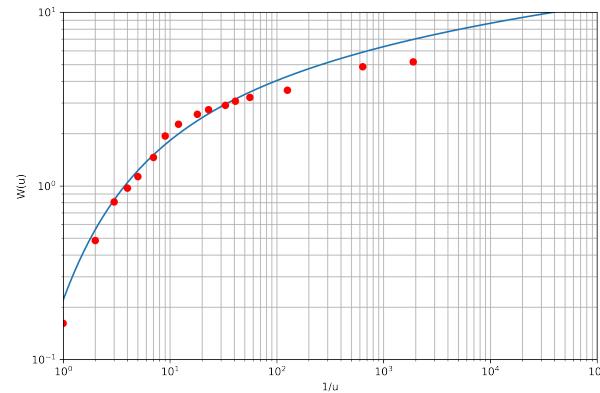
with: $W(u) = \int_u^\infty \frac{e^{-\tilde{u}}}{\tilde{u}} d\tilde{u}$ and $u = \frac{Sr^2}{4Tt}$

- ▶ The plot of **log-transformed** form of eqs. $s(r, t)$ and $W(u)$ leads to so-called the **Type-Curve**

- ▶ log transformed forms:

$$\log s(r, t) = \log \frac{Q}{4\pi T} \cdot \log W(u)$$

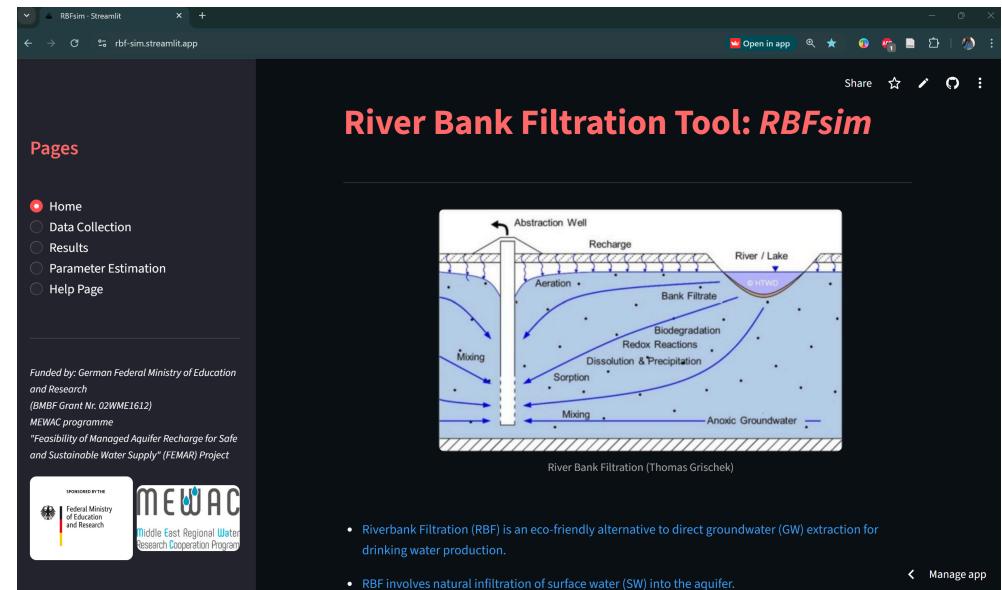
$$\log \frac{t}{r^2} = \log \frac{S}{4T} + \log \frac{1}{u}$$
- ▶ Type curve allows to quantify S and T



(Check the Web-App)

Hybrid solution for River Bank Filtration cases

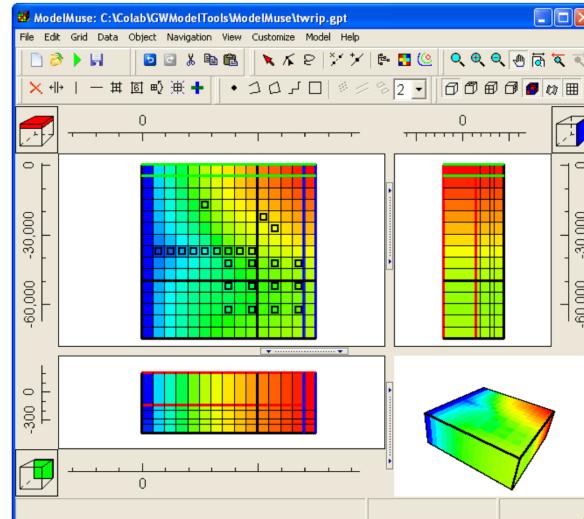
- ▶ **Hybrid solution methods** attempts to combine Analytical and/or Numerical methods
- ▶ **Hybrid Method** can economically provide to some GW flow problems
- ▶ **RBFsim** implements Analytic Element Method (AEM) to solve several Riverbank filtration scenario.
- ▶ **RBFsim** can be simulated on-line from <https://rbf-sim.streamlit.app/>



