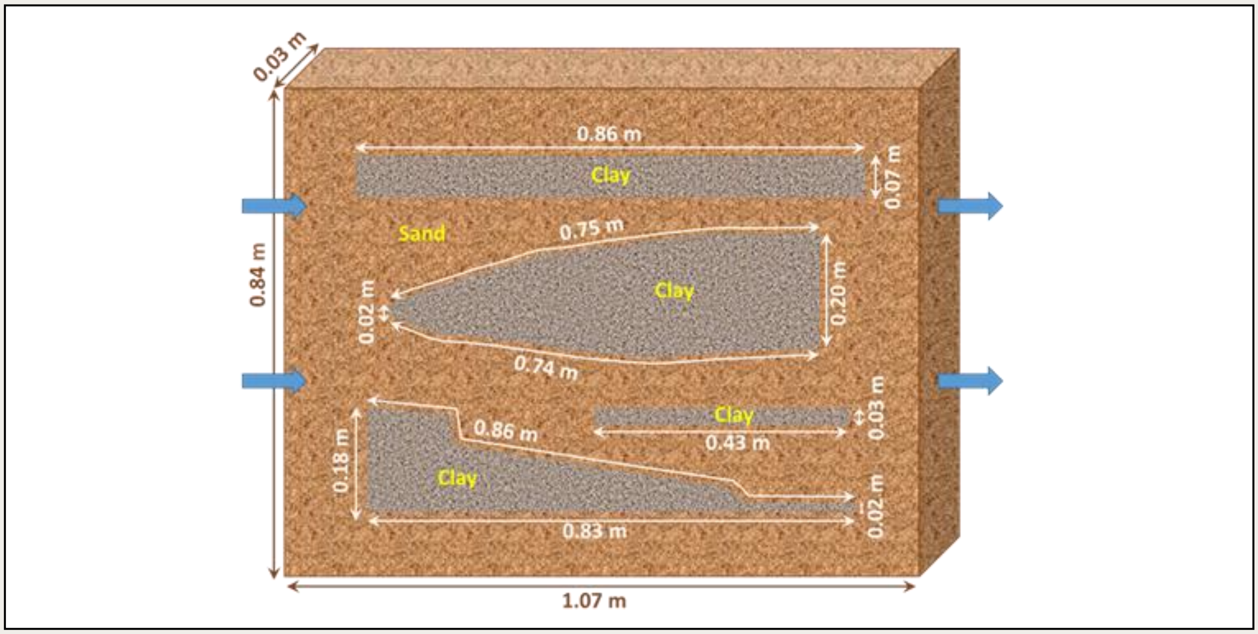
GMS 10.8 Tutorial

MODFLOW-USG Transport – MDT Matrix Diffusion

Use the Matrix Diffusion Transport (MDT) package in GMS to simulate matrix diffusion in heterogeneous sand/clay system using a semi-analytic approximation



Objectives

Learn how to use the Matrix Diffusion Transport (MDT) package with MODFLOW-USG Transport to simulate matrix diffusion in a heterogeneous sand/clay system.

Prerequisite Tutorials

- MODFLOW-USG Transport
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Required Components

- GMS Core
- MODFLOW-USG Transport

Time

- 30–40 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 heterogeneous porous media system where the heterogeneity occurs at the sub-gridblock scale. 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/

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For this example, a simulation of the Doner[5] (2008) laboratory matrix diffusion experiment is performed. The experiment was conducted in a 1.07 x 0.03 x 0.84m tank filled with sand and four embedded clay lenses. A tracer solution consisting of 400 mg/L of fluorescein was injected into the sand box for 22 days, followed by clean water for 100 days. Diffusion of the fluorescein into the clay lenses resulted in extensive back diffusion during the clean water flushing period. Chapman[6] et al. (2012) simulated this experiment using high resolution 2-D numerical models with 9,000 to 24,000 elements.

