

Groundwater modeling : Introduction to ModelMuse

Installation and introduction

The following exercises are designed to give a first insight into groundwater modeling and help you to learn how to build a model with the software ModelMuse. They do not include model calibration with real observation data as will be done during the project.

- 1) Download the latest version of ModelMuse (a graphical interface to ModFlow to automatically build the input files and read the output files) and install it on your computer <https://water.usgs.gov/nrp/gwsoftware/ModelMuse/ModelMuse.html>
- 2) Since ModelMuse is only an interface, you should also download Modflow itself (be careful to download MODFLOW 6, <https://water.usgs.gov/water-resources/software/MODFLOW-6/>), and MODPATH (latest version) (HYPERLINK "<https://water.usgs.gov/ogw/modpath/>").
- 3) The first time you open ModelMuse, you have to specify the location of those programs on your disk so that ModelMuse can locate and run them: open ModelMuse (click OK to everything) Model → Modflow program locations → specify the path on your computer where the above-mentioned programs were installed.
- 4) It is necessary to select a package for solving the flow problem. Model → MODFLOW Packages and Programs → Flow Packages → Select NPF: Node Property Flow package, deselect the 'Save Saturation' option in the NPF pane . In the same Window, also select a Solver : Solvers → IMS: Iterative Model Solution. If you want to solve transport equations, you also will have to select the transport packages you want to use.

One specificity of ModelMuse is to have two distinct levels : the **grid** itself which will be used to solve the equations and **objects** that will be used to define the different properties, stress factors and geometries in the model. This approach is powerful to build model independently from the grid. For example, if you have a zone of with higher hydraulic conductivity, you can define it using an object instead of changing the parameter value in each cell of the zone. If for some reason, you want to change the shape of this zone, you can just change the geometry of the object, the corresponding cells will be automatically modified on the grid. Your objects are thus grid independent, it means that you can make modifications to your grid (for example refine it), cells within a specified object will always take the value as defined by the object.

You will quickly realize that a lot of objects are needed to build a relatively simple model (for the geometry of the model, the geology, the boundary conditions, the wells, etc. and this for all the layers). It is therefore recommended to adequately name the objects, for example using standard names and abbreviation (BC for boundary conditions, OBS for observation wells, etc.).

ModelMuse has also advanced features to define properties based on formula. It means that within an object, you don't need to specify constant values, but can use the formula to make the property location-dependent. As an example, you can define boundary conditions whose value depends on the coordinate of the boundary using an appropriate formula.

Exercise 1: First model with Modflow

As shown in Fig. 1, an aquifer system with two stratigraphic units is bounded by no flow boundaries 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 fixed head boundaries. The hydraulic heads on the west and east boundaries are 9 m and 8 m above reference level, respectively. The aquifer system is unconfined and isotropic. The horizontal hydraulic conductivities of the first and second stratigraphic units are 0.0001 m/s and 0.0005 m/s, respectively. The vertical hydraulic conductivity of both units is assumed to be 10% of the horizontal hydraulic conductivity. The effective porosity is 25%. The elevation of the ground surface (top of the first stratigraphic unit) is 10m. The thickness of the first and the second units is 4 m and 6 m, respectively. A constant recharge rate of 8×10^{-9} m/s is applied to the aquifer.

A contaminated area lies in the first unit next to the west boundary. The task is to isolate the contaminated area using a fully penetrating pumping well screened between 0 and 3 m and located next to the eastern boundary.

A numerical model has to be developed for this site to calculate the required pumping rate of the well. The pumping rate must be high enough so that the contaminated area lies within the capture zone of the pumping well.

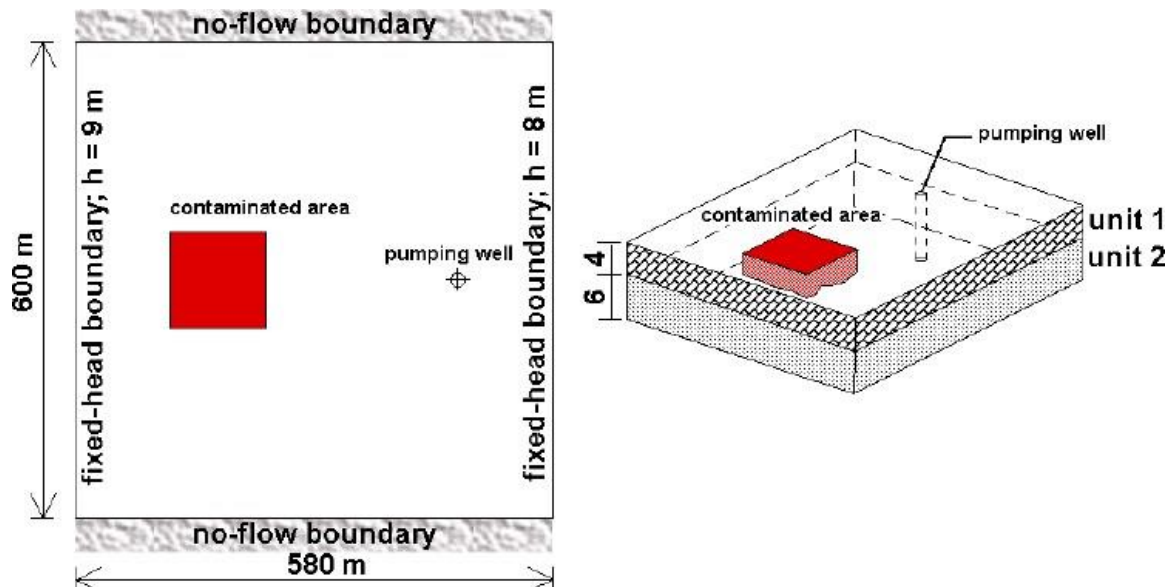


Figure 1. Fate of contaminant prediction

I. Flow simulation

A. Creating a new model and a new grid

- 1) Open ModelMuse. 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 **anew project** and so we will create a new MODFLOW project. The first screen is not important and can be used to add details on the project.
- 2) In the second screen, **create the grid** with the extent corresponding to your problem definition as illustrated in Figure 2. We will use a relatively coarse model with 30 rows and columns, all 20 m wide (so a model of 600 x 600 m in total) and an appropriate number of layers or hydrogeological units (2 in this case, the two aquifer units). Note that a layer can be later subdivided in several sub-layers, so what is important is to define the correct number of hydrogeological units. You will be able to change the grid later. Specify the elevation of the model top and of the boundaries between layers, this can be adjusted later as well. Note that the grid can be modified at any moment as all the properties are set using objects. Click on [Finish](#).

