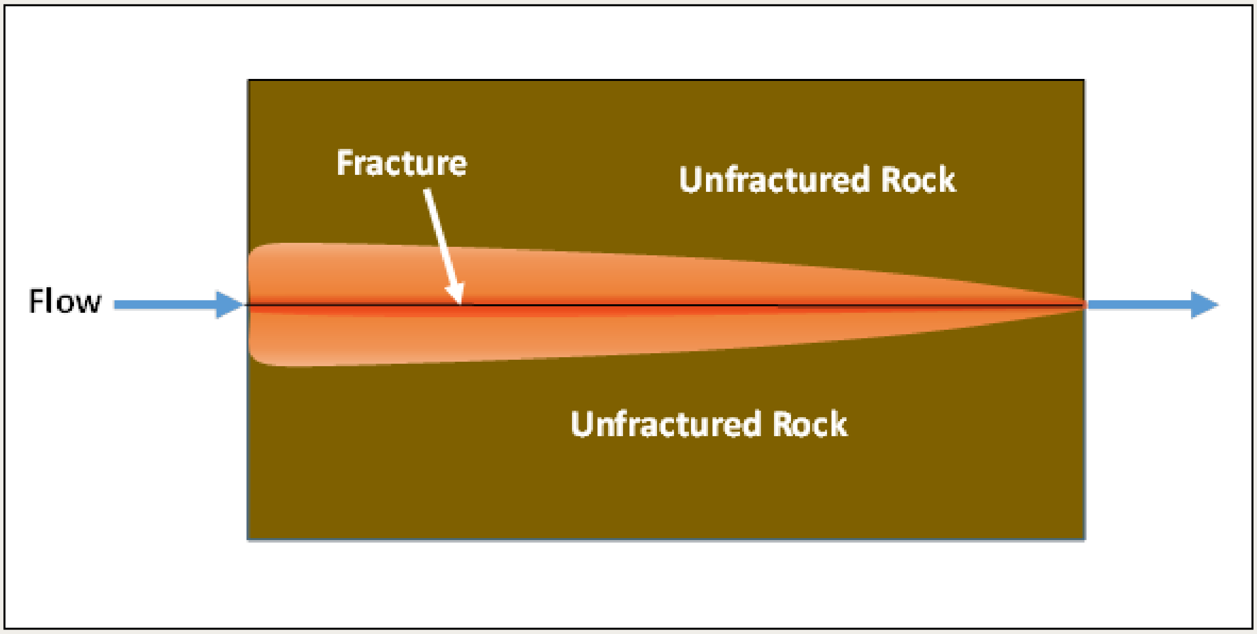
GMS 10.8 Tutorial

MODFLOW 6 – MDT Discrete Fracture

Use the Matrix Diffusion Transport package (MDT) in GMS to simulate diffusion from a fracture using a semi-analytic approximation



Objectives

Learn how to use the Matrix Diffusion Transport package (MDT) with MODFLOW 6 to simulate diffusion from a single fracture.

Prerequisite Tutorials

- Getting Started
- MODFLOW 6 – Conceptual Model Approach
- MODFLOW 6 – Grid Transport

Required Components

- GMS Core
- MODFLOW Interface

Time

- 20–30 minutes

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1 Introduction

The Matrix Diffusion Transport package (MDT) works with MODFLOW 6. The MDT package allows existing flow and chemical transport models to be upgraded to include a full accounting of matrix diffusion effects. The MDT package is based on the semi-analytic matrix diffusion method implemented in the REMChlor-MD model[1, 2, 3]. The development of this simulation capability has been supported by the Department of Defense Environmental Security Technology Certification Program (ESTCP) and it represents a collaborative effort between Clemson University, GSI Environmental, and Aquaveo.

The MDT matrix diffusion method is conceptually similar to dual porosity methods, where the volume of each element is divided into "mobile" and "immobile" fractions. Solute transport occurs by advection, and dispersion in the mobile fraction, but only by diffusion in the immobile fraction. With the MDT package, the concentration profile in the immobile fraction is approximated using a dynamic function that expresses the concentration as a function of distance from the mobile/immobile interface. This function is recomputed at each time step in each element using the current and previous concentrations in the mobile fraction, along with the integral of the concentration profile in the immobile fraction. The mass transfer to or from the mobile/immobile fractions is then computed as a linear concentration-dependent source term.

This tutorial demonstrates how the MDT package can be used with a MODFLOW 6 simulation to simulate diffusion in a single fracture. This example is based on a benchmarking problem that was developed with REMChlor-MD. For a more detailed description of the semi-analytic method used in the MDT package, please refer to the REMChlor-MD user's guide[1] and related journal papers[2, 3].

The problems in this tutorial consist of a single layer, one-dimensional unstructured grid (UGrid) with a MODFLOW 6 simulation. The head values have been set for the grid.

