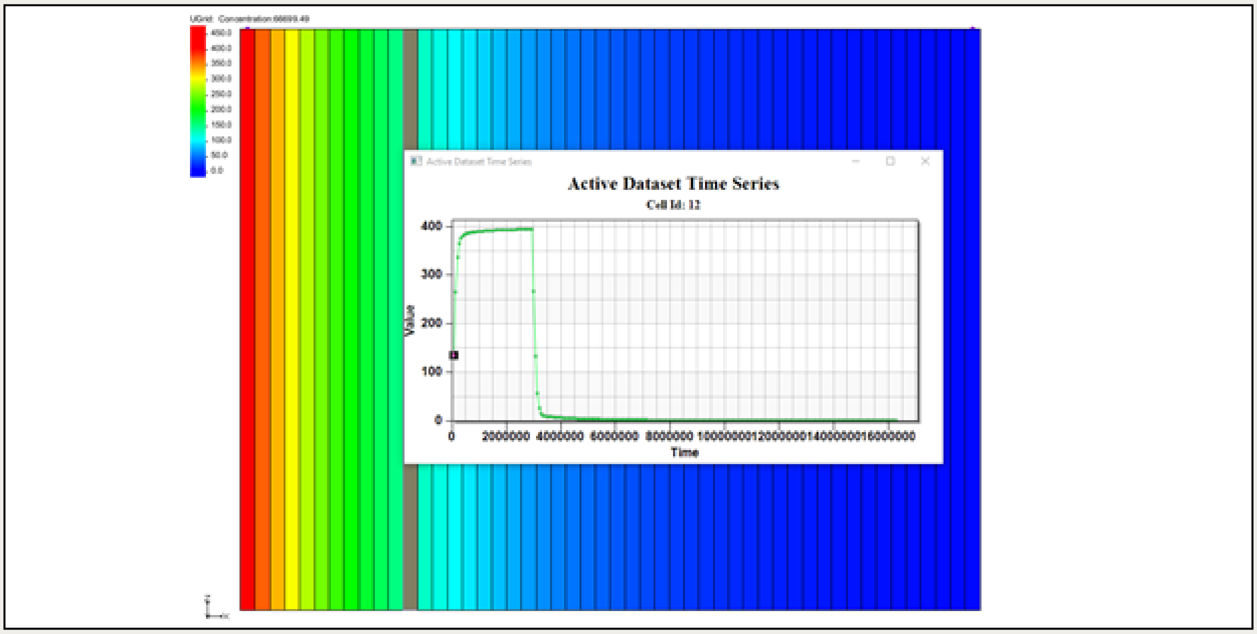
GMS 10.8 Tutorial

MODFLOW 6 – MDT Sand Tank

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



Objectives

Learn how to use the Matrix Diffusion Transport package (MDT) with MODFLOW 6 to simulate matrix diffusion in a heterogeneous sand/clay system.

Prerequisite Tutorials

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

Required Components

- GMS Core
- MODFLOW-USG Model & 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 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 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

---

[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.*

 © Aquaveo 2024

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].

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:

---

[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/

[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.

 © Aquaveo 2024

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_sank_tank* 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). The project contains a MODFLOW 6 simulation that has observation data.

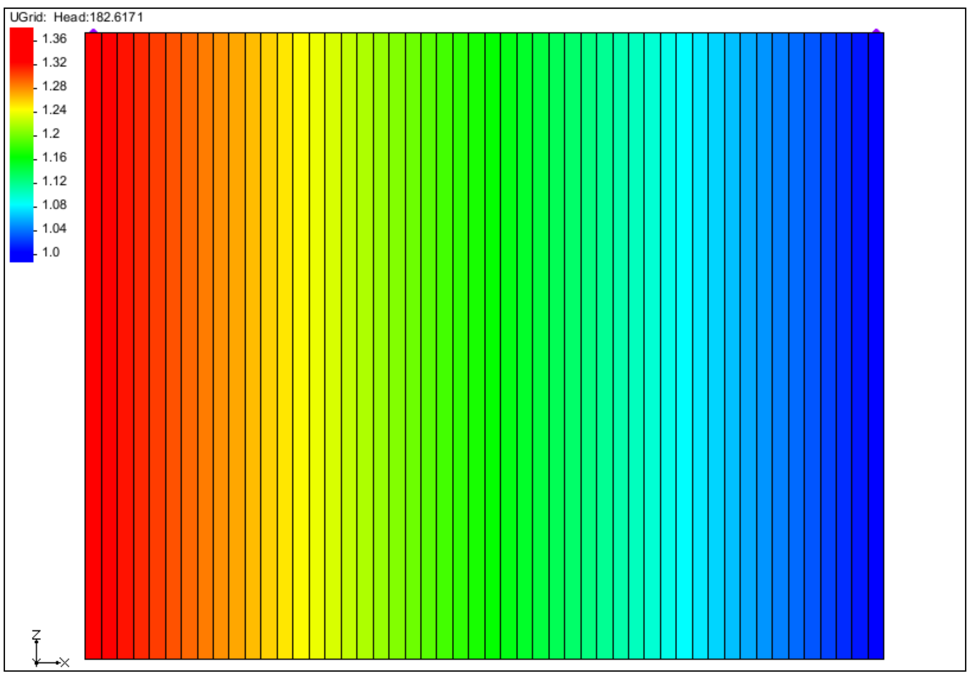


Figure 1 Initial project for the MODFLOW 6 model

This model has a single layer UGrid. Specified heads (CHD) have been set at each end. A total of 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 left-most element is maintained at a constant head of 1.3281 m using the CHD package, while the right-most 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.

 © Aquaveo 2024

Before continuing, save the project with a new name.