Initial Grid

MODFLOW 6 MODFLOW Version

Specify initial grid (optional)

30 Number of columns 20 Column width

30 Number of rows 20 Row width

2 Number of layers

Grid origin: Upper left corner

0 X 0 Grid angle (degrees)

0 Y Vertical exaggeration

0 Z

Layer group name	Bottom elevation
Model_Top	10
Unit 1	6
Unit 2	0

? Help No grid Finish →

Figure 2. Grid extent

- 3) Now that the model is created, save it so that you can recover your work at any time (it is suggested to **save your work regularly** anyway). [File](#) → [Save](#) → select the folder where to save the results and give a name to your model (for example Exo_1.gpt).
- 4) Define the **units** of the model. Note that you should **be consistent** and always define your property with the according units (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](#).

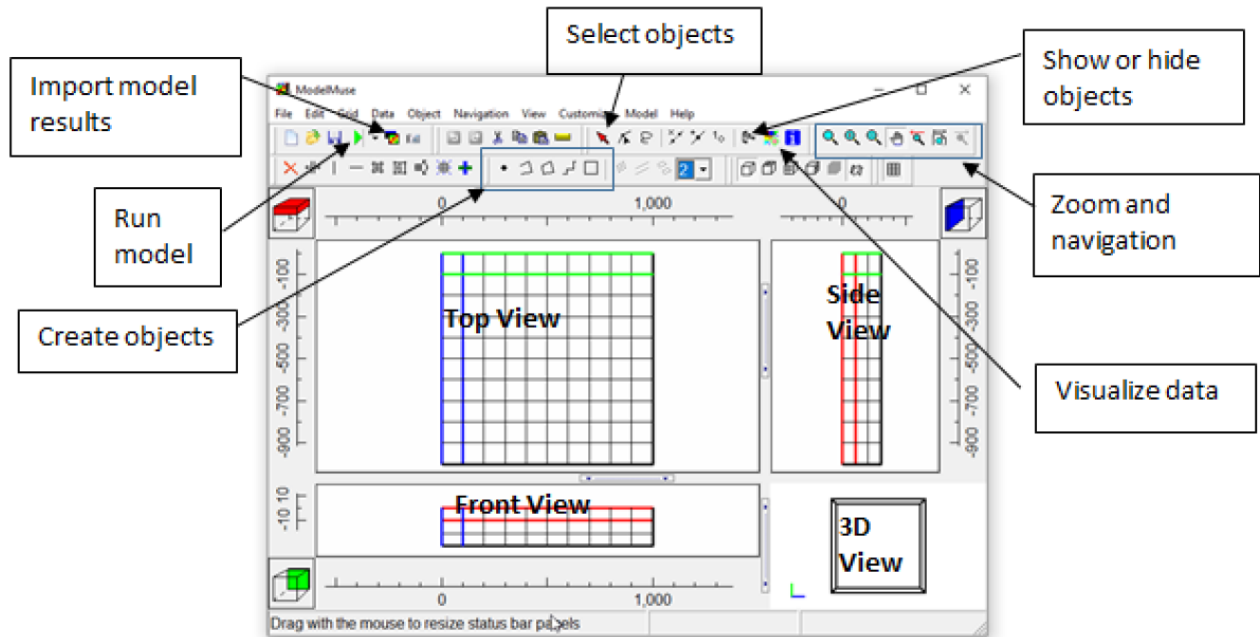


Figure 3. The ModelMuse main screen

B. Specify the parameters of the simulations.

To assess the behavior of the contaminant and estimate the required pumping rate, we have to simulate a steady-state pumping in the well. Transport will induce change of concentration with time and thus require a time component and we will simulate a period of 3 years (94 608 000 seconds). We use seconds to be consistent with our units.

- 1) Select **Model** → **MODFLOW Time** → The first stress period start at -1 and finish at 0. You can modify it to let it start at 0 and continue for **9.4608E+07 s**. Make sure the simulation type is steady-state and the unit is second. At this stage, you can use a single time step (remember that in steady-state, there is no variation with time), so set the length of the first step to **9.4608E+07 s**.

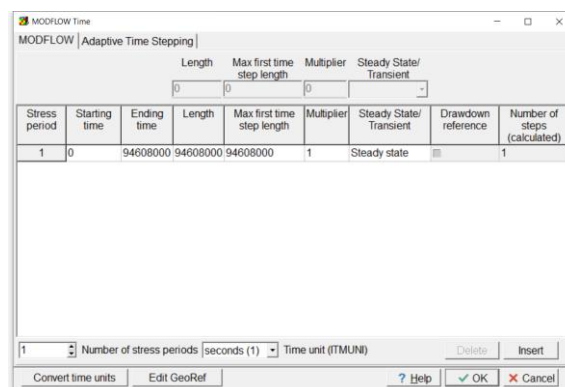


Figure 4. The time setting

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

Data → Edit Data sets → Expand “Required” and “Hydrology” → Select “Modflow_Initial-Head”. We will use an initial value of 8 m everywhere in the model → Enter 8 in “Edit Formula” with the Edit button (Figure 5).