For this example, only the fracture itself is discretized, and the semi-analytic method is used to compute the matrix diffusion from the fracture into the adjacent rock matrix. This example is based on a test problem presented by Falta and Wang[2] where water containing tritium is injected into a 100µm fracture at a pore velocity of 0.1 m/day. The tritium concentration is maintained at the upstream end of the grid for a period of 30

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[1] Farhat, S.K., C.J. Newell, R.W. Falta, and K. Lynch, 2018. REMChlor-MD User's Manual, developed for the Environmental Security Technology Certification Program (ESTCP) by Clemson University, Clemson, SC and GSI Environmental Inc., Houston, TX, https://www.serdp-estcp.org/Program-Areas/Environmental-Restoration/Contaminated-Groundwater/Persistent-Contamination/ER-201426

[2] Falta, R.W., and W. Wang, 2017, A semi-analytical method for simulating matrix diffusion in numerical transport models, J*ournal of Contaminant Hydrology, V. 197, p. 39-49.*

[3] Muskus, N., and R.W. Falta, 2018, Semi-analytical method for matrix diffusion in heterogeneous and fractured systems with parent-daughter reactions, *Journal of Contaminant Hydrology*, *V. 218, p. 94-109.*

years, followed by injection of clean water. Additional model parameters are given in Table 1.

Table 1. Parameters used in the fractured rock matrix diffusion comparison

Parameter	**Fracture**	**Matrix**
Fracture aperture, µm	100	
Porosity, ϕ	1.0	0.01
Tortuosity, τ	1.0	0.1
Retardation factor, R	1.0	1.0
Darcy velocity, v_x (m/d)	0.1	0
Diffusion coefficient of tritium, D (m^2/s)	1.6E-9	1.6E-9
tritium decay rate (1/yr)	0.0561	0.0561
Loading period, t_1, (years)	30	

This tutorial will demonstrate the following topics:

1. Opening an existing MODFLOW 6 simulation.
2. Activating the MDT package.
3. Running the simulation and examining the results.

2 Opening a MODFLOW 6 Simulation

Start with opening a MODFLOW 6 model:

1. If necessary, launch GMS.
2. If GMS is already running, select the *File* | **New** command to ensure that the program settings are restored to their default state.

Start with a previously created project.

4. Click **Open** to bring up the *Open* dialog.
5. Select “Project Files (*.gpr)” from the *Files of type* drop-down.
6. Browse to the *mf6_mdt_discrete* folder and select “start.gpr”.
7. Click **Open** to import the project and exit the *Open* dialog.

The project should be visible in the Graphics Window (Figure 1).

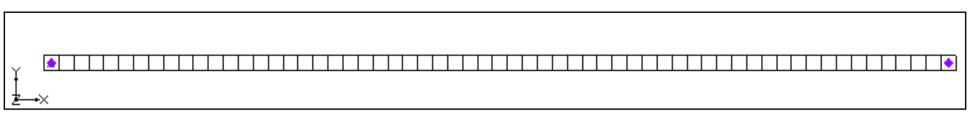

Figure 1 Initial project for the MODFLOW 6 model

A total of 61 elements are used in this 1D grid. These elements have dimensions of 1 m in the direction of flow (x-direction), 1 m perpendicular to the flow (y-direction), and 0.0001 m vertically (z-direction). The very small vertical dimension reflects the 100 µm fracture aperture.

The hydraulic head in the leftmost element is maintained at a constant head of 11 m using the CHD package, while the rightmost element is maintained at a head of 10 m. The horizontal hydraulic conductivity was set to a value of 2190 m/yr, resulting in a Darcy velocity of 36.5 m/yr or 0.1 m/d. Since the fracture porosity was set to 1 in the MST package, the pore velocity is equal to the Darcy velocity in this example.

Before continuing, save the project with a new name.

8. Select *File* | **Save As…** to bring up the *Save As* dialog.
9. Browse to the *Tutorials\MODFLOW 6\mf6_mdt_discrete* directory.
10. Enter "discrete_fracture.gpr" as the *File name*.
11. Select "Project Files (*.gpr)" from the *Save as type* drop-down.
12. Click **Save** to save the project file and close the *Save As* dialog.

3 Adding the MDT Package

The MODFLOW 6 simulation has been setup without the MDT package. Both a groundwater flow model and a groundwater transport model have been added. The MDT package can be added by doing the following:

1. Right-click on " trans" and select *New Package* | **MDT** to add the package.

Notice the " MDT" package is now shown in the Project Explorer under the groundwater transport model. Make certain the package is not locked before continuing.

