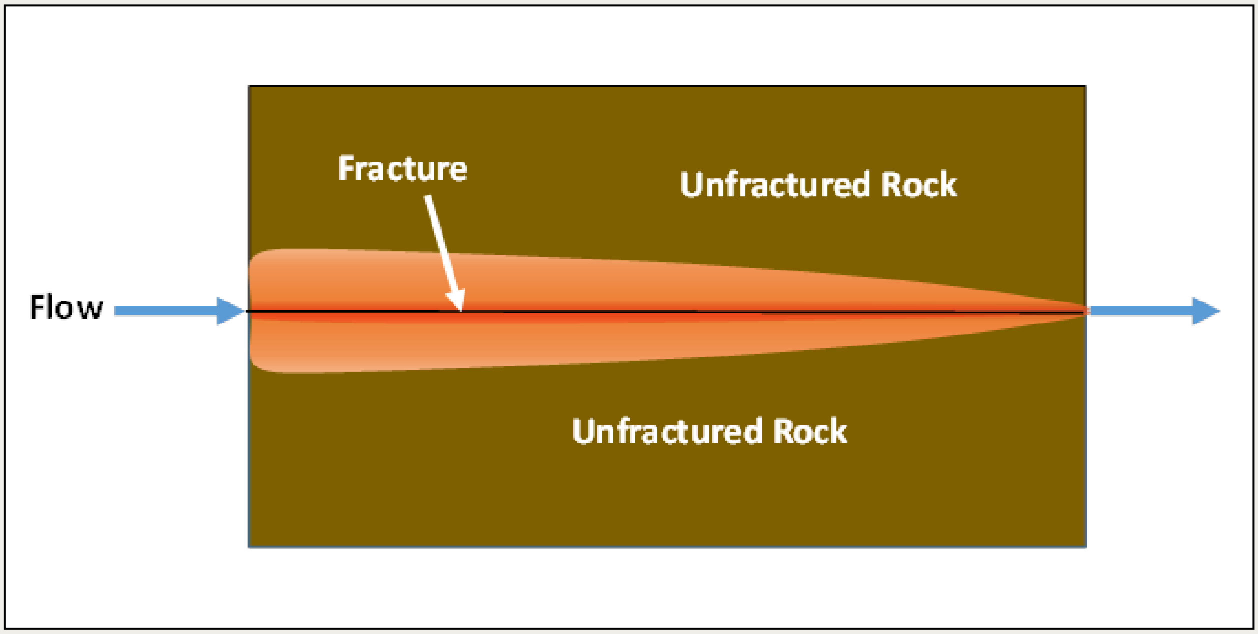
GMS 10.8 Tutorial

MODFLOW-USG Transport – MDT Equivalent Porous Media Approach

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



Objectives

Learn how to use the Matrix Diffusion Transport (MDT) package with MODFLOW-USG Transport to simulate diffusion from a single fracture or from a set of parallel fractures.

Prerequisite Tutorials

- MODFLOW-USG Transport

Required Components

- GMS Core
- MODFLOW-USG Transport

Time

- 15–30 minutes

1 Introduction

The Matrix Diffusion Transport package (MDT) works with MODFLOW-USG Transport. 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-USG Transport 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 input variables used in the MDT package are described in the MDT Process for MODFLOW-USG Transport User's Guide[4].

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

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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*

[4] Panday, S., R.W. Falta, S. Farhat, K. Pham, and A. Lemon, 2021, Matrix Diffusion Transport (MDT) Process for MODFLOW-USG Transport, https://www.gsienv.com/product/modflow-usg/

This tutorial will demonstrate the following topics:

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

2 Getting Started

Do the following to get started:

1. If necessary, launch GMS.
2. If GMS is already running, select *File* | **New** to ensure that the program settings are restored to their default state.
3. Click **Open** (or *File* | **Open…**) to bring up the *Open* dialog.
4. Browse to the data files for this tutorial and select “start.gpr”.
5. Click **Open** to import the file and close the *Open* dialog.

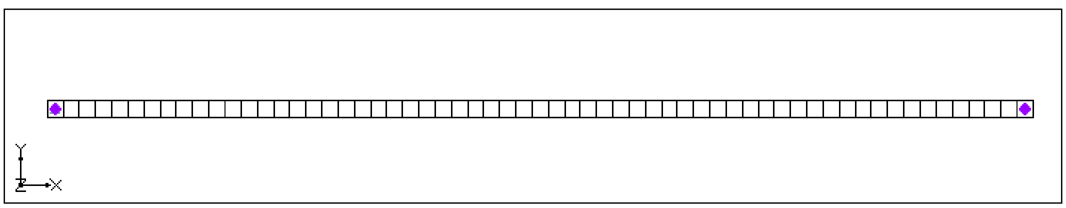

Figure 1 Imported MODFLOW-USG Transport model

The Graphics Window should appear as in Figure 1. 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.

The tracer (Species 1) is introduced at the upstream end of the grid using a transient concentration boundary (PCB package) with a value of 1 for 50 years, followed by a value of 0 for 150 more years.

A general modeling 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. This is the VOLFRACMD variable in the MDT package. The characteristic diffusion length used in the MDT package, DIFFLENMD 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 a 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 2.

Table 2. Parameters used in the fractured rock matrix diffusion simulation

Parameter	**Fracture**	**Matrix**
Fracture aperture, µm	100	
Porosity, ϕ	1.0	0.1
Tortuosity, τ	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.

6. Select *File* | **Save As…** to bring up the *Save As* dialog.
7. Enter “model-mdt_parallel.gpr” as the *File name*.
8. Select “Project Files (*.gpr)” from the *Save as type* drop-down.
9. Click **Save** to save the project file and close the *Save As* dialog.

3 Activating the MDT Package

With the flow model set up, the MDT package can now be activated and added to the MODFLOW simulation. To activate the MDT package:

1. Switch to the **UGrid** module.
2. Select *MODFLOW* | **Global Options…** to bring up the *MODFLOW Global/Basic Package* dialog.
3. Click **Packages…** to bring up the *MODFLOW Packages / Processes* dialog.
4. In the *Optional packages / processes* section, turn on *MDT – Matrix Diffusion Transport*.
5. Click **OK** to exit the *MODFLOW Packages / Processes* dialog.
6. Click **OK** to exit the *MODFLOW Global/Basic Package* dialog.

4 Defining the MDT Package

Now the new matrix diffusion package parameters can be entered. The retardation factor value of 2.0 in the matrix will be achieved by entering a bulk density value (RHOBMD) of 2.0 and a soil-water distribution coefficient (KDMD) value of 0.05.

1. Select *MODFLOW* | *Optional Packages* | **MDT – Matrix Diffusion Transport…** to bring up the *MDT Package* dialog.
2. In the list on the left, select *Aquifer Properties*.
3. Enter the following for the *Constant Value* column:
    a. *MDFLAG*: “2.0”. 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 in this example.
    b. *VOLFRACMD*: “0.0002”. This is the volume fraction of high permeability material in the element. In this case it is the fracture aperture divided by the fracture spacing.
    c. *PORMD*: “0.1”.
    d. *RHOBMD*: “2.0”.
    e. *DIFFLENMD*: “0.25”. The characteristic diffusion length is one-half of the fracture spacing
    f. *TORTMD*: “0.1”.
4. In the list on the left, select *Species Properties*.
5. Enter the following for the *Constant Value* column:
    a. *KDMD*: “0.05”.
    b. *DECAYMD*: “0”. No decay.
    c. *DIFFMD*: “0.03159”.
6. Click **OK** to close the *MDT Package* dialog.

It is necessary to change the decay rate in the high permeability zone using the BCT package.

7. Select *MODFLOW* | *Optional Packages* | **BCT – Block Centered Transport…** to bring up the *BCT Process* dialog.
8. In the list on the left, select *Species Properties*.
9. For the *Constant Value* column, under *FODRW*, enter “0.0”. This variable is the decay rate for the species.
10. Click **OK** to close the *BCT Process* dialog.

5 Run MODFLOW and Examine the Results

The changes should now be saved before running MODFLOW-USG Transport.

1. Click **Save** to save the project.
2. Click the **Run MODFLOW** macro in the toolbar to bring up the *MODFLOW* model wrapper dialog.

3. When MODFLOW finishes, check the *Read solution on exit* and *Turn on contours (if not on already)* boxes.
4. Click **Close** to close the *MODFLOW* model wrapper dialog.
5. Click **Save** to save the project with the new solution.

The solution set should appear in the Project Explorer. In order to more clearly see how the MDT package impacted the simulation, compare the results. As before, this can be done by using the *Plot Wizard* to create a time series plot.

6. In the Project Explorer, select the " Species 1" dataset to make it active.
7. Click the **Plot Wizard** macro to open the *Plot Wizard* dialog.
8. Under *Plot Type*, select the *Activity Dataset Time Series* option.
9. Click **Finish** to close the *Plot Wizard* dialog and generate the plot.
10. Using the **Select Cells** tool, select the second cell from the left.

The *Active Dataset Time Series* plot should appear similar to Figure 2.

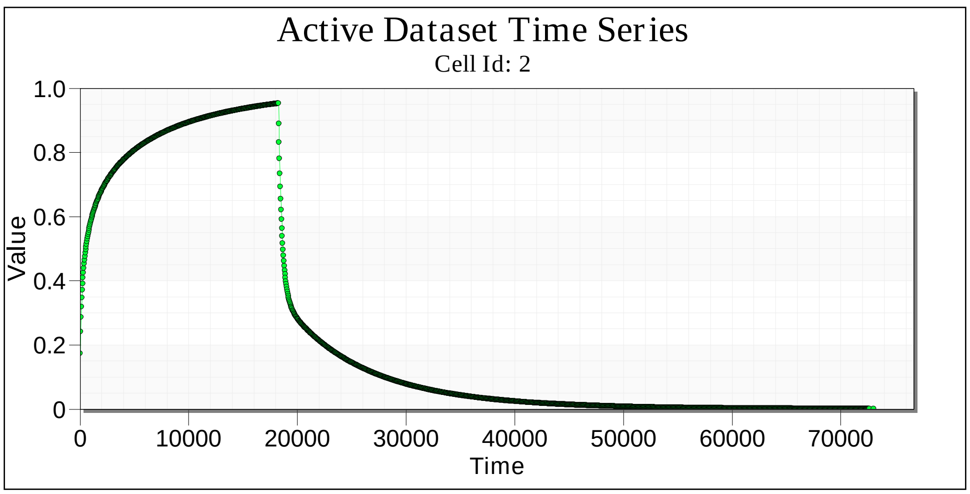

Figure 2 The Active Dataset Time Series for the second cell

6 Conclusion

This concludes the tutorial. Here are the key concepts from this tutorial:

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

