Groundwater modelling with ModelMuse

The project of the course Groundwater modelling will be carried out using MODFLOW and related programs such as MODPATH and the interface provided by ModelMuse. The software is developed mostly by the USGS and are is free of use. For the installation and introduction you are referred to the introductory exercise.

You can use Python to avoid repetitive work for plotting and processing the results. If you are not sure how to get started you can follow the python instructions available on Ufora.

In the next sections, we will see the necessary steps to define a model and solve the project. As we go further in the project, it will be considered that previous steps are understood and can be reproduced, so that some of the instructions will not be repeated. This document is designed to help you with the technical side of ModelMuse, but it will not solve the project for you. During each session, it is expected that you learn how to use the software to accomplish the task, but some personal work will probably be needed to get a satisfactory model (i.e., calibrated)

! Start by making a folder for each step of the project ! Save the model itself and the results in the appropriate folder. You can use the following structure:

- Steady_state
- Transient_state
- Transport
- Problem solution
    - Flowrate
    - Time
    - Modpath

(Continue building on the model of the previous step, do not start a new model for each step 😉)

A. Create a new grid

1) When you open ModelMuse, you have the choice to do several things. You can open an existing project or create a new model. At this stage, we are beginning a new project and so we will create a new project. The first screen is not necessary. In the second screen we will now **select "No Grid".** This will allow us to create the grid using an object. In this way the grid will be easier to modify later on in the project.

   Select Object → Create → Rectangle to **create an object** for the grid. Change the object name and select "**Use to set grid cell size**". As grid size you choose the largest cell size that you want in your model. You also have to **adjust the vertices** (coordinates) so the extent of the grid corresponds to your problem definition (upper left corner of your model: X = 0, Y = 1000, lower right corner: X = 1000, Y = 0). **You may want to refine** the grid around the pumping well (see later). Note that the grid can be modified at any moment as all the properties are set using objects.

2) Now **create the layers**. Model → Modflow layer groups. By default there are 3 layers. You

can add/remove layers and change their names. Make sure you have the appropriate number of layers according to your project (= number of hydrogeological units). Note that a layer can be later subdivided in several sub-layers.

3) To generate the grid: Grid → Generate Grid

4) **Define the units** that are going to be used. Be consistent: if you use meter and second as length and time unit, then you should define the hydraulic conductivity in m/s
Model → MODFLOW options → Options tab → time length and mass unit

5) It is general useful to have a graphical representation of the conceptual model to help build the model. A **base map** is available on the folder on Ufora "basemap.png". Load this base map:
File → Import →Image. Select the image and set the coordinates of minimum two points (corners). You can do this by clicking on the image and specifying the location you want this point to correspond with in the grid. Make sure this reference system is in adequation with your definition of the grid. Now you should see the position of the well, piezometers and limits of the model on the figure.
You should **refine the grid** around the pumping wells to increase the accuracy of the model in this zone. Grid → Subdivide grid cells (or use the short-cut icon) **or** you can create an object to set the grid cell size in a zone around the pumping wells (same workflow as step 1).
Do not forget to select Grid→ Generate Grid and Grid →Smooth Grid for a gradual change in cell size. Be careful to keep the size of the cells in reasonable limits (the higher the number of cells is, the longer a simulation will take) and follow the recommendations for an appropriate grid (for example neighboring cells).

B. Edit the grid

1) The geometry of the layers is a requirement for the model to run. So far, default values were used during the grid generation. We still need to **specify the correct elevation** of the model top, bottom and boundaries between layers. To do this: Data → Edit Data Sets → Required → Layer Definition. The elevation of the **model top and the model bottom** can each be fixed to a single value (horizontal layers).

   For **the limit between the top and bottom aquifer**, the values are changing depending on the location (the thickness of the alluvial aquifer is not constant). Therefore, we have to specify the value where it is known (borehole) and interpolate the values in between. To do that, the easiest way is to define objects at the location of the boreholes.

   - For each borehole/piezometer
     Object → Create → Point (or use the icon) → click on the borehole location on the basemap

     Properties :
     - Name : choose a name for your object so that you find it easily (example: BRF1 for bedrock at location F1)
     - Number of Z formulas = 0
     - Set values of cells by interpolation

Data sets :

- expand « Required|Layer Definition|Upper Aquifer Bottom »
- Set the value of the elevation in 'Formula for …'
- Adjust the vertices
- If a dialog box pops up, just say yes

You can also use polyline or polygon to set elevations using the same procedure.

Once all the points are entered, you can interpolate the layer. Go to Data → Edit Data Sets → Required → Layer Definition. Expand the Upper_aquifer_bottom and choose an interpolation method.

Use the data visualization tool to see the results of interpolation
Data → Data Visualization (or the icon) → Expand Data Sets|Required|Layer definition|Upper_aquifer_bottom → click OK

2) **Define the model limit.** Some cells within the model are going to be **inactive** because they are located out of the interesting zone. You can set them inactive.
The default value for a cell is to be active. First change the **default value to inactive** Data → Edit Data sets → Expand Required|Hydrology|Active and set the value to False .Then **create** a polygon **object** covering the zone that should be **active** (between the hillslope andthe river). Define the enclosed cells as active. Don't forget to adjust the Z formulas in a way that the object applies to the all model layers.
Use the data visualization tool to color the active cells and verify that your settings are correct.

You now have a proper model in terms of layer geometry. However, to be able to run it, you have to define the type of simulation you want to do. You also have to specify the time parameters, stress factors, boundary conditions, observation wells and aquifer properties.

C. Specify the time parameters and initial conditions of the simulations

1) The first step is to assign the **time characteristics** of the simulation.
Model → MODFLOW Time
Here you can select the number of stress-period (a stress period = a period during which stress factors such as recharge, pumping and boundary conditions are constant) and the duration of each stress period.
For the first part of the project, you have to calibrate the model in **steady-state** conditions **with and without pumping**. This means that you need to start with steady-state conditions and two stress periods (natural flow + pumping). For steady-state, the duration of the period is not important, so you can choose -1 – 0 for the first period and 0 – 1 for the second. If you want to simulate some advective transport in steady- state, then the length of the period becomes important.
You can also choose the time unit used in the simulations. Be consistent.

2) The solution (final hydraulic head) is computed with an iterative process. This means that Modflow must start with a first guess, called the initial hydraulic head. Change the default

initial head for your model. Data → Edit Data sets → Expand "Required" and "Hydrology" → Select "Modflow_Initial-Head".

D. Set the boundary conditions

By default, Modflow uses no flow boundary conditions. If some of the boundary conditions you want to apply are no flow boundaries, nothing has to be done.

For other types of boundary conditions, it is first necessary to activate the corresponding modflow packages.

Model → MODFLOW Packages and Programs

On the left side, you have all the available modflow packages. Expand Boundary conditions and activate the desired packages. Most used packages are CHD (constant specified head), RCH (recharge = specified flux, generally on top of the models), WEL(well package, also used to apply a specified flux other than recharge). Other packages are available for head-dependent fluxes such as the drain, the lake and the river (RIV) package. Keep in mind that there is not one single solution/option for the boundary condition.

Now you can proceed and specify the boundary conditions. The easiest way to proceed is to **create an object for each boundary.**

Once the dialogbox opens, specify the name of the object, **make sure you select the correct options** (z-formulas, intersected or enclosed cells, direct/total per layer/calculated boundary condition/…). **Check that you apply the BC to the correct layer(s) and cells**. (use the visualization tool! Data → Data Visualization → Expand Boundary conditions)

Tip: if you do not want a constant value along you can use the formula editor to specify the head. For example, if you know that the head variesbetween 47.3 at x = 0 to 47.5 at x = 1000, you can use a formula defined as BC = 0.0002 X + 47.3

The "X" value is available in the right panel of the formula editor under GIS when you use the formula. Other parameters are also available.

Do this for all boundaries. Be careful at the intersection because the values are additive (do not let multiple boundary objects end/start in the same cell).

Some extra info on the River boundary condition (if you want to use it): The conductance is the hydraulic conductivity of the river bed divided by the thickness of the river bed. If you used a line, you should multiply it by the width of the river (Make sure the conductance is calculated). The river bottom is the elevation of the river bed (eg. x m below the river stage).

Do not forget to specify the pumping rate at the well. You have to specify a different pumping rate for the two stress periods. Negative values mean that water is extracted.

E. Change the parameters of the layers

1) Define the **aquifer type confined/unconfined**. You should have at least two layers, one for each aquifer. Create an object that covers the entire layer (set the Z-formulas correctly!) and change the Cell_type as you learned in the introductory exercise.
   Check if your settings have the desired outcome by visualizing the Cell_type.

2) Now that the geometry, the stress factors, time parameters and the boundary conditions are defined, we still have to define the value of the properties in the different layers. We will give a starting value, then the process of calibration will be used to adapt the value so that the calculated values fit (hopefully 😊) the observed data.

For steady-state simulations, all we need to do isto define **hydraulic conductivity**. For transient state and transport, we also have to definethe **specific storage coefficient, specific yield and effective porosity and dispersivity respectively**.

It is helpful to define as the **default value** the lithology with the highest surface area in the system (Data → Edit Data Sets → Required → Hydrogeology). Here, we can use the sandy gravel deposits. 10^{-3}

To define other zones, we will use **polygon objects**. One nice thing with objects is that you can define them and change their shape, it will automatically modify the value in the grid. Remember that the default value applies for all layers, so make sure you also modify the second layer with your objects (pay attention to the specified z formulas). By default, Ky = Kx(no horizontal anisotropy) and Kz = Kx/10.

For example: to define a zone with clean gravel, we will draw a polygon going around the corresponding boreholes (make sure the shape is geologically realistic, not a simple rectangle). Give an appropriate name, check 'enclosed cells', verify that the Z-formulas are correctly set, and go to the tab Data Sets and give the desired value of Kx.

Repeat the process **for every lithology and for each layer**. Make sure you draw something geologically realistic. You can later select a polygon and modify its shape, it might be necessary to calibrate your model.

F. Define the observation wells

Now, we can define the location where we have observation well. First, make sure the package observation well is activated. Model → MODFLOW Package and programs → Observations → OBS : Observation Utility

Create a **punctual object** at the location of the observation well. Give it an appropriate name (names must be unique, for instance: P1_O), Select one Z formula (middle of the aquifer in absence of more information), go to the model feature tab and select **OBS**.
Then you can enter the name of the piezometer. Select the option '**head observation'**. For every simulation a *.ob_gw_out_head.csv file will be created with the observed head at the end of each stress period for every observation utility.

Repeat for all wells. Be careful, Pz12 is drilled in the bottom aquifer.

G. Calibrate with steady state simulation

1) Run a simulation

If all the parameters where properly set, you should be able to run the Modflow simulation. You just have to click on the **"Play" icon**.

ModelMuse will prompt you to save the file. If the "Execute Model" option is checked, the simulation will start automatically.

Modflow will first check that all necessary files are created (for every package used, a file will be generated and used for simulation) and make a list of error and warnings (correct the error and read the warning), it might point to problems in your input files. Then, it will show you the results of simulations with the error in the water budget for every time-step. The latter should be as low as possible (no water should be created). A high value might mean that the discretization grid is too large, or that some boundary conditions are not properly set, or that the initial head is badlychosen, or that the solver tolerance is too high (this can be changed in Modflow packages and programs → solver).

When you close that window, the file "ProjectName.lst" opens. It contains a summary of all the input and the results of the simulations, including the water budget, and at the end the calculated head at the observation wells. You can use it tocheck the quality of the results.

It is recommended to use another program, such as an excel spreadsheet to make a **comparison between the observed and calculated head** (or a plot of the residuals compared to the observed head). Then you will be able to compute indicator such as the average error/objective function (sum of squared errors) and make further analysis. If you want to avoid repetitive work you can also use the Python script that is available on Ufora to read the output files and process the results.

2) Visualize the results

After the simulation, you can import the results.First, you have to import the results

File → Import → Model Results → select the file "ProjectName.bhd"

Then, you can select the stress period for which you want to import the results.

You can use the Data Visualization tool to adapt the view. You can also add contour lines and display the results for each layer using this tool.

3) Start the calibration process

Depending on the discrepancy between your observed and calculated heads, modify the hydraulic conductivity of the model, and re-run the model until you are satisfied by the calibration. You can of course modify the properties (hydraulic conductivity) of your objects/layers, but also their geometry. If you have strange results, make sure your boundary conditions are properly defined. Once calibrated, you can modify the values of the parameters to see which ones are the most sensitive (local sensitivity analysis).

H. Now that the model is calibrated in steady-state, we are going to calibrate it in transient flow conditions to derive the Specific yield/Specific storage.

It is advised to save your model in a new folder so you do not overwrite your results of the steady state simulations.

1) **Set transient-state simulations**

   You have to modify the simulation type

   Model → MODFLOW Time

   Adjust the stress period as required. Be careful, in transient state, the length of the period is important. You can use a steady-state simulation for the natural flow from -1 to 0 do the model gets the correct starting conditions, then start a transient state simulation from 0 to at least 432000 s (see the data).

   Adjust the time steps. The time steps are important to ensure convergence, it might be necessary to reduce the time-steps if the solution does not convergence. Generally, we start with a relatively small time step, which can be multiplied as we go further towards the steady-state solution.

   Remember that it will change accordingly the time of your boundary conditions, so it is important to check that those are still correct.

2) **Set new parameters**

   In transient state, two new parameters are required: the specific yield (~effective porosity) and the specific storage. They characterize the storage capacity of the aquifer and should be calibrated for each zone that was defined previously and for both layers. However, given the data restricted in the pumping well, some parameters might be insensitive (you may want to check that through a sensitivity analysis as well).

3) **Calibrate** the curve (drawdown in P1 and Pz12) using Excel or the available Python script. Here we only have data in P1 and Pz12 so you can deactivate the other observation wells.

I. Transport

It is advised to save your model in a new folder so you do not overwrite your results of the transient simulations.

On top of advection, solute transport is also influenced by diffusion and dispersion processes (+ adsorption/desorption, degradation/reaction, etc.). We will use the GWT (groundwater transport) package of MODFLOW 6 to solve the transport equations. In practice, GWT will use the computed head/flows from GWF (groundwater flow), at each time-step, to calculate advection-dispersion processes in the aquifer. The GWT Model can access these flows in a GWF Model that is running in the same simulation as the GWT Model. Alternatively, the GWT Model can read the output files created from a previous GWF Model simulation. In the last case it is therefore always necessary to first run the GWF model and afterwards the GWT model.

1) Activate GWT. Model → MODFLOW Packages and programs → activate all the necessary packages (basic transport package, advection and dispersion packages, sink and sources mixing packages solver package, constant concentration/mass source loading package, etc.).Pay attention to the options for the different packages. For example, it is here that you canchoose which method is going to be used to solve the advection-dispersion equation (seetheory). You can also specify the name of the chemical species.
2) Activate GWT

   Model → MODFLOW Packages and programs → activate all the necessary packages (basic transport package, advection and dispersion packages, sink and sources mixing packages solver packages, concentration packages etc.)
3) Check the unit that are used for mass Model → model options → should be gram (g)

4) If you go to Data → Edit data sets à MT3DMS,MT3D-USGS, or GWTGWT you will see that new parameters are available. The most important are the longitudinal dispersivity and the (effective) porosity (also used for MODPATH).The latter should be close to the specific yield but can differ slightly (it correspond to a transport properties). Both should be calibrated using the tracing experiment data. You can change the default value of the model and the specific values of your lithology objects.
5) If you go to Data → Edit data sets → GWT, you will see that also the transverse dispersivity and diffusion coefficient are now available as object parameters. In there you can define the anisotropy of the dispersivity (1 by default). You can also note that the diffusion coefficient is set to zero by default, it means that diffusion is neglected (this can be modified if desired). You can change the default value of the model and the specific values of your lithology objects.
6) During the tracing experiment, there is an injection occurring at Pz2 (at 32 m depth).Pz2. You thus have to create an object at Pz2 crossing the middle part of the alluvial aquifer (when it is divided into 3 equal layers Model→Layer Groups→Discretization). You have to make sure that the correct source package is activated. Also make sure that if you set WEL/RIV/… boundary conditions they still have the correct value when dividing the upper aquifer into three layers. For example if you used 'direct'/'total per layer' as option and the object crosses 3 layers now the rate should be divided by 3. You can check if it has the desired results by checking the budgets in the listing file (.lst) after the model has completed running.

Now, everything is ready to define the transport simulations. The first step is to adapt the simulations time. Transport simulations are always transient simulations. Here, you have to make sure that the pumping has reached steady-state first (thus the first stress period can be steady-state), then you can have an injection period of one hour at the correct concentration, then the pumping continues for at least the time for which measurements are available

1) Model → MODFLOW time →Define the appropriate time control for MODFLOW **AND** GWT
2) Verify that the boundary conditions are still valid
3) Don't forget to think about the boundary conditions for transport! By default the cell will be active so that the concentration will be calculated. The default value is zero concentration gradient, but it means that some mass can flow out through advection. The other possibility is to impose concentration (through sink/source).
4) At the pumping well, you can define concentration observations using the corresponding object and the OBS package. Check the concentration observation in Modflow Features|OBS in the dialog box of the object.the OBS utility.
5) At the injection well, you have to specify the injected mass of eosin. Use the mass- loading option and calculate the injected mass flux in g/s.
6) If you want to reduce computation time, you can try playing with the ATS option in the Modflow Time dialog box.
7) Run the flow and transport model.Run the simulation

Once the simulation is done, you can analyze the results. The concentration at the chosen time-steps are stored in the file ProjectName.ucn. You can visualize them in ModelMuse. For more options, you can also use the graphic software GW chart (https://water.usgs.gov/nrp/gwsoftware/GW_Chart/GW_Chart.html)

If observations were activated, the file ProjectName.eosin.ob_gw_out_concentration.csv contains the observation. You can easily use it to plot the results and compare them to observation in an excel spreadsheet. You can also make use of the available Python script on Ufora to quickly make these plots. Do not forget to pay attention to the difference in units.

Calibrate the model against observed concentration data.

J. Estimate the minimum flow and time

You can now use the calibrated models from the previous steps to formulate an answer to the problem.

1) Use the steady state model to estimate the **minimum flowrate**.

2) Create an object that represents the pit (with the correct dimensions!) and give it a high hydraulic conductivity value (0.1 m/s or higher) to represent the excavated zone.

3) Create a well object (make sure to delete the pumping well from the calibration process). There are multiple wells placed at the boundaries of the excavation pit and they are filtered right underneath the pit (in the middle part of the alluvial aquifer). Divide the alluvial aquifer into 3 equal layers (Layer groups→discretization). Make sure that if you set WEL/RIV/… boundary conditions they still have the correct value when dividing the upper aquifer into three layers. For example if you used 'direct'/'total per layer' as option and the object crosses 3 layers now the rate should be divided by 3. You can check if it has the desired results by checking the budgets in the listing file (.lst) after the model has completed running.

4) Make sure you set all the parameters ready for the steady-state simulation (Time, boundary conditions, ..). Always start with a steady state stress period to let the model evolve to natural conditions.

5) Run a full flow simulation and look at the groundwater level in the *.bhd file and rerun the model with an increased pumping rate until the pit becomes dry (only the pit).

6) Use the calibrated transient state model to estimate the **minimum time**. You can copy the pit_Kx objects and the final pit_WEL object from the previous model. Edit→Copy // Edit→Paste. Make sure to delete the pumping well from the transient calibrations and make sure the alluvial aquifer is divided into 3 equal layers.

7) Make sure you set all the parameters ready for the transient-state simulation (Time, boundary conditions, ..). Always start with a steady state stress period to let the model evolve to natural conditions.
8) Run a full transport simulation and look at the water level at the pit in the *.bhd file. Increase

the time until the pit becomes dry (only the pit).

You are free to model additional scenarios in order to provide an answer to other questions or to quickly try out if your estimation/thoughts make sense.

K. Determine if the contaminant will end up in the well

Use MODPATH to estimate if the contaminant present at the surface might reach the pit during the construction time of 4 months. It is advised to save your model in a new folder so you do not overwrite your results of the transport simulations. Start from the model you used to estimate the time and make sure you change de default value of the porosity.

1) Activate the MODPATH package
Model → MODFLOW packages and programs → expand post processors and select Modpath. We will use backtracking to see from which zone the water particles are coming, we will use forward tracking to see where the particles are going in natural conditions. Make sure you set the reference time correctly for backtracking. Don't forget to select the 'pathlines' option if you want to generate the pathline output file for visualization later on.

2) MODPATH will use the solution of flow from Modflow to compute the pathlines, but it can only read the binary file format. You thus have to change the MODFLOW options. Model → Modflow Output control → Head →External File Type = Binary.

3) Make sure the time of simulation (stress-periods) and the pumping rates are correctly set according to the problem definition. Model → MODFLOW Output Time.

4) Create an object that represents the contamination at the surface.

5) Open the object you want to track the particles for. In Modflow features|Modpath, you can specify the initial location of the particles. Several options are available. You set the particle within the specified cell, around a cylinder, on faces, etc. Choose the option you find the most appropriate.

6) Make sure you define the porosity in the data set. It should be defined from GWT (>< SULAMA has to choose a porosity value now), but it is important to check that it is correctly set. Don't forget that you have different lithologies.

7) If you would run Modpath now you would probably get an 'invalid grid structure' error. This is because Modpath is adding an unnecessary restriction to MF6 DIS grids. To work around this, create a grid that is will pass the restriction. Delete the objects you created to refine the grid around the well and generate a new grid with a constant cell size. Grid → Generate grid.

8) Once everything is ready you can run Modflow. Modpath should be executed automatically after that. If you want to change the geometry of the particle, you don't have to re-run modflow but you can directly run modpath.

9) To visualize the results
Data → Data Visualization → MODPATH pathlines → load the file created during simulations.It will show you the pathlines, the color being proportional to the time. You can also display the end location of the particles using Endpoint (a file is also createdduring simulation).

You are free to model additional scenarios in order to provide an answer to other questions or to quickly try out if your estimation/thoughts make sense.