MODULE 9. Groundwater modelling

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— What changes can be expected in groundwater levels in the aquifers beneath Lisbon, Portugal, in the year 2030?

— How will a change in river Tagus stage affect the water table in the adjacent alluvial aquifers?

— What is the capture area for a well field that supplies the “Estufa fria” garden in Lisbon?

— What is the most likely pathway of contaminants if there is a leak in the proposed underground repository for high-level radioactive waste in Salamanca, Spain?

Hydrogeologists are often called upon to predict the behaviour of groundwater systems by answering questions like these.

And, the best tool available to help hydrogeologists meet the challenge of prediction is usually a groundwater model.
What is a model?

It is any device that represents a naive approximation of a field situation. Due to the inherent complexity of the world and the interactions in it, models are created as a simplified, manageable view of reality.

Models help you understand, describe, and predict the consequences of a proposed action.

Models can also be used in interpretive sense to gain insight into the controlling parameters in a site-specific setting; or, can be used to study processes in generic geological conditions.

In order for hydrogeologists to provide answers for those seemingly questions involves formulating a correct concept model; selecting parameter values to describe spatial variability within the groundwater flow system, as well as spatial and temporal trends in hydrologic stresses and past and future trends in water levels.
Examples of models

- Geological map
- Geological cross/sections
- Physical model of a lake or river
- Model of gas and oil exploitation
- Hydrological model
- Model of a mineral deposit
- Model of a urbanism project
- Model of a mine
Groundwater models

• calculate the value of variables such as the potentiometric level, the discharge of a spring or the volume of water transferred to a river, the recharge, the concentration of a pollutant, based on the resolution of an equation or series of equations, which describe the behavior of the aquifer system, based on a series of simplifications.

• if the model is a good representation of the reality and is well calibrated, then it may be an important tool for prediction and management of groundwater resources.

• allow you to test different scenarios and assess the risk of some actions

• but, the validity of the predictions of the model predictions will always depend on the quality as the model represents reality, nature.
Type of groundwater models

- **physical models**
  - Laboratory sand tanks (simulate groundwater flow directly)

- **analogical models**
  - models that use similar methods to simulate groundwater flow (for ex., use of electrical current or heat flow simulation)

**Problems:**
- scale
- change of the in situ conditions

- one model per aquifer type
Type of groundwater models

- **mathematical models**

Simulate groundwater flow indirectly by means of a governing equation thought to represent the physical processes that occur in the system, together with equations that describe heads or flows along the boundaries of the model (**boundary conditions**). For time-dependent problems, an equation describing the initial distribution of heads in the system is also is needed (**initial conditions**).

Matemathical models can be solved using:

- **analytical solutions**

These are the exact solutions of the set of differential equations for very specific and restrictive conditions (for ex. homogeneous and isotropic media). They are always a very simplified version of the reality.

Example: Theis method

\[ h_0 - h = \frac{Q}{4\pi T} W(u) \Rightarrow T = \frac{Q}{4\pi(h_0 - h)} \]

\[ u = \frac{r^2}{4Tt} \Rightarrow s = \frac{4Tut}{r^2} \]
Type of groundwater models

- **mathematical models**

Simulate groundwater flow indirectly using a group of *differential equation* that are believed to represent the physical processes in the aquifer, associated with equations that describe the variation of groundwater levels or flow in the limits of the model (boundary conditions).

Mathematical models can be solved using:

- **numerical methods**

The numerical models use approximations (by *finite difference* or *finite elements*) to solve the set of differential equations that describe the flow or transport of solutes in groundwater.

These approximations require that the model domain is *discretized*, being represented by a grid of elements or cells. And the time of simulation is represented by time intervals.
Numerical methods

1. Finite difference method

2. Finite difference method
Steps in a protocol for model application

1. Define purpose
   - Field data

2. Conceptual model
   - Mathematical model
   - Analytical solutions
   - Numerical Formulation
   - Code verified?
     - yes
     - no
     - CODE SELECTION

3. Computer programme
   - Code verified?
     - no
     - yes

4. Model design
   - Field data
   - (includes sensitivity analysis to evaluate effect of uncertainty)

5. Calibration
   - (uncertainty in a predictive simulation arises from uncertainty in the calibrated model)

6. Verification

7. Prediction
   - Presentation of the model design and results
   - Postaudit
     - (Model redesign?)

Postaudit
   - Field data

Presentation of the model design and results
   - (It is essential for effective communication)
"The fascinating impressiveness of rigorous mathematical analysis, with its atmosphere of precision and elegance, should not blind us to the defects of the premises that condition the whole process."
- T.C. Chamberlin, 1899

1) Darcy law

\[ q = v = K \frac{\Delta h}{L} \left[ \mathbf{D}^{-1} \right] \]

2) Continuity equation

\[ \frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z} = 0 \]

3) Laplace equation

\[ \frac{\partial}{\partial x} \left( K_x \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left( K_y \frac{\partial h}{\partial y} \right) + \frac{\partial}{\partial z} \left( K_z \frac{\partial h}{\partial z} \right) = S_s \frac{\partial h}{\partial t} - R^* \]
Boundary conditions

1. Neumann conditions or constant flow

\[ \frac{\partial h}{\partial x} = 0 \text{ or } \frac{\partial h}{\partial y} = 0 \text{ or } \frac{\partial h}{\partial n} = 0 \]

- flow is parallel to the border
- the equipotentials are perpendicular to the border

\[ q_n(x_b, y_b, z_b, t) = q_b(t) \]

2. Dirichlet condition or constant level: \( h = \text{constant} \)

\[ H(x_b, y_b, z_b, t) = H_b(t) \]

- flow is perpendicular to the border
- the equipotentials are parallel to the border

3. Cauchy (Fourier or mixed conditions)
Integration of the field data

Type of information:

- soils
- geology
- logs boreholes
- digital model of terrain
- geological limits;
- hydrogeology;
- potentiometric heads;
- surface water bodies.

Fonte: http://www.interaeng.ca/
Hydrostratigraphic units
Model construction

Model grid

• regular (finite difference)
  
  ![3D regular grid with variable layer thickness generated from DEM. Fracture elements selected from intersecting fracture polygon sets.](image)

• irregular (finite elements)
  
  ![Vertical Slice of Finite Element Grid through Deep Disposal Vault](image)

Fonte: http://www.interaeng.ca/
Run the model to get the head contours (and vectors):
Visualization of the results in plane and slices (head contours and vectours):
Calibration (compare the results of the simulations vs measured)
Highly parameterized groundwater models can create calibration difficulties.

Regularized inversion—the combined use of large numbers of parameters with mathematical approaches for stable parameter estimation—is becoming a common approach to address these difficulties and enhance the transfer of information contained in field measurements to parameters used to model that system.

Similar to classical parameter estimation of overdetermined problems, regularized-inversion approaches are grounded on principles of least-squares minimization, where a best fit is defined by the minimization of the weighted squared difference between measured and simulated observations.

For further reading on PEST:
PEST for Groundwater-Model Calibration

About PEST

PEST stands for parameter estimation; it is a non-linear inverse modeling code, developed by John Doherty, Watermark Numerical Computing.

Generally, it is often easier in hydrogeology to measure model output (heads, fluxes, concentrations) than it is to measure input parameters (hydraulic conductivity, storativity, porosity, etc.). As a result, we try to infer system inputs, or parameters, from system outputs (results). This is called the “inverse problem”. PEST uses a powerful mathematical technique to estimate a new set of parameters by comparing model results to a set of observations, and provides valuable insight into the conceptual model. PEST is model-independent and is a public domain code. It can be used with any numerical simulator. PEST is well-documented and supported.

When should PEST be used?

There are several important places in the modeling process where PEST is really useful:

• at the beginning of the calibration process, when the model is first developed and a gross calibration to the hydrogeologic conceptualization is needed;
• at the end of the calibration process when “tweaking” the model to obtain the “best” set of model parameters;
• during sensitivity analysis and uncertainty analysis to understand the implications of model input uncertainty on the predicted results.

For more details, visit: http://www.pesthomepage.org.
Flow Models. Example 01. East Texas

Setting up the conceptual model

Converting the conceptual model (grid finite difference)

Running the model

Converting the conceptual model (grid finite element)
Flow Models. Example 01. East Texas

Exporting the results to ArcGIS or QGIS
Flow Models. Example 02. Estarreja

Spatial discretization

Cross-sections

Source: Barreiras et al. 2019 SOIL TAKE CARE project

Grid, borders and surface water bodies

Níveis piezométricos e calibração
Flow Models. Example 02. Estarreja

Rivers and drains, boundary conditions, hydraulic parameters, etc

Hydraulic Heads

Source: Barreiras et al. 2019 SOIL TAKE CARE project
Flow Models. Example 02. Estarreja

Source: Barreiras et al. 2019 SOIL TAKE CARE project
Flow Models. Example 02. Estarreja

T=0; L2; Tracer (chloride) 5000 < C < 10000 mg/L

T= 5 years

T= 10 years

T= 20 years

Source: Barreiras et al. 2019 SOIL TAKE CARE project
Flow Models. Example 03. Aveiro Cretaceous aquifer

Hydrostratigraphic units

Five layers are considered:
- layer 1
- layer 2
- layer 4
- layer 3 & 5
- impermeable base and inactive

Conceptual model

Model domain: goes from the shelf break (considered vertical) to the most eastern outcrop of the Cretaceous. It measures 65km horizontal, subdivided in 260 columns of 25 m, and 760 m vertical, subdivided in 76 layers of 10 m.

Source: Vandanbohede & Condesso de Melo, 2018
Flow Models. Example 03. Aveiro Cretaceous aquifer

Model input parameters: $Kh$, $Kv$ & $\theta$

<table>
<thead>
<tr>
<th>Layer</th>
<th>Type</th>
<th>$Kh$ (m/d)</th>
<th>$Kv$ (m/d)</th>
<th>$\theta$ (-)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Layer 1</td>
<td>Quaternary</td>
<td>20</td>
<td>0.40</td>
<td>0.35</td>
</tr>
<tr>
<td>Layer 2</td>
<td>Clay</td>
<td>0.005</td>
<td>0.0001</td>
<td>0.35</td>
</tr>
<tr>
<td>Layer 3</td>
<td>Semi-pervious 1</td>
<td>0.25</td>
<td>0.02</td>
<td>0.15</td>
</tr>
<tr>
<td>Layer 4</td>
<td>Cretaceous Aquifer</td>
<td>5</td>
<td>0.1</td>
<td>0.15</td>
</tr>
<tr>
<td>Layer 5</td>
<td>Semi-pervious 2</td>
<td>0.25</td>
<td>0.02</td>
<td>0.15</td>
</tr>
</tbody>
</table>

And, **hydraulic conductivity** ($K$) and **porosity** ($\theta$) are a function of depth $d$ (m).
Flow Models. Example 03. Aveiro Cretaceous aquifer

Distribution of parameters in model domain

Source: Vandanbohede & Condesso de Melo, 2018
Modelling results

SCENARIO 1. Fresh-saltwater with current boundary conditions

• In a first step, current day boundary conditions are used to calculate evolution fresh-saltwater distribution and the ages of the water.

• Heads and C-14 corrected ages are used to “calibrate” the flow model.

• We start with saltwater in the complete aquifer (also on land).

• Model is run for 60 000 years
Flow Models. Example 03. Aveiro Cretaceous aquifer

Source: Vandanbohede & Condezzo de Melo, 2018
Flow Models. Example 04. Seixal

Source: Barreiras 1999
Problem: An aquifer system with two stratigraphic units is bounded by impermeable boundaries (no flow boundary) on the North and South sides. The West and East sides are bounded by rivers, which are in full hydraulic contact with the aquifer and can be considered as constant head boundaries. The hydraulic heads on the west and east boundaries are 9 m and 8 m above reference level, respectively.
EXERCISE WITH PROCESSING MODFLOW 11

Build and Run a Steady-State Flow Model

In this section, we will walk you through the following steps to build your first groundwater model with PM.

1. Create a groundwater model and load the area.shp shapefile;
2. Specify layer types;
3. Modify the layer elevation of the model cells;
4. Assign cell types, such as constant-head or no-flow cells, to the flow model;
5. Assign the initial hydraulic head values, and aquifer parameters, such as hydraulic conductivity, to model cells;
6. Add the pumping well to the model, and
7. Carry out the flow simulation with MODFLOW.
EXERCISE WITH PROCESSING MODFLOW 11

To create a new model

1. Start PM if it is not already started and select **File > New** to start a new project.

2. **Turn off the maps** by unchecking the Base Maps group on the Table of Contents (TOC), as we will not use the base map feature in this tutorial.

3. **Select File > Create Model.**
   - PM displays a dialog box and asks you to save the project before creating a model, click OK on the dialog box.
   - In the Save As dialog box, create or find a folder (for example, C:\MyModels), enter a filename for the PM file, and then click Save.

4. As soon as the file is saved, the Create Model dialog box appears. We use the **Time tab** to define the temporal discretization and use the and **Grid tab** to define the spatial discretization of the model. All values may later be modified when necessary. For this tutorial, the following values are used. The default values are used if they are not mentioned below.

   - **Internal Flow Package: Layer-Property Flow (LPF).**
   - **Time Tab:**
     - Model Start Date/Time: **2018-01-01 00:00:00**
     - Length of simulation = **94672800** and Time Unit = Second (that is about 3 years.)
EXERCISE WITH PROCESSING MODFLOW 11
EXERCISE WITH PROCESSING MODFLOW 11