Source: [Yadav et al. \(2024\)](#)

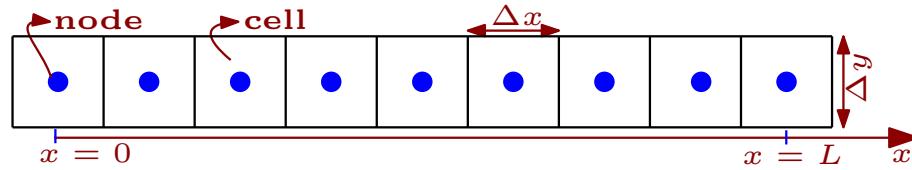
Numerical methods for solving GW flow problems

- ▶ Numerical methods can solve almost all types of GW flow problems
- ▶ Finite Different Method (FDM) is very generally the numerical method of choice, due to:
 - ▶ Simplified **adaptation** of the problem
 - ▶ **Economical** also for large domains
 - ▶ Sufficiently **accurate** and **stable**
- ▶ Other (to FDM) methods e.g., **Finite Element Method, Finite Volume Method** are also actively developed and used.
- ▶ MODFLOW - an open-source FDM software has been an industry-standard for decades

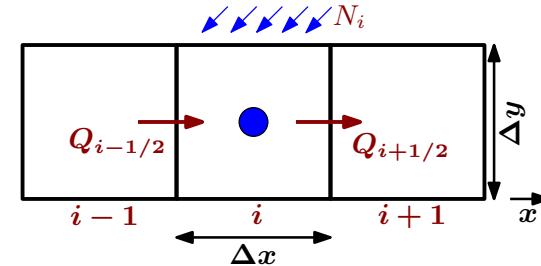


- ▶ ModelMuse - the GUI for MODFLOW simplifies the use of MODFLOW.

MODFLOW (FDM) methods - the 1D case



- ▶ Based on two fundamental principles:
 - ▶ conservation of volume and
 - ▶ Darcy's Law
- ▶ Space is discretized ($\Delta x, \Delta y \dots$) in **Grids**
- ▶ Hydraulic head is computed at the **node**, which here is **block-centred**



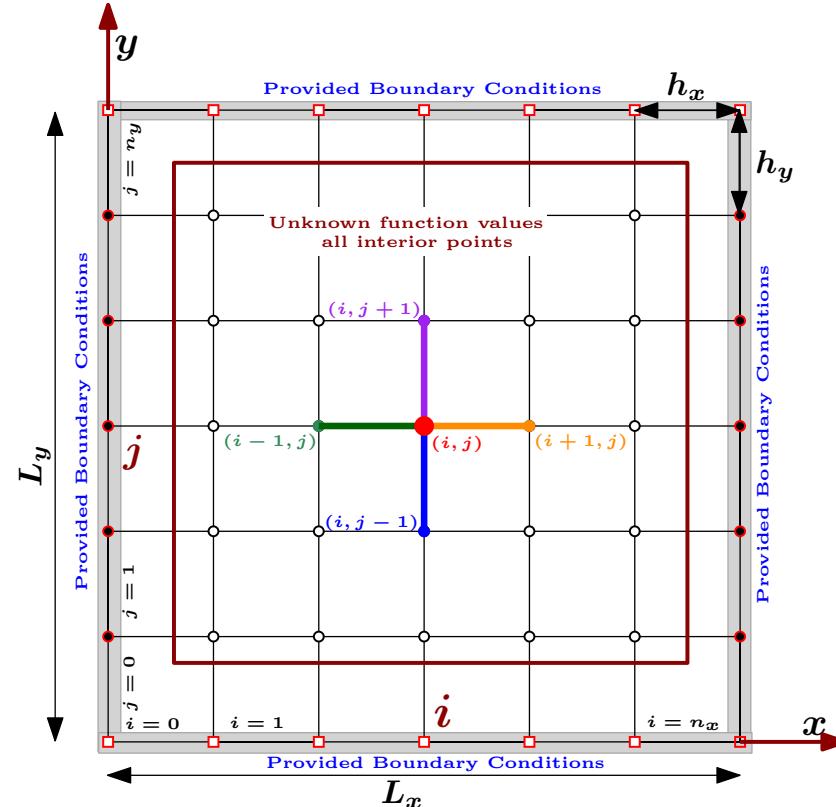
- ▶ Volume conservation:
$$Q_{i-\frac{1}{2}} + N_i \cdot \Delta y \cdot \Delta x = Q_{i+\frac{1}{2}}$$
- ▶ Darcy's law:
$$Q_{i-\frac{1}{2}} = -T \cdot \Delta y \cdot \frac{(h_i - h_{i-1})}{\Delta x}$$