2. In the Project Explorer, right-click on " model-mdt" and select **Unlock All**.

4 Defining the MDT Package

The MDT package can be defined during the process of setting up the GWT model or after the GWT model has been created as in this case. To define the MDT package, do the following:

1. Double-click on the " MDT" package to bring up the *Matrix Diffusion Transport (MDT) Package* dialog.
2. On the *MD_TYPE_FLAG* tab, set the *Constant* value to "4". This variable is a flag that tells the MDT package how matrix diffusion will be handled. Choosing a value of 4 tells the package to allow matrix diffusion from both the top and bottom of the element into an infinite media. This example uses this option because it is directly modeling only the fracture volume.
3. On the *MD_FRACTION* tab, set the *Constant* value to "0". This is the volume fraction of low permeability material in the element. Since this example is only modeling the fracture, the value is zero.

   Note: this convention is different from that used in REMChlor-MD and in the MODFLOW-USG MDT package where the MDT volume fraction is the fraction of high permeability material in the element.
4. On the *MD_POROSITY* tab, set the *Constant* value to "0.01". This is the porosity of the unfractured rock.
5. On the *BULK_DENSITY* tab, set the *Constant* value to "2.0". This is the dry bulk density of the rock, which is not used in this simulation of tritium transport.
6. On the *MD_DIFF_LENGTH* tab, set the *Constant* value to "1e-10". The characteristic diffusion length is used with other MD_TYPE_FLAG options, but is not needed for MD_TYPE_FLAG-4. Nonetheless, a small non-zero value has been added.

7. On the *MD_TORTUOSITY* tab, set the *Constant* value to "0.1". This is the tortuosity in the rock matrix
8. On the *MD_DIST_COEFF* tab, set the *Constant* value to "0.0". This is the adsorption distribution coefficient, which is not used in this example.
9. On the *MD_DECAY* tab, set the *Constant* value to "0.0561". This is the tritium decay rate, 1/yr.
10. On the *MD_DIFF_COEFF* tab, set the *Constant* value to "0.05046". This is the tritium molecular diffusion coefficient, m^2/yr.
11. Click **OK** to close the *Matrix Diffusion Transport (MDT) Package* dialog.

The MDT Package is now set up for the discrete fracture and ready for the simulation run.

5 Saving and Running the Simulation

Save and run the simulation by doing the following:

1. Right-click on " model-mdt" and select **Save Project, Simulation and Run** to start the *Simulation Run Queue*.
2. If it appears, click **OK** on the *Info* dialog to unload the previous solution.
3. Click **Load Solution** to import the solution files.
4. Click **Close** to exit the *Simulation Run Queue*.

6 Examining the Solution

Now examine the results of the MDT package being included in the transport model.

1. Switch to the **UGrid** module.
2. In the Project Explorer, select the " Concentration" dataset in the " trans" folder under the " model-mdt (MODFLOW 6)" folder.
3. Using the **Select Cells** tool, select cell 2 (the second cell on the left).
4. Click the **Plot Wizard** macro to open the *Plot Wizard* dialog.
5. Under *Plot Type*, select "Active Dataset Time Series".
6. Click **Finish** to close the *Plot Wizard* and generate the plot.

The generated plot should appear similar to Figure 2.

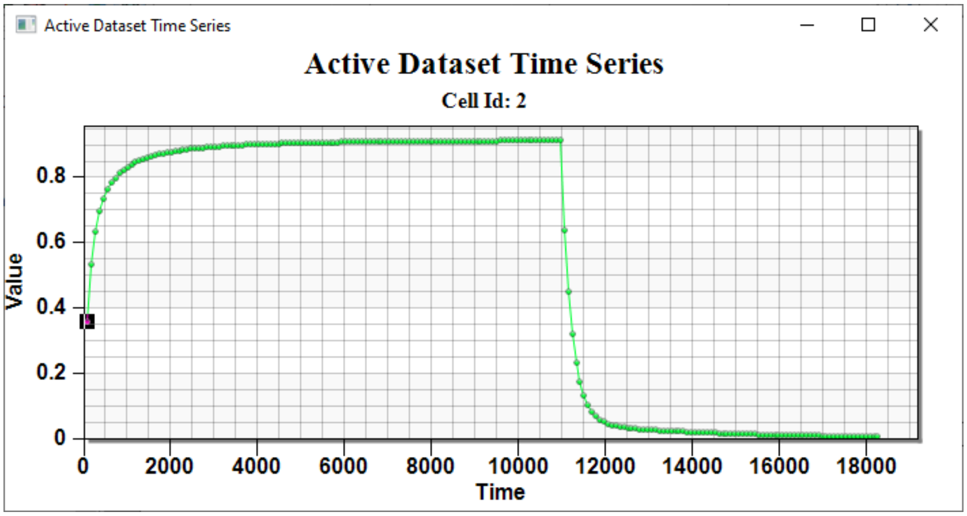

Figure 2 The active dataset time series plot

7 Conclusion

This concludes the "MODFLOW 6 – MDT Discrete Fracture" tutorial. The following topics were discussed and demonstrated:

- Adding the MDT Package to MODFLOW 6.
- Defining the MDT Package.
- Running MODFLOW 6.
- Reviewing the MODFLOW 6 solution.