Using the semi-analytic matrix diffusion method in MDT, the laboratory experiment is simulated using a one-dimensional grid (UGrid) with only 50 elements. With this approach, the flow and transport in the sand is simulated with localized matrix diffusion into and out of the clay lenses using the semi-analytic method. The clay lenses are not specifically discretized; rather they are represented in the model in an average sense, using the volume fraction (VOLFRACMD) of sand, and the characteristic diffusion length in the clay (DIFFLENMD). This example is based on a test problem presented by Muskus and Falta[3]. Additional model parameters are given in Table 1.

Table 1. Input parameters used to simulate Doner[5] (2008) experiment

Parameter	**Value**
Darcy velocity, v_x (m/yr)	31.29
Sand porosity, ϕ	0.45
Matrix porosity, ϕ_l	0.6
Sand retardation (fl), R	1.39
Matrix retardation, R_l	1
Matrix tortuosity, τ_l	0.3
Diffusion coefficient (fl), D (m^2/yr)	1.73E-02
Source concentration (fl), C_0 (mg/L)	400
Δx (m)	0.0214
Δy (m)	0.03
Δz (m)	0.84
Sand volume fraction, V_f	0.711
Characteristic diffusion length, L (m)	0.0405
Number of elements (x-dir)	50
Δt (d)	0.5
Number of time steps	244

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.

[5]Doner, L.A., 2008, Tools to Resolve Water Quality Benefits of Upgradient Contaminant Flux Reduction, MS thesis, Colorado State University, Fort Collins, CO.

[6]Chapman, S.W., B.L. Parker, T.C. Sale, and L.A. Doner, 2012, Testing high resolution numerical models for analysis of contaminant storage and release from low permeability zones, Journal of Contaminant Hydrology, 136-137, 106-116.

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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.
6. Click on the **Front View** macro to show the sand tank model from the side.

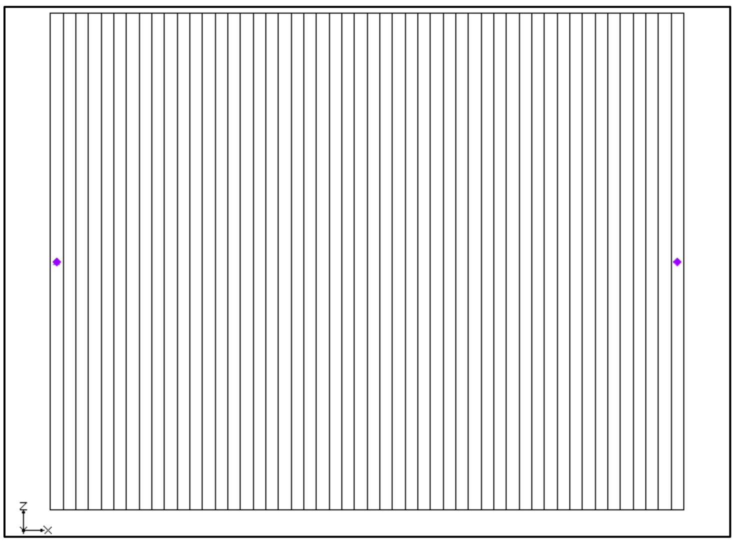

Figure 1 Imported MODFLOW-USG Transport model

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 50 elements are used in this 1D grid. The elements have dimensions of 0.0214 m in the direction of flow (x-direction), 0.03 m perpendicular to the flow (y-direction) and 0.84 m vertically (z-direction).

The hydraulic head in the leftmost element is maintained at a constant head of 1.3281 m using the CHD package, while the rightmost element is maintained at a head of 1 m. The horizontal hydraulic conductivity was set to a value of 100 m/yr, resulting in a Darcy velocity of 31.29 m/yr.

The fluorescein (Species 1) is introduced at the upstream end of the grid using a transient concentration boundary (PCB package) with a value of 400 for 0.06023 years (22 days), followed by a value of 0 for the remaining 0.2738 years (100 days).

Before continuing, save the project with a new name.