$$Q_{i+\frac{1}{2}} = -T \cdot \Delta y \cdot \frac{(h_{i+1} - h_i)}{\Delta x}$$
- ▶ Leading to FD equation (fixed **h** BCs):

$$h_i = \frac{h_{i-1} + h_{i+1}}{2} + \frac{N_i}{2T} \cdot \Delta x^2$$

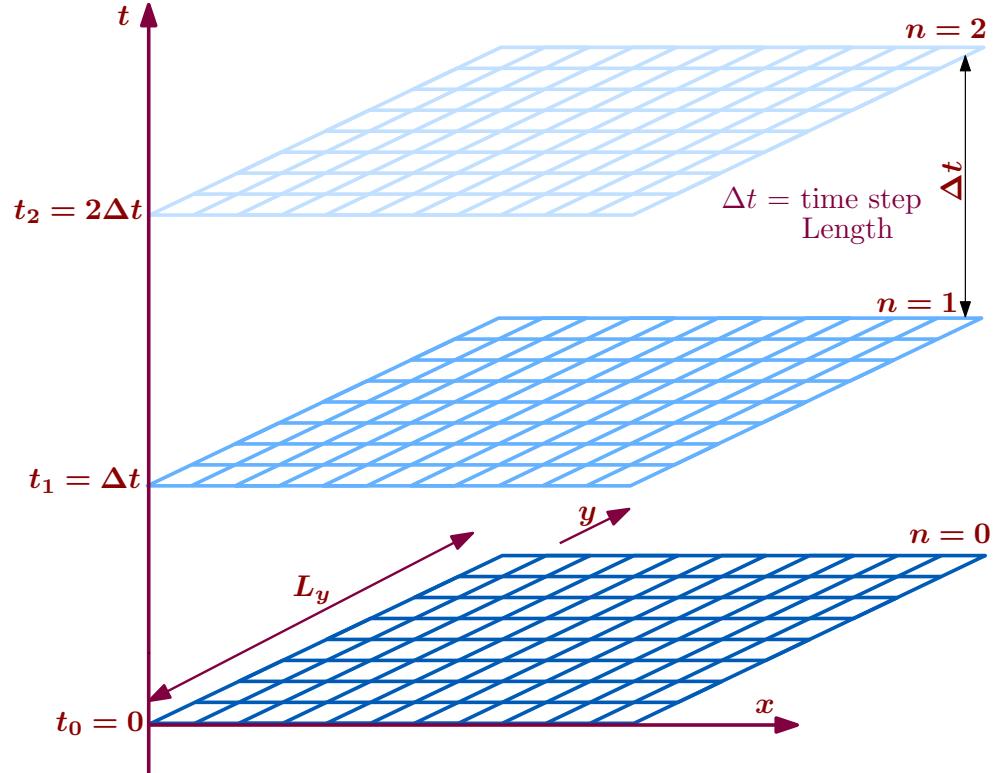
MODFLOW (FDM) methods - the 2D Case

- ▶ GW flow is **generally** modelled as a 2D system
- ▶ 2D system normally is a single layer
- ▶ Multi-layer systems can be developed by varying K in each layer
- ▶ T or K are calculated at the cell edges
- ▶ The 2D (or 3D) FD equations are developed similar to 1D case
- ▶ FD equation for interior cells depends on BCs and processes



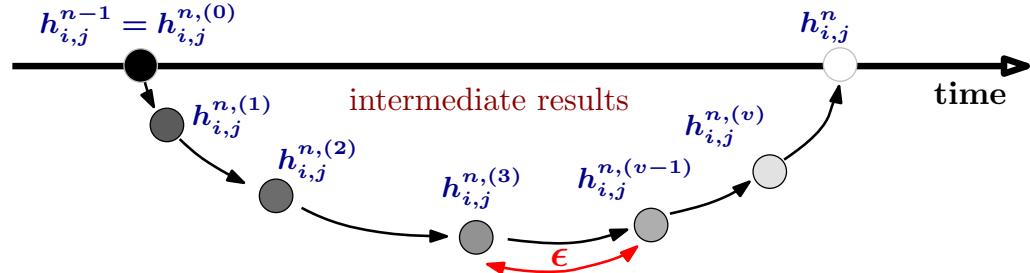
MODFLOW (FDM) methods - time derivative

- ▶ Transient problem requires discretization of **time**
- ▶ For **stability** of the solution it is required that: $C = v \frac{\Delta t}{\Delta x} < 1$
with Courant number **C**[-] and GW flow velocity **v** [LT^{-1}]
- ▶ Internally, the **time-stepping** (in MODFLOW) follows the *fully implicit backward Euler* method



MODFLOW (FDM) methods - Iteration and Solver

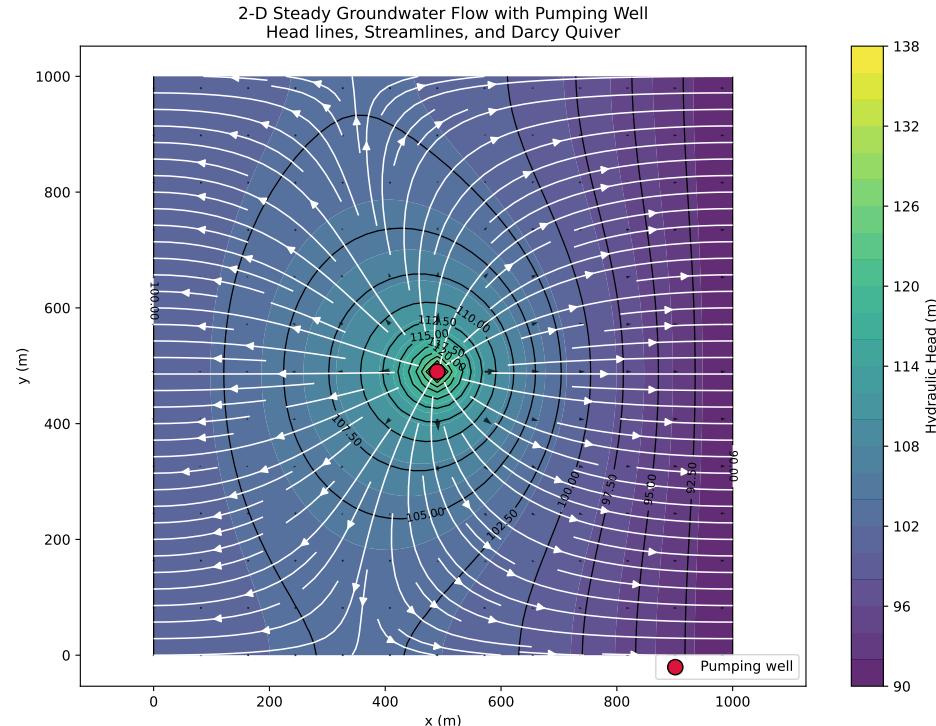
- ▶ MODFLOW iteratively solves the **well-posed** GW flow problem
- ▶ Each numbered (*in bracket*) iterative time-step improves the solution until **acceptable error-tolerance** or **maximum iteration (max-itr)** is reached.
- ▶ Error criterion ϵ :
$$\max \left| h_{ij}^{n,(v)} - h_{ij}^{n,(v-1)} \right| < \epsilon$$
- ▶ ϵ or **max-itr** can be problem-type specific



Solvers	Problem-type
Preconditioned Conjugate Gradient (PCG)	Confined aquifer
Geometric Multigrid Solver (GMG)	Large 3D Grid
Newton Formulation (NWT)	Complex nonlinear model

Post-Processing GW flow results

- ▶ Visualization of MODFLOW (or numerical) results normally requires use of complex codes
- ▶ Generally (for GW flow problems):
 - ▶ head contour lines are plotted
 - ▶ flowlines (vector) provide flow direction in the domain
 - ▶ streamlines, tangent to flowlines, provide speed of flow
- ▶ Visualization can be computationally intensive





Computing interfaces for GW flow Problems

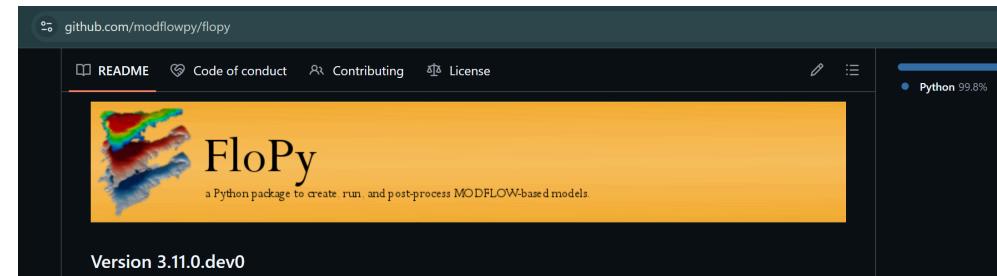
- ▶ GW flow problem using FD method have a simple code structure
- ▶ For simple problems computational codes can be easily developed
- ▶ More complex problems will require MODFLOW-type code
- ▶ FloPy allows scripting MODFLOW
 - ▶ Scripting helps in automatization
 - ▶ Not suitable for problems (e.g.) with complex geometries
 - ▶ Requires programming skills

Computational code for 1D GW flow problem

python

```
1 import numpy as np
2 import matplotlib.pyplot as plt
3 from typing import Literal
4 } # check the attached 1D-flow.py
```

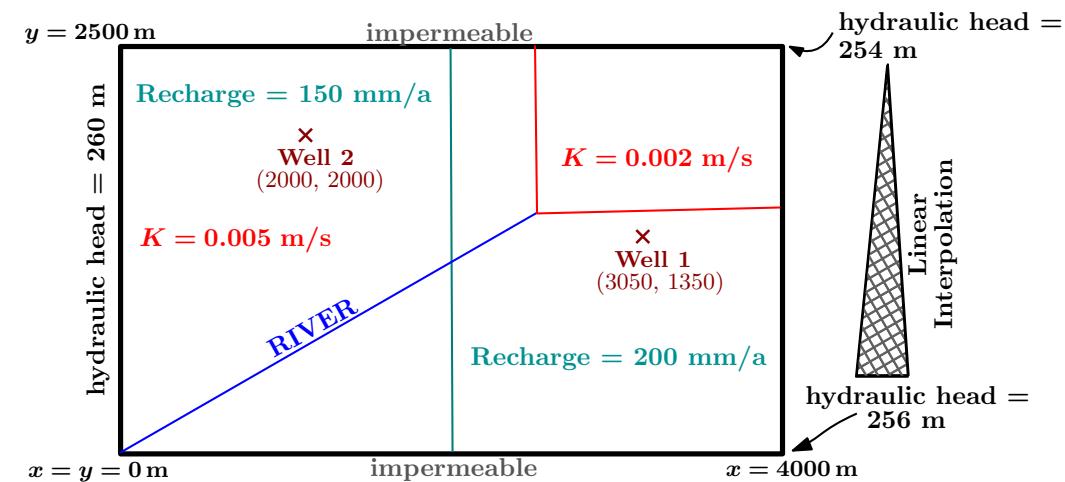
FloPy has been developed since 2001



Modeling GW flow with MODFLOW and ModelMuse

- ▶ ModelMuse provides an excellent user-interface for MODFLOW
 - ▶ It is Open-source code (**flexibility**)
 - ▶ Developed by **USGS** since 2006
 - ▶ Extensively documented and cost-free
- ▶ In the next two sessions we use **MODFLOW** with **ModelMuse** to
 - ▶ 2D horizontal GW flow model
 - ▶ 2D vertical GW flow model
 - ▶ 3D GW flow model
 - ▶ Include Riverbank filtration scenario

- ▶ The first 2D model conceptual setup



Download the required files from [here](#)

REFERENCES

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