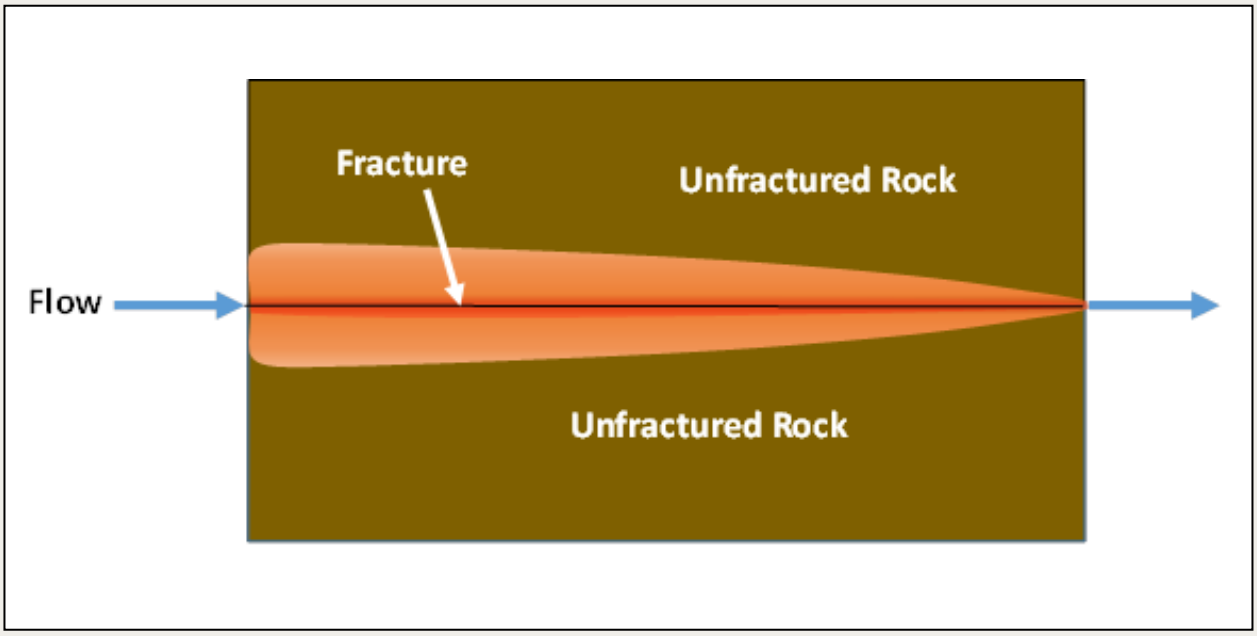
*GMS 10.8 Tutorial*

# *MODFLOW 6 – MDT Equivalent Porous*

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




## Objectives

Learn how to use the Matrix Diffusion Transport package (MDT) with MODFLOW 6 to simulate diffusion from a set of parallel fractures.

## Prerequisite Tutorials

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

## Required Components

- GMS Core
- MODFLOW Interface

## Time

- 20–30 minutes

AQUAVEO™

# 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 with collaboration 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 series of parallel fractures. 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.

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.

---

[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*

# 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_equivalent_porous* 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).

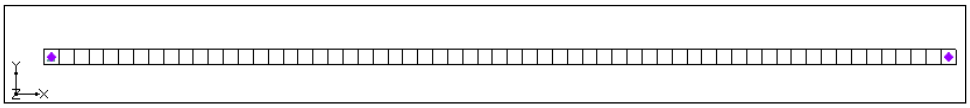


*Figure 1 Initial project for the MODFLOW 6 model*

This model has a single layer UGrid. Specified heads (CHD) have been set at each end. 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 1 m vertically (z-direction).

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.

A general simulation approach, which can be used for systems with multiple fractures, involves using an equivalent porous media approach. With this method, normal full-sized elements are used with the fractures embedded inside the elements. From a flow perspective, it is possible to calculate an equivalent porous media hydraulic conductivity that gives the same overall flow, averaged over the entire area (the Darcy velocity). Since the fractures occupy only a small fraction of the volume, the pore velocity in the fractures is much higher than the Darcy velocity of the entire rock mass.

The MDT package can simulate matrix diffusion in a system of embedded parallel fractures using the method described in Muskus and Falta[3]. In order to do this, it is necessary to generate a numerical grid with full-sized dimensions, and then specify the fracture characteristics, namely the fracture spacing and aperture. Then the volume fraction of high permeability material (the fractures) is equal to the fracture aperture divided by the fracture spacing. In REMChlor-MD and in the MODFLOW-USG MDT package, this is the VOLFRACMD variable. In the MODFLOW 6 MDT package, a different convention is used, and the volume fraction of the low permeability is specified as the MD_FRACTION variable, where MD_FRACTION = 1 – VOLFRACMD . The characteristic diffusion length used in the MDT package, MD_DIFF_LENGTH is equal to one-half of the fracture spacing.