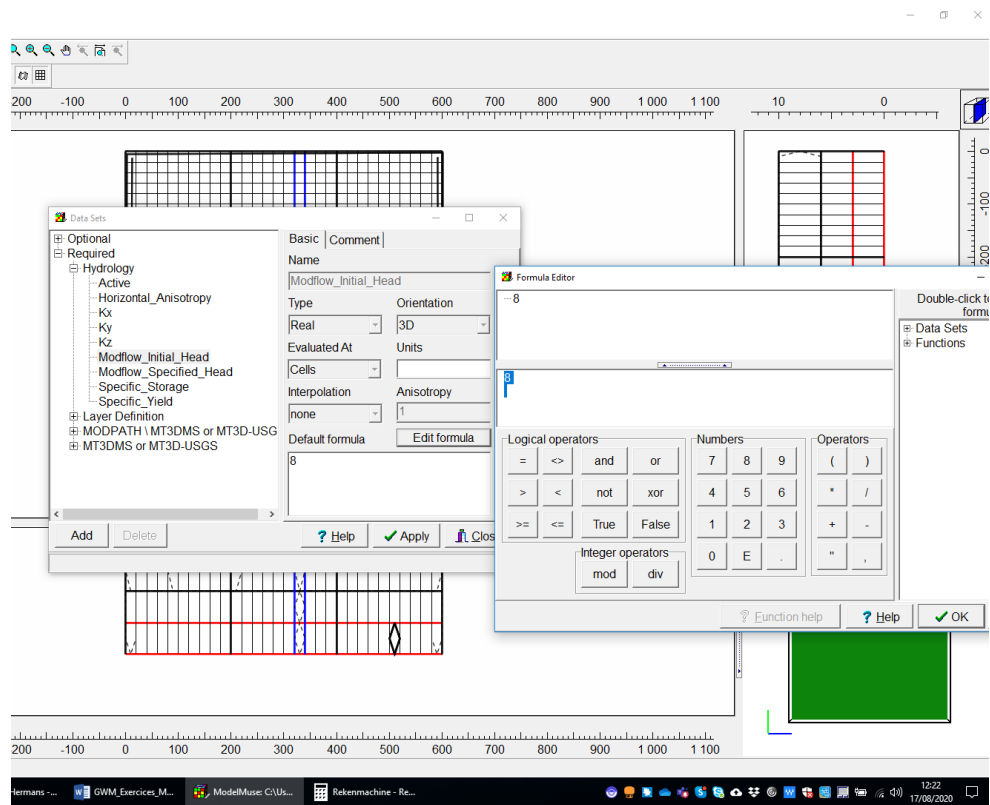


Figure 5. Modflow_Initial- Head

C. Edit the grid

- 1) You can subdivide the hydrogeological unit in several layers. For example, you can divide Unit 2 in two layers so that it accounts for the location of the screen interval between 0 and 3 m. [Modflow](#) → [Modflow Layer Groups](#) → [Unit 2](#) → [Discretization](#). In vertical discretization, choose 2 and click OK, the default is uniform spacing. Your model now contains 2 aquifer units but three layers. You can check this in the front and side view of the grid (Figure 6).

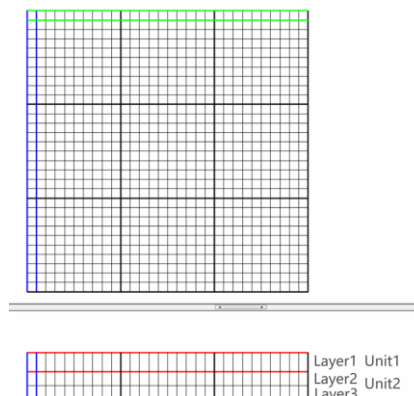


Figure 6. The Grid of Units

- 2) If you want to modify the geometry of the grid layers: [Data](#) → [Edit Data Set](#) → [Expand "Required|Layer definition"](#). Here you can modify the elevation of the Model Top, or the aquifer top and bottom. Note that it is not necessary to define constant value, it can be defined from interpolation or using mathematical formula (for example if the limit is not horizontal).

D. Change the parameters of the layers

- 1) Define the **aquifer units and type**. Choose which type of aquifer must be simulated. In MODFLOW 6, modelers specify individual cells as being confined or unconfined using the Cell_Type data set.
 - **Create an object** that covers the entire model: [Object](#) → [Create](#) → [Rectangle](#) (double-click to finish drawing). **Change the name** of the object to for example "Unit 1" and make sure the box "set values of enclosed cells is selected". Also make sure you **apply the object to unit 1**: adjust the number of Z formulas and the values (elevation) accordingly. Here we want to specify the top and bottom of the cells to which we want to apply the object so we need 2 Z-formulas, the higher one will correspond to the top and the lower one to the bottom. (don't close it yet)

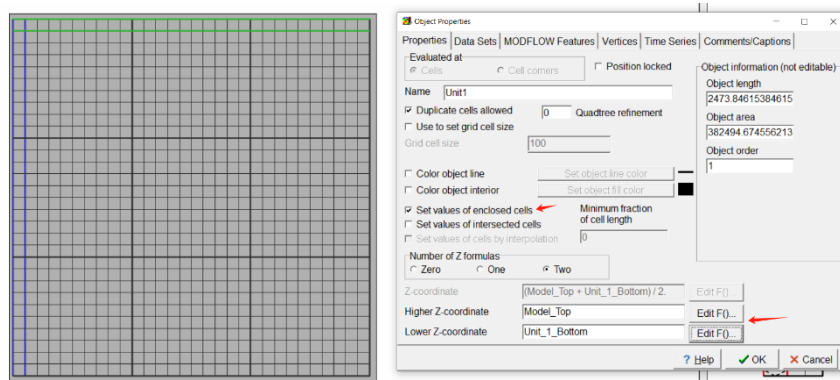


Figure 7. Create Unit1

(Tip: you can specify the elevation value or you can also find the Z-coordinates if you click [Edit F\(\)](#) → [Data Sets](#) → [Required](#) → [Layer Definition](#))).

- Now we still have to **change the Cell_Type feature of the object**. In the object dialog box: [Data Sets](#) pane → [Required](#) → [Hydrogeology](#) → [Cell_type](#). In this case Unit 1 will be unconfined (the water level can drop below the top of the layer so an unsaturated zone can be present). The cell (saturated) thickness will change, therefore we have to specify a value larger than 0 (such as 1).

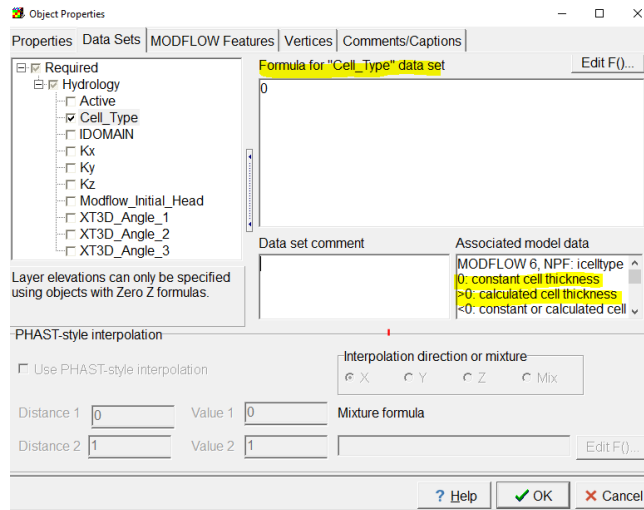


Figure 8: modflow features in the object dialog box showing where you can change the cell-type

Tip: if you closed the object you can open it again by double-clicking it in the show or hide object dialog box.

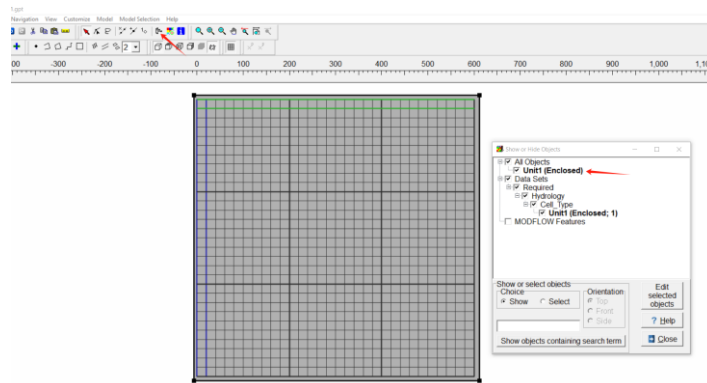


Figure 9. How to open the show/hide object tab

! Follow the **same workflow for unit 2(cell type=0)**. The Middle aquifer is Unit 2.

- 2) Use the **data visualization** dialog box to color the grid to check whether your object had the desired effect. When the cursor is placed over a cell the value will be shown at the bottom of the modelmouse main screen.

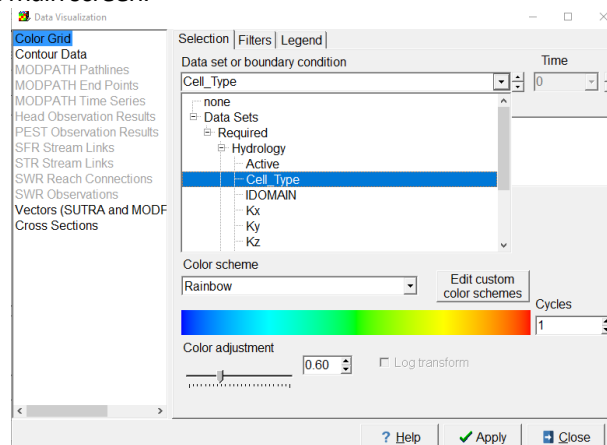


Figure 10. Data visualization tab

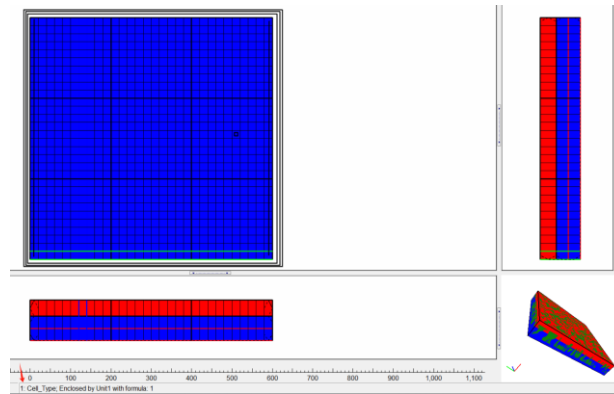


Figure 11. Data visualization of cell type

- 3) We now have to specify the **hydraulic conductivity** of the different layers. The default value in the model is 0.0001 m/s. Unit 2 (Layers 2 and 3) should have a value of 0.0005 m/s. So let's change the default value to 0.0005.
 - [Data](#) → [Edit Data sets](#) → [Required](#) → [Hydrology](#) → [Kx](#) . Change the **default value** (edit formula) to 0.0005.
 - To **change the hydraulic conductivity for specific layers/locations** you have to create objects. For layer 1, we can re-use the object of Unit 1 which was defined in the first layer. You can use the Object list to select it. When the window opens, go to the tab "[Data Sets](#)". Opens the "[Hydrology](#)" menu and edit the value for Kx for this object to 0.0001. You could also create new objects to set the properties if you want to define more complex geometries.
 - Using the Data Visualization tool, check that the distribution of Kx follows what you expect.
 - By default, the vertical hydraulic conductivity is 1/10 of the horizontal hydraulic conductivity and there is no horizontal anisotropy (check in [Data](#) → [Edit Data sets](#) the default formula for Ky and Kz). We can keep this like that. Otherwise, you would have to change the Ky and Kz property.

E. Setting boundary conditions

Modflow has a variety of packages that can be used to simulate different features in a model such as rivers, wells, recharge, etc.. **Activate the packages** you will need for this exercise by checking the boxes. [Model](#) → [Modflow Packages and Programs](#) → [Boundary conditions](#) → [activate the desired package](#). In this case, you want to activate the "specified head [CHD](#) package", the "specified flux [RCH](#) package" and the "[WEL](#) well package".

1) Set-up the boundaries.

By default, cells at the side and bottom of the model are set as zero-flux boundary condition (no-flow). This is OK for the North and South boundaries. For the **West and East boundaries**, we need instead to specify a fixed hydraulic head because we want to establish a hydraulic gradient.

- **Create an object for each boundary.** [Object](#) → [Create](#) → [Polyline](#) → [draw a line on the West boundary \(for the last point, double-click to finish the drawing\)](#). In the window, change the name of the boundary to for example "West_boundary", select the box "set values in intersected cells" (this make sure the intersected cells will be defined by this object) and make sure you apply the boundary condition to all layers (Higher Z-

coordinate= Model_Top, Lower Z-coordinate = Unit2_Bottom).

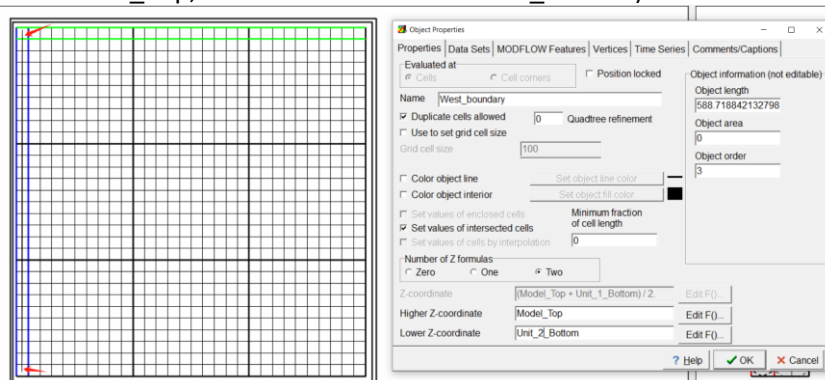


Figure 12. Create boundary conditions

- In the Modflow features tab of the object you can specify the hydraulic head (Click on CHD and specify the starting and ending head of 9 m, choose the same start and end time as you specified for the stress period in the time dialog box). The boundary conditions can be different according to stress periods.

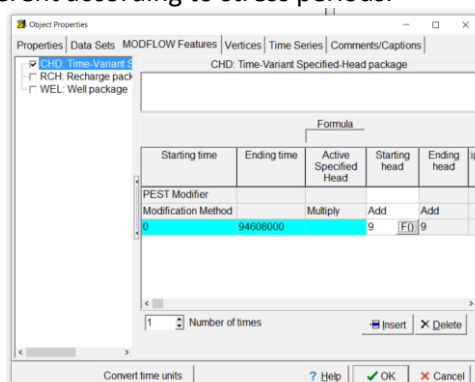


Figure 13. Specify the hydraulic head

- Repeat the same procedure for the East Boundary, (head is 8 m!).

2) Visualize the CHD boundaries to check if your objects have the desired effect.

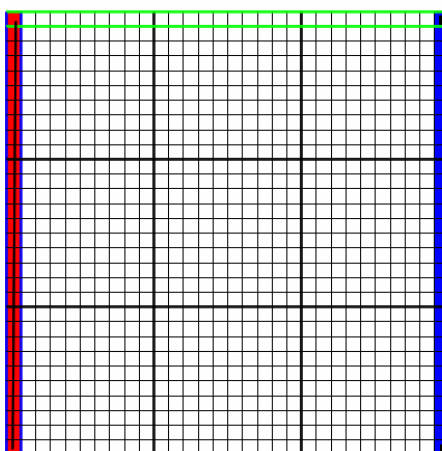


Figure 14. Boundary conditions

3) Set-up the recharge.

The recharge is uniformly distributed on the top of the model.

Create a **new object** for the recharge **Object** → **Create** → **Polygon** → **Draw a polygon**


encompassing the whole model (for the last point, double-click to finish the drawing). In the window, name the object “Recharge”, check the box “Set values of enclosed cells”, this will ensure that all the cells within the polygon will be defined by the object, and select the first layer using the Z formulas, the recharge is by default applied to the top layers (Higher Z-coordinate = Model_Top, Lower Z-coordinate = Unit1_Bottom). In the tab MODFLOW features select the RCH package and specify the starting and ending times and the recharge rate of $8\text{E-}9$ m/s.

4) Set-up the well.

The well will cross the three layers, but the **screen is located in the third layer**, so the pumping rate will be specified in the third layer. We will start with a pumping rate of -0.006 m³/s. It will later be adapted to make sure all the contamination can be captured.

- **Create a new point object.** Object → Create → Point → Select the cell where the well is located (**x = 510 m, y = -290 m**). You can adjust the coordinates in the tab “Vertices” of the object. The third layer should be selected through the Z-formulas layers (Higher Z-coordinate = 3, Lower Z-coordinate = 0). In **Modflow features**, specify the starting and end time and a pumping rate at -0.006 m³/s (the negative sign means that water is extracted from the model). Select “Direct” as the method for pumping rate interpretation.

F. Perform flow simulation

The model is now ready to run. Save your model, then click on the “Play button” in the menu bar 

- 1) **Models → Modflow → Run.** A dialog box appears. Click OK to run the simulation. Modflow creates the input files and launches the simulation.
- 2) When prompted, **save the model results.**
- 3) If Modflow runs correctly, you should see the following screen with a green smiley face :). In case something went wrong during the simulation the monitor and listing tabs contain useful information.

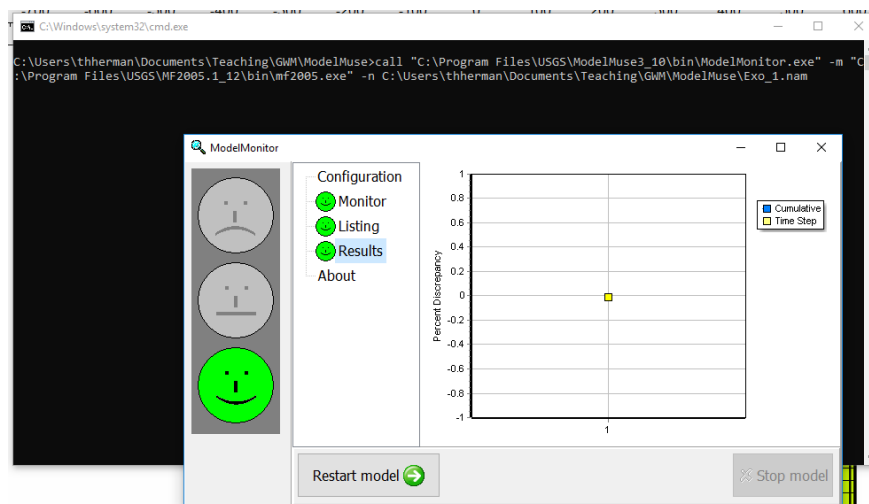


Figure 15. Model monitor

- 4) When closing this window, a file “*.lst” opens. It contains a summary of the simulation. At the end of this file, you can see the water budget of the simulation. It summarizes how much water goes in and out of the model. No water should be created (mass

conservation principle), so the budget should be as close to zero as possible. Since the simulation is not transient, the storage is 0. Water is entering from the west boundary (constant head) and recharge, and is going out at the eastern boundary (constant head) and the well. The discrepancy between the two is 0.01%, which is acceptable. If the error is larger, it might be necessary to change the solver parameters (any error is coming from the numerical approximation of the problem).


-----				-----			
IN:				IN:			
---				---			
STORAGE =	0.0000	STORAGE =	0.0000				
CONSTANT HEAD =	447860.8125	CONSTANT HEAD =	4.7306E-03				
WELLS =	0.0000	WELLS =	0.0000				
RECHARGE =	254480.4844	RECHARGE =	2.6880E-03				
TOTAL IN =	702341.3125	TOTAL IN =	7.4186E-03				
OUT:				OUT:			
---				---			
STORAGE =	0.0000	STORAGE =	0.0000				
CONSTANT HEAD =	134400.7500	CONSTANT HEAD =	1.4196E-03				
WELLS =	568036.8125	WELLS =	6.0000E-03				
RECHARGE =	0.0000	RECHARGE =	0.0000				
TOTAL OUT =	702437.5625	TOTAL OUT =	7.4196E-03				
IN - OUT =	-96.2500	IN - OUT =	-1.0165E-06				
PERCENT DISCREPANCY =	-0.01	PERCENT DISCREPANCY =	-0.01				

TIME SUMMARY AT END OF TIME STEP	1 IN STRESS PERIOD	1
SECONDS MINUTES	HOURS DAYS	YEARS
-----	-----	-----
TIME STEP LENGTH 9.46728E+07 1.57788E+06	26298. 1095.8	3.0000
STRESS PERIOD TIME 9.46728E+07 1.57788E+06	26298. 1095.8	3.0000
TOTAL TIME 9.46728E+07 1.57788E+06	26298. 1095.8	3.0000

run end date and time (yyyy/mm/dd hh:mm:ss): 2020/08/10 15:36:58
lapsed run time: 0.017 Seconds

Figure 16. Mass conservation

- 5) Import the results in ModelMuse. [File](#) → [Import](#) → [Model results](#) → [Select the file with extension "*.bhd"](#).
- 6) Display the results. It should be displayed automatically. You can see the larger drawdown around the well. Otherwise, use the tool Data Visualization. There you can also change visualization option. You can switch from Layer 1 to the other layer using the small box at

the top left corner of the graphical window. 

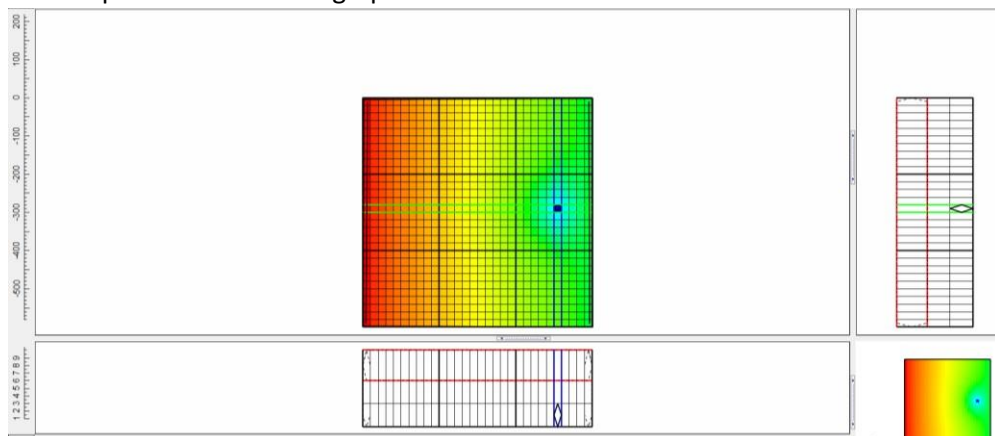


Figure 17. Flow simulation result.

G. Draw Pathlines

Pathlines represent the trajectories followed by water particle and pollutants through advection. This gives very important information on the flow path, the origin and the fate of dissolved species in groundwater, without the need to solve the full transport equations. Modflow has a package that solves pathlines through particle tracking (MODPATH). We will estimate the capture zone of the well

by backtracking the particles, i.e. we are going to simulate where the particle arriving in the well are coming from.

- 1) Activate MODPATH. [Model](#) → [Modflow Packages and program](#) → [Select Post processors](#) → [MODPATH](#). Select backward direction. In backward mode, Modpath has a time axis reversed compared to Modflow. It is therefore interesting to set the reference time at the end of the simulation period (for example 94 608 000 seconds). Choose Pathlines as the simulation method. In the Version 6 & 7 option tab, you can select when to end the tracking. You can choose at termination point (meaning when particles are going to go out of the model). This can happen after the end of the simulation period if the model is steady-state.
- 2) For advective transport, the effective porosity will influence the actual flow velocity, although it has no influence on the flow solution. We thus have to set a value. [Data](#) → [Edit Data Sets](#). Under the [MODPATH](#) tab that now appears, you can select [porosity](#). You can keep the default value of 0.25.
- 3) Now we have to set the particles. Open the object corresponding to the well. You can use the icon to show or hide object to find the list of objects you created. You can find the well under [Modflow features](#) → [WEL package](#). Double click on the well you created and choose [Model Features](#) → [MODPATH](#). Here you can set particles around the well. You can set them as shown on Figure 18 or test other geometries.

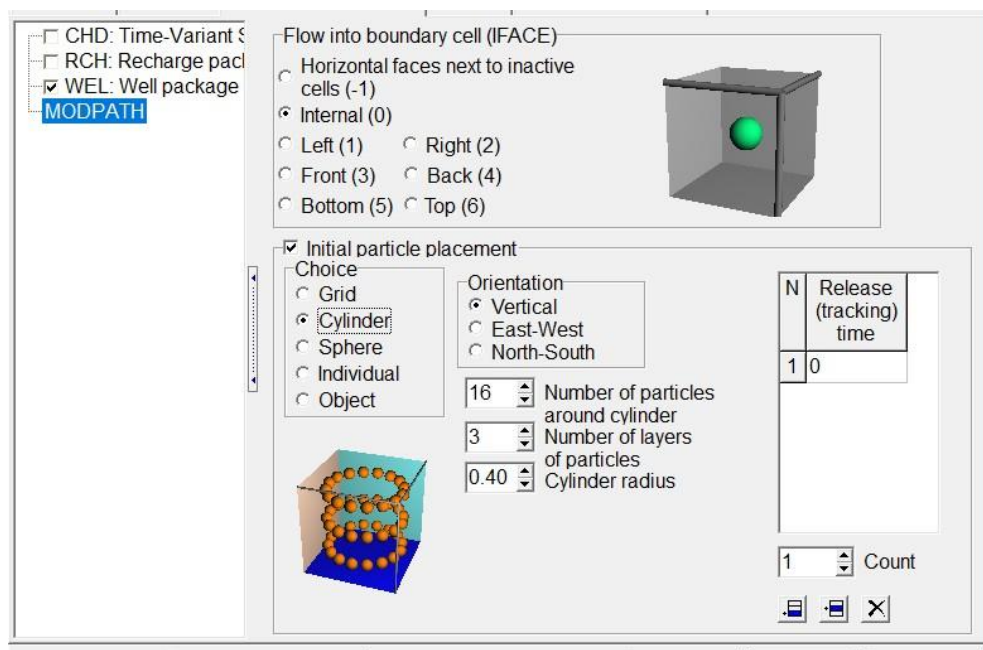


Figure 18. Setting particles for backtracking.

- 4) 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 ([File](#) → [Export](#) → [Modpath](#)) as the flow solution is not affected.
- 5) To visualize the results, [Data](#) → [Data Visualization](#) → [MODPATH pathlines](#) → [load the file created during simulations \(*.path\)](#). It will show you the pathlines, the color being

proportional to the time. Since the particles were released in layer 3, choose that layer for better visualization.

You can now adapt the pumping rate so that it is just large enough to recover the pollution coming from the contaminated zone (see Figure 19).

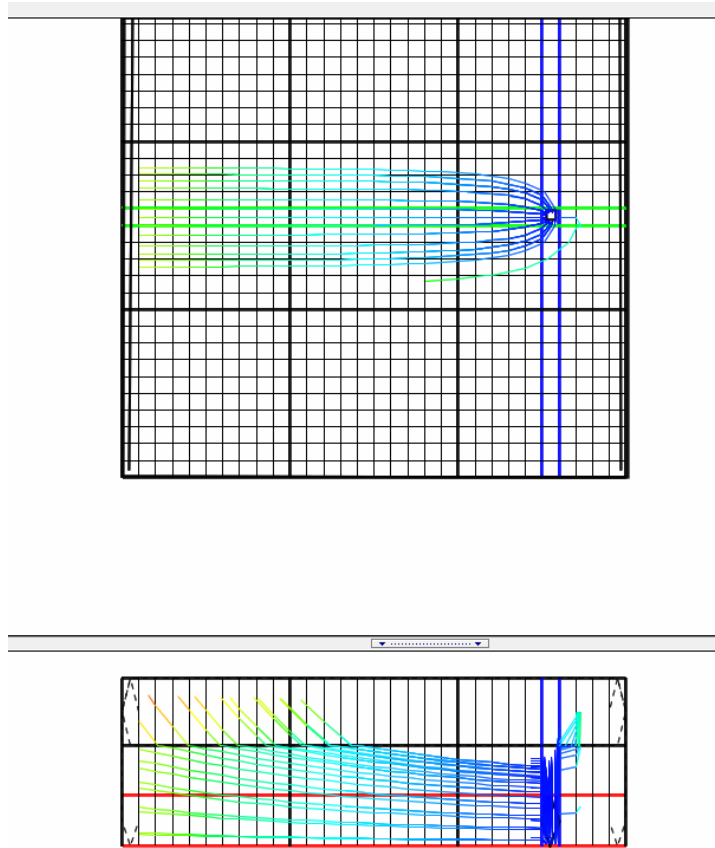


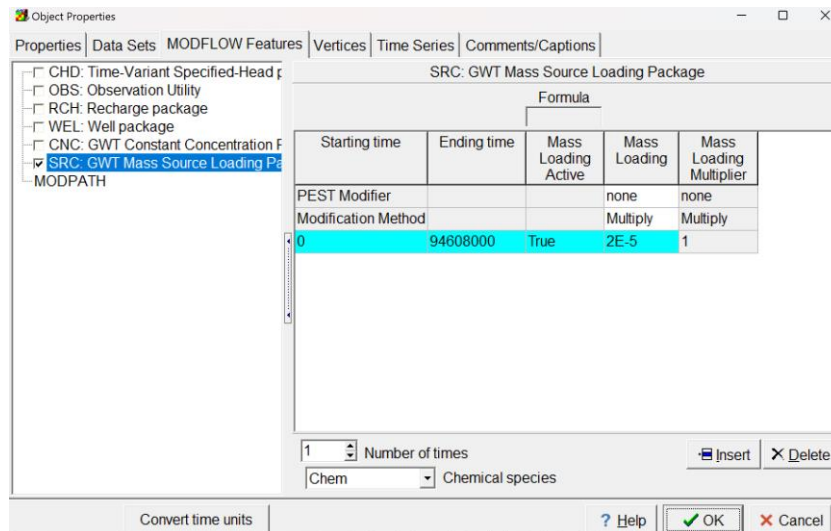
Figure 19. Capture zone at a pumping rate sufficient to recover the pollutant.

II. Solute transport

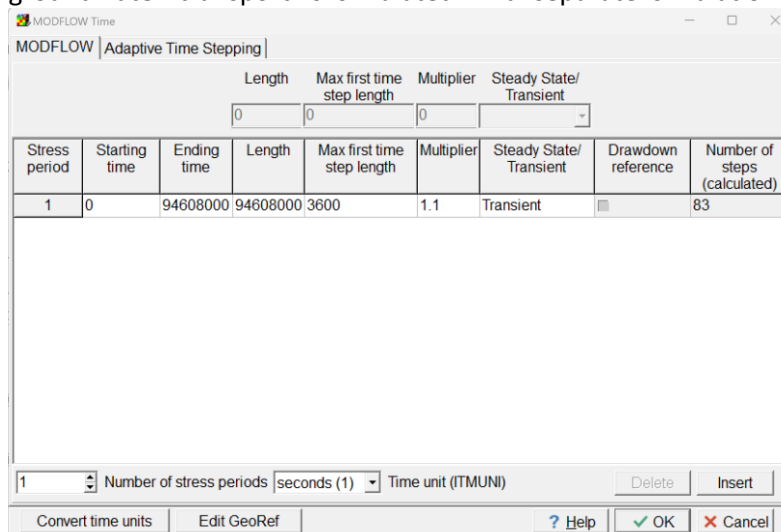
H. Setting transport parameters

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.

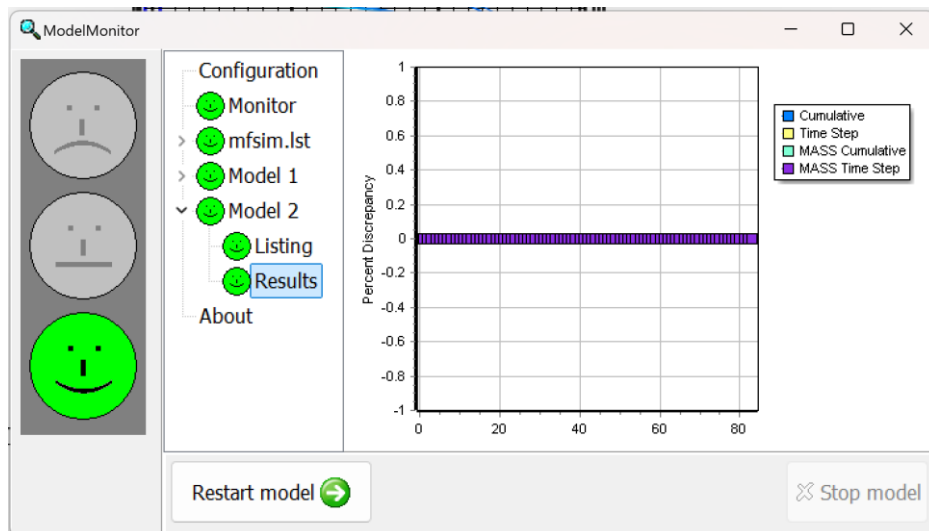
- 1) Activate GWT. [Model](#) → [MODFLOW Packages and programs](#) → [activate all the necessary packages](#) (basic transport package, advection and dispersion packages, sink and sources mixing packages solver package, constant concentration/mass source loading package, etc.). Pay attention to the options for the different packages. For example, it is here that you can choose which method is going to be used to solve the advection-dispersion equation (see theory). You can also specify the name of the chemical species.
- 2) If you go to [Data](#) → [Edit data sets](#) → [MT3DMS, MT3D-USGS, or GWT](#) you will see that new parameters are available. The most important are the longitudinal dispersivity and the (effective) porosity. The latter was already defined for Modpath. You can change the default value of the model and the specific values of your lithology objects.
- 3) 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.
- 4) We will monitor the concentration of a contaminant in the subsurface using one observation borehole with a screen in the three layers. We can create it using an object crossing all three layers. [Object](#) → [Create](#) → [Point](#). Choose a location which you think is interesting. Also activate the OBS (observation utility package) and select it in the object dialog box and check the concentration observation in [Modflow Features|OBS](#). This will ensure that a file is created with the concentration at the different time steps (easiest way to export the data to another program such as Excel).
- 5) We specify a contaminant input through recharge. First create an object in the corresponding zone. [Object](#) → [Create object](#) → [Polygone](#) → Create a 7 x 7 square in the first layer, with its upper left corner at **row 11/column 6**. The contaminant will enter through recharge. Specify a mass loading of 0.00002 g/s (mass rate of contaminant), therefore use the appropriate SRC package.



- 6) Change the Time control for Modflow and GWT. **Model → MODFLOW Time → Choose Transient simulation**. Switch the simulation type to transient and choose a first step length of 3600 s with multiplier of 1.1. Then adapt the parameters for transport simulation (the end period should be the same as for flow). Note that in the Time pane for modflow 6 there is also a tab for adaptive time stepping. It can be used to optimize the simulation time or to make the simulation more accurate if necessary. It should not be used if groundwater transport is simulated in a separate simulation from the flow model.



- 7) Run the transport (and flow) simulation. It might take a while, transport simulation requires smaller time steps and more computation. Similar to flow, the document opening at the end can be used to check the mass conservation (go to the end of the file).



I. Check transport results

- 1) [File](#) → [Import](#) → [Model Results](#) → [Select the *conc file](#). Visualize the concentration in the aquifer. You can choose at which output time to observe the results.

Check the file *.ob_gw_out_head (for instance in Notepad/excel). It contains the concentration at the observation wells for every simulation time.

- 2) You can draw a concentration curve at the wells in Excel (or using Python)

Now you can play with the model, change the parameters (K_x , dispersivity), the pumping rate, the boundary conditions and see how it changes the output of the model.