7. Select *File* | **Save As…** to bring up the *Save As* dialog.
8. Browse to the directory for this tutorial.
9. Enter "model-mdt2.gpr" as the *File name*.
10. Select "Project Files (*.gpr)" from the *Save as type* drop-down.
11. Click **Save** to save the project file and close the *Save As* dialog.

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3 Activating the MDT Package

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

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 values:

    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 low permeability zones with a finite diffusion length.

    a. *VOLFRACMD*: “0.711”. This is the volume fraction of sand in the laboratory experiment tank. This value was calculated by subtracting the clay volume from the total tank volume and dividing by the tank volume[3].

    b. *PORMD*: “0.6”. This is the porosity of the clay.

    c. *RHOBMD*: “1.6”. Dry bulk density of the clay.

    d. *DIFFLENMD*: “0.04052”. This characteristic diffusion length in the clay lenses was estimated using the surface area (A_{md}) of the clay lenses[3] of 0.193 m^2. Given the total tank volume (V) of 0.027 m^3 and the sand volume fraction (V_f) of 0.711, the characteristic diffusion length (L) can be estimated from a volume balance on the clay[3]: $(1 - V_f) = A_{md}L$.

    e. *TORTMD*: “0.3”. Tortuosity of the clay.

5. In the list on the left, select *Species Properties*.
6. Enter the following values:

    a. *KDMD*: “0.0”. K_d value for fluorescein in the clay; set to zero for R=1.

    b. *DIFFMD*: “0.0173”. The fluorescein diffusion coefficient, m^2/yr.

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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 on 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 *Active 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 last cell on the right in the Graphics Window.

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

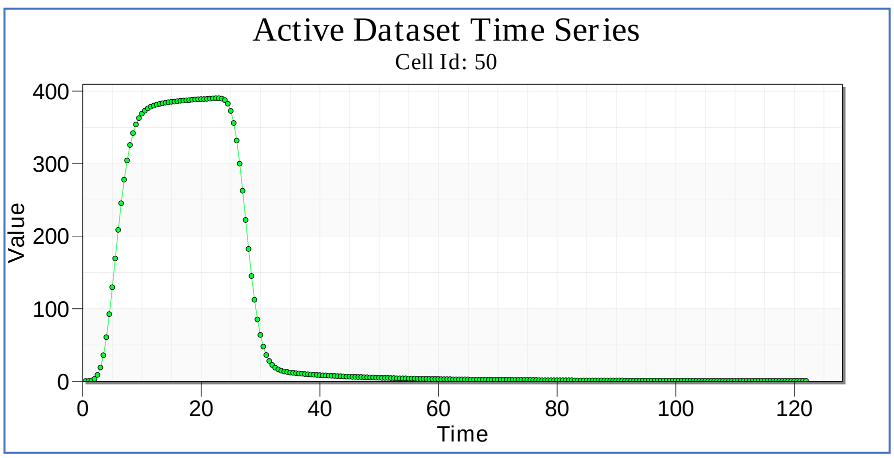

Figure 2 The Active Dataset Time Series for the last cell

6. Right-click in the plot and select **Display Options** to open the *Active Dataset Time Series Customization* dialog.
7. Select the *Axis* tab.

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8. Change the *Y Axis* to *Log* scale.
9. Under *Y Axis*, select the button next to *Min/Max* and set *Min* to "0.01" and *Max* to "1000".
10. Click **OK** to exit the *Active Dataset Time Series Customization* dialog.

The *Active Dataset Time Series* plot should update to appear similar to Figure 3. The extensive tailing of fluorescein that occurs after about 35 days is due to matrix diffusion.

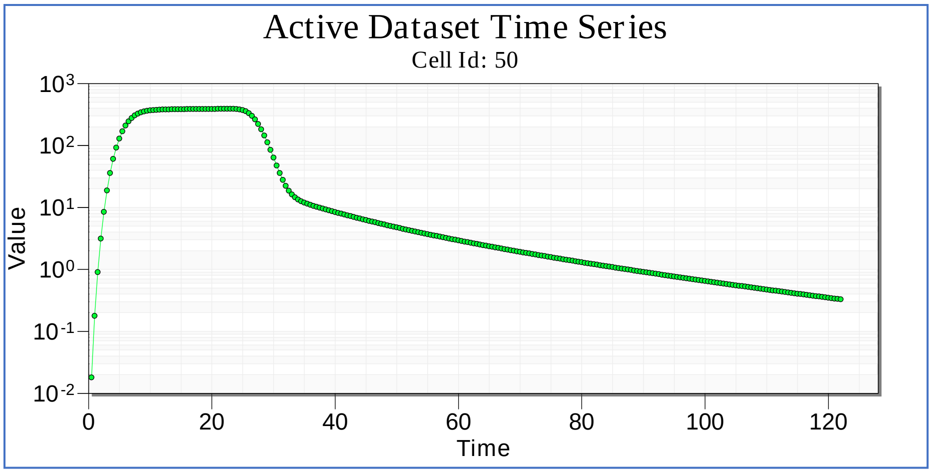

Figure 3 The Active Dataset Time Series with applied log scale

The results calculated using the MDT Package in MODFLOW-USG Transport[4] are compared to the experimental results and to the REMChlor-MD solution in Figure 4. The MDT package results are identical to the REMChlor-MD results and approximate the laboratory data. Results from a fine-grid MODFLOW/MT3DMS numerical model that discretized the individual clay lenses (8,988 model cells) by Chapman[6] et al. (2012) are shown as the yellow line.

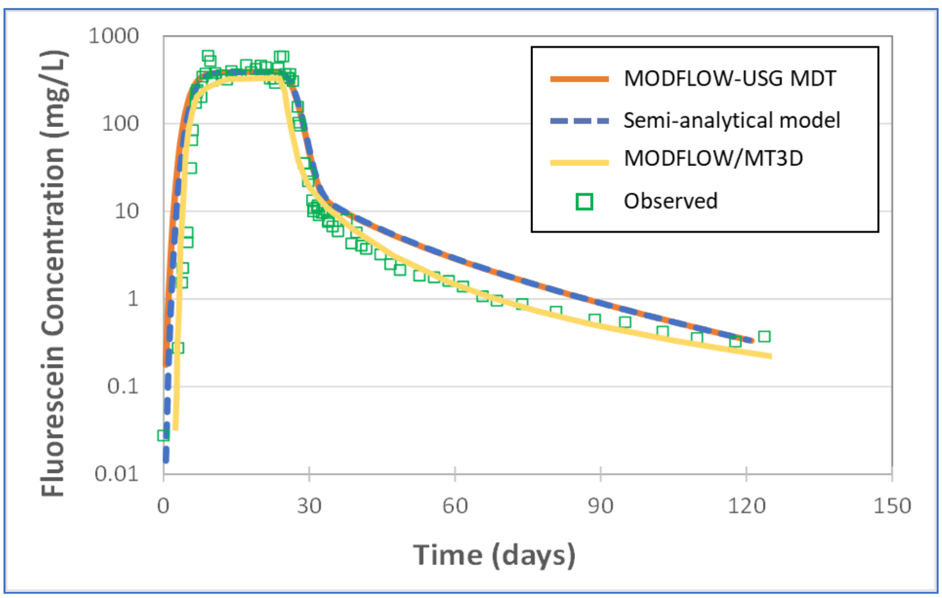

Figure 4 Comparison of MODFLOW-USG MDT model (50 model cells) output with Chapman et al. (2012) MODFLOW/MT3DMS model (8,988 model cells), REMChlor-MD (semi-analytic) model (50 model cells), and observed concentrations

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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 in heterogeneous porous media for cases where diffusion occurs at the sub-gridblock scale.
- Normal grid elements are used with embedded matrix diffusion occurring over a finite distance in the matrix material in each element.

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