This example of using the equivalent porous media approach is based on a test problem from Muskus and Falta[2] involving a system of parallel fractures with a fracture spacing of 0.5 m and fracture apertures of 100 µm.

With an equivalent porous media approach, the hydraulic conductivity value reflects the value averaged over the entire rock mass. Following the example in Muskus and Falta[3], the pore velocity in the fractures is 100 m/yr. The volume fraction of the fractures is 0.0001m/0.5m = 0.0002. Then the bulk Darcy velocity is 0.02 m/yr. With our previous

hydraulic gradient of 1/60, this Darcy velocity is achieved with a hydraulic conductivity (HK) of 1.2 m/yr.

Additional parameters used in this example are given in Table 1.

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

| **Parameter** | **Fracture** | **Matrix** |
|---|---|---|
| Fracture aperture, µm | 100 | |
| Porosity, $\phi$ | 1.0 | 0.1 |
| Tortuosity, $\tau$ | 1.0 | 0.1 |
| Retardation factor, $R$ | 1.0 | 2.0 |
| Pore velocity, (m/yr) | 100 | 0 |
| Diffusion coefficient, $D$ ($m^2$/s) | 1.0E-9 | 1.0E-9 |
| decay rate (1/yr) | 0.0 | 0.0 |
| Loading period, $t_1$, (years) | 50 | |

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_equivalent_porous* directory.
10. Enter "equivalent_porous.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_parallel" 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 "2". This variable is a flag that tells the MDT package how matrix diffusion will be handled. Choosing a value of 2 tells the package to allow matrix diffusion into embedded matrix blocks with a finite diffusion length. This example uses this option because it is using an equivalent porous media approach.

3. On the *MD_FRACTION* tab, set the *Constant* value to “0.9998”. This is the volume fraction of the low permeability material.

   ***Note***: that this definition is different from the *VOLFRACMD* variable that is used in REMChlor-MD and the MODFLOW USG MDT package. *MD_FRACTION = 1 – VOLFRACMD*.

4. On the *MD_POROSITY* tab, set the *Constant* value to “0.1”. 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 unfractured rock.
6. On the *MD_DIFF_LENGTH* tab, set the *Constant* value to “0.25”. This is the characteristic diffusion length, which is one-half of the fracture spacing.
7. On the *MD_TORTUOSITY* tab, set the *Constant* value to “0.1”.
8. On the *MD_DIST_COEFF* tab, set the *Constant* value to “0.05”. This is the rock/water distribution coefficient for the chemical. This value, combined with the bulk density of 2.0 and porosity of 0.1 gives a retardation factor of 2.
9. On the *MD_DECAY* tab, set the *Constant* value to “0.0”. The solute is not undergoing decay.
10. On the *MD_DIFF_COEFF* tab, set the *Constant* value to “0.03159”. This is the 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 parallel fracture system 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_parallel” 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_parallel (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.

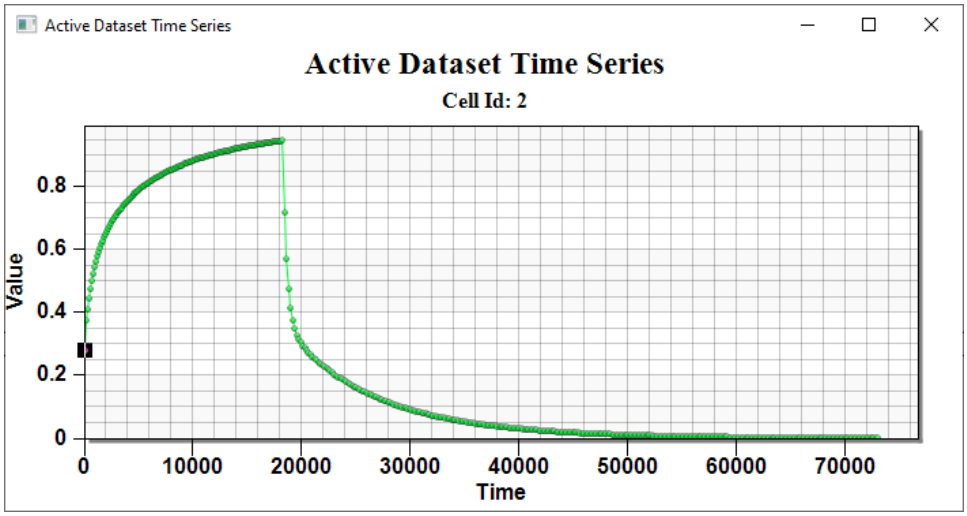



*Figure 2 The active dataset time series plot*

# 7 Conclusion

This concludes the “MODFLOW 6 – MDT Equivalent Porous” tutorial. The following topics were discussed and demonstrated:

- The MODFLOW 6 MDT package can be used to simulate matrix diffusion from multiple fractures in fractured porous materials.
- The MDT package allows for an equivalent porous media approach to be used for fractured systems where normal grid elements are used with embedded matrix diffusion occurring over a finite distance in the matrix material in each element.