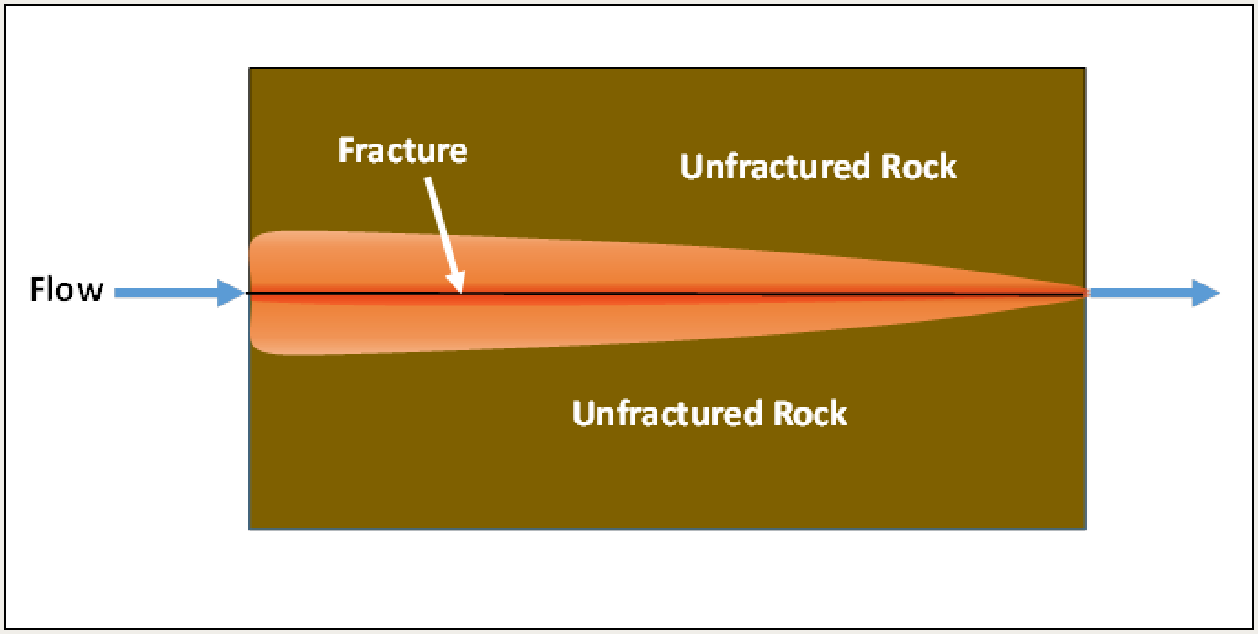
GMS 10.8 Tutorial

MODFLOW-USG Transport – MDT Discrete Fracture

Use the Matrix Diffusion Transport (MDT) package in GMS to simulate diffusion from a fracture 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.

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 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 input variables used in the MDT package are described in the MDT Process for MODFLOW-USG Transport User's Guide[4].

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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/

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

For the 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 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-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.

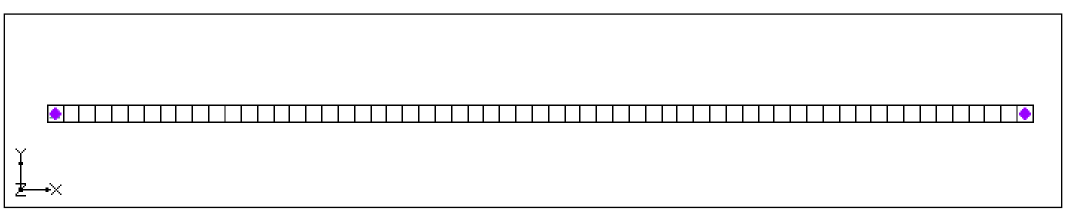

Figure 1 Imported MODFLOW-USG Transport model

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 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 BCT package, the pore velocity is equal to the Darcy velocity in this example.

The tritium (Species 1) is introduced at the upstream end of the grid using a transient concentration boundary (PCB package) with a value of 1 for 30 years, followed by a value of 0 for 30 more years.

Before continuing, save the project with a new name.

6. Select *File* | **Save As…** to bring up the *Save As* dialog.
7. Browse to the data files for this tutorial.
8. Enter “model-mdt.gpr” as the *File name*.
9. Select “Project Files (*.gpr)” from the *Save as type* drop-down.
10. 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 – Discrete Fracture Model

With the MDT package activated, the parameters for the MDT package can now be defined.

1. Select *MODFLOW* | *Optional Packages* | **MDT – Matrix Diffusion Transport…** to bring up the *MDT Package* dialog.
2. In the list on the left, select *Variables*.

Review the options here. For this example, the default settings will be used.

3. In the list on the left, select *Aquifer Properties*.
4. Enter the following for the *Constant Value* column:
    a. *MDFLAG*: “4.0”. 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 in this example.

b. *VOLFRACMD*: “1.0”. This is the volume fraction of high permeability material in the element. Since this example is only modeling the fracture itself, use the value of 1.

c. *PORMD*: “0.01”. This is the porosity of the unfractured rock.

d. *RHOBMD*: “2.0”. This is the dry bulk density of the rock, which is not used in this simulation of tritium transport.

e. *DIFFLENMD*: “1.0e-010”. The characteristic diffusion length is used with other MDFLAG options but is not needed for MDFLAG=4. Nonetheless, a small non-zero value has been added.

f. *TORTMD*: “0.1”. This is the tortuosity on the rock matrix.

5. In the list on the left, select *Species Properties*.
6. Enter the following for the *Constant Value* column:
    a. DECAYMD: “0.0561”. This is the tritium decay rate, 1/yr.
    b. DIFFMD: “0.0504576”. This is the tritium molecular diffusion coefficient, m^2/yr.
7. Click **OK** to close the *MDT Package* dialog.

5 Saving and Running MODFLOW

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.

6 Examining the Results

In order to more clearly see how the MDT package impacted the simulation, compare the results. This can be done by using the *Plot Wizard* to create a time series plot.

1. In the Project Explorer, select the “ Species 1” dataset to make it active.
2. Click the **Plot Wizard** macro to open the *Plot Wizard* dialog.
3. Under *Plot Type*, select the *Activity Dataset Time Series* option.
4. Click **Finish** to close the *Plot Wizard* dialog and generate the plot.

5. Using the **Select Cells** tool, select the first cell on the left in the Graphics Window.

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

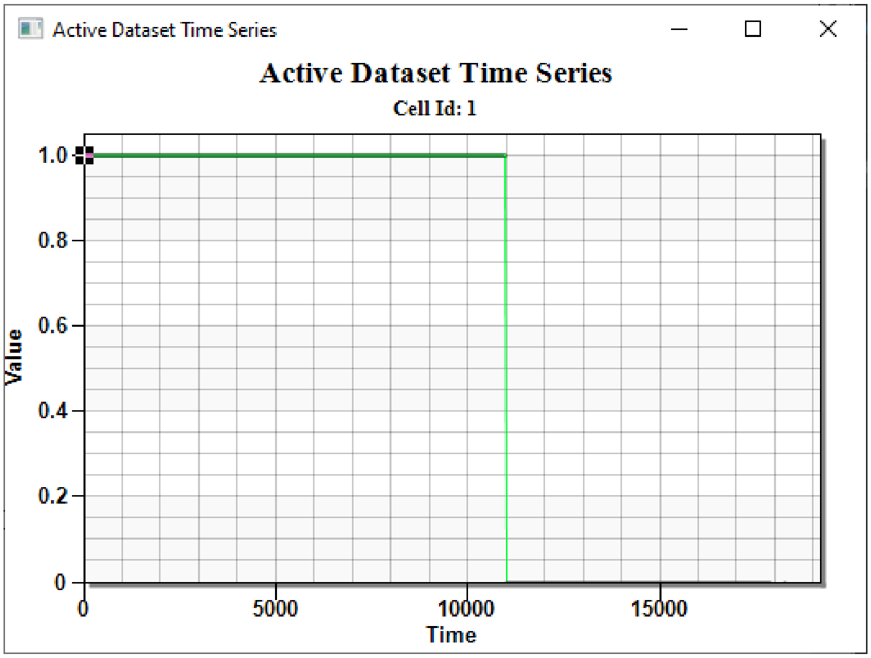

Figure 2 The Active Dataset Time Series for the first cell

6. Using the **Select Cells** tool, select the second cell on the left.

The *Active Dataset Time* Series plot should update to appear similar to Figure 3. Note how the solution changes. If desired, select additional cells moving to the right to further see how the solution changes.

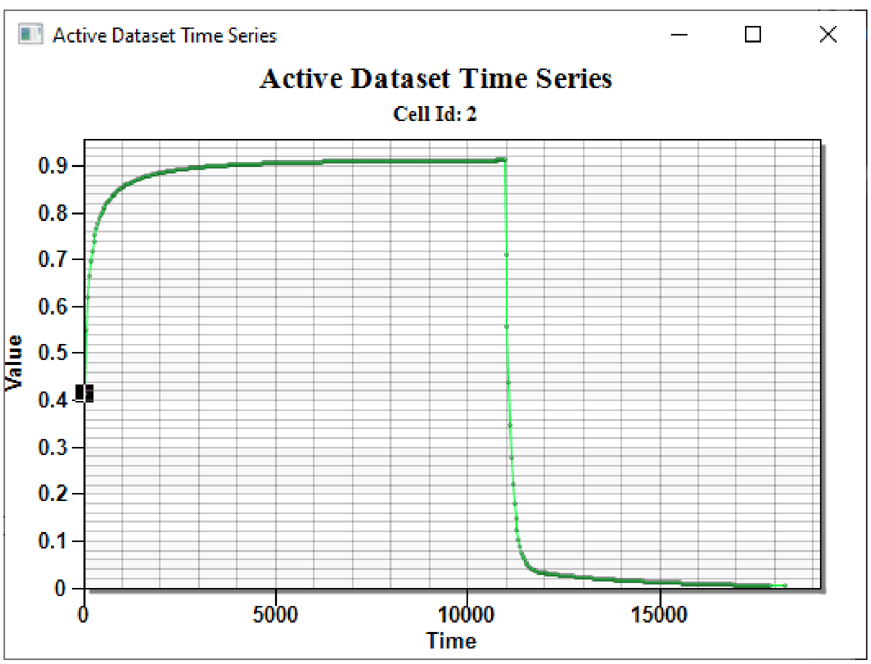

Figure 3 The Active Dataset Time Series for the second cell

The results calculated using the MDT Package in MODFLOW-USG Transport[4] are compared to an analytical solution and to the REMChlor-MD solution in Figure 4. The MDT package results are identical to the REMChlor-MD results and closely approximate the exact analytical solution.

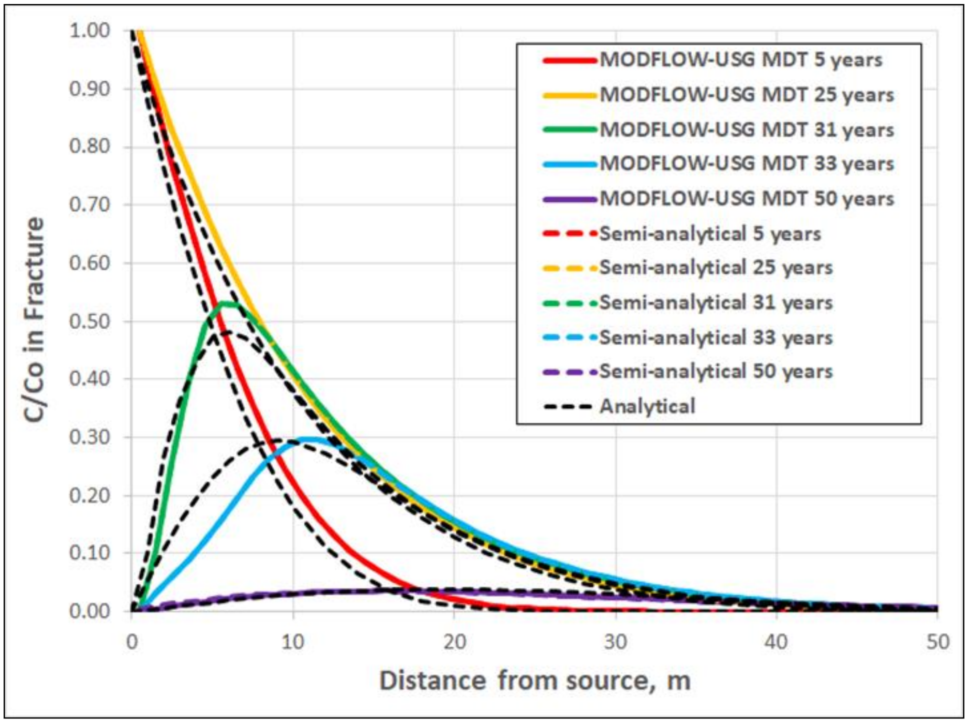

Figure 4 Comparison of MODFLOW-USG MDT Package output with REMChlor-MD (semi-analytical) and the analytical solution.

7 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 a single or multiple fractures in fractured porous materials.
- The MDT package allows for two main simulation approaches: a discrete fracture approach, where the fracture is directly simulated and matrix diffusion occurs into infinite surrounding matrix material, and 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.