1. Select *File* | **Save As…** to bring up the *Save As* dialog.
2. Browse to the *Tutorials\MODFLOW 6\mf6_mdt_sand_tank* directory.
3. Enter “sand_tank.gpr” as the *File name*.
4. Select “Project Files (*.gpr)” from the *Save as type* drop-down.
5. Click **Save** to save the project file and close the *Save As* dialog.

3 Adding a New GWT Model

With the MODFLOW 6 open, a groundwater transport (GWT) model is necessary to use the MDT package. The GWT model can be added by doing the following:

1. Switch to the **UGrid** module.
2. Right-click on “ sand_tank” and select *New Package* | **GWT** to bring up the *New Groundwater Transport (GWT) Model* dialog.
3. In the *Select UGrid* section, turn on the “UGrid” grid.
4. In the *GWT – Groundwater Transport Model* section, turn on the following packages: *ADV, CNC, DSP, MDT,* and *SSM*.
5. Click **OK** to close the *New Groundwater Transport (GWT) Model* dialog.

Notice the “ trans” model is now shown in the Project Explorer along with the selected packages.

6. In the Project Explorer, right-click on “ sand_tank” and select **Unlock All**.

3.1 The TDIS Package

The TDIS package defines the temporal discretization for the groundwater transport model. The package has already been defined for this example.

3.2 The ADV Package

Review the ADV package before continuing.

1. Double-click on the “ ADV” package to bring up the *Advection (ADV) Package* dialog.
2. Check that the *SCHEME* option is turned on.
3. Click **OK** to close the *Advection (ADV) Package* dialog.

3.3 The CNC Package

Define the constant concentration by doing the following:

1. Double-click on the “ CNC” package to bring up the *Constant Concentration (CNC) Package* dialog.
2. Click the **Add Rows** button to bring up the *Add Stresses* dialog.

 © Aquaveo 2024

3. Accept the default settings (adding 1 row to all defined periods) and click **OK** to close the *Add Stresses* dialog.
4. In row *1*, enter the following:
   - *LAY* set to “1”
   - *CELL2D* set to “1”
   - *CONC* set to “400.0”
5. Change the *Period* to “2”.
6. Click **Define Period** to bring up the *Define Period* dialog.
7. Make certain *Copy from previous period* is selected and click **OK** to close the *Define Period* dialog.
8. Change the *CONC* column to be “0.0”.
9. Click **OK** to close the *Constant Concentration (CNC) Package* dialog.

3.4 The DSP Package

Define the dispersion by doing the following:

1. Double-click on the “ DSP” package to bring up the *Dispersion (DSP) Package* dialog.
2. On the *DIFFC* tab, turn on the *Define* option and set the *Constant* value to “0.03844444”.
3. Under *Sections*, turn on *OPTIONS.*
4. Turn on the *XT3D_OFF* option.
5. Click **OK** to close the *Dispersion (DSP) Package* dialog.

3.5 The IC Package

The IC Package default settings are sufficient for this example. No changes are needed, though the settings may be reviewed if desired.

3.6 The MST Package

Define the mobile storage and transfer by doing the following:

1. Double-click on the “ MST” package to bring up the *Mobile Storage and Transfer (MST) Package* dialog.
2. On the *POROSITY* tab, set the *Constant* value to “0.45”.
3. On the *BULK_DENSITY* tab, turn on the *Define* option and set the *Constant* value to “1.6”.
4. On the *DISTCOEF* tab, turn on the *Define* option and set the *Constant* value to “0.109693”.
5. Under *Sections*, turn on *OPTIONS.*
6. Turn on the *SORPTION* option.
7. Click **OK** to close the *Mobile Storage and Transfer (MST) Package* dialog.

 © Aquaveo 2024

3.7 The SSM Package

Define the source mixing for this example by doing the following:

1. Double-click on the " SSM" package to bring up the *Source and Sink Mixing (SSM) Package* dialog.
2. Under *Sections*, turn on *OPTIONS.*
3. Turn on the *SAVE_FLOWS* option.
4. Click **OK** to close the *Source and Sink Mixing (SSM) Package* dialog.

4 The MDT Package

The MDT package can be defined during the process of setting up the GWT model.

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".
3. On the *MD_FRACTION* tab, set the *Constant* value to "0.289".
4. On the *MD_POROSITY* tab, set the *Constant* value to "0.6".
5. On the *BULK_DENSITY* tab, set the *Constant* value to "1.6".
6. On the *MD_DIFF_LENGTH* tab, set the *Constant* value to "0.04052".
7. On the *MD_TORTUOSITY* tab, set the *Constant* value to "0.3".
8. On the *MD_DIST_COEFF* tab, set the *Constant* value to "9.33e-09".
9. On the *MD_DIFF_COEFF* tab, set the *Constant* value to "0.0173".
10. Under *Sections*, turn on *OPTIONS.*
11. Turn on the *SORPTION* option.
12. Click **OK** to close the *Matrix Diffusion Transport (MDT) Package* dialog.

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

5 Output Control

Before running the MODFLOW 6 simulation, set the output option for the GWT model.

1. Under the " trans" model, double-click on the " OC" package to bring up the *Output Control (OC) Dialog*.
2. Change the *Preset output* to be "At every time step".
3. Click **OK** to close the *Output Control (OC) Dialog*.

6 Adding a Second IMS Package

A second iterative model solution package will be used in this example.

1. Right-click on " sand_tank" and select *New Package* | **IMS**.
2. Double-click on the " IMS (2)" package to bring up the *Iterative Model Solution (IMS)* dialog.

© Aquaveo 2024

3. Under *Sections*, turn on *OPTIONS*.
4. Turn on the *COMPLEXITY* option and change to be "COMPLEX".
5. Click **OK** to close the *Iterative Model Solution (IMS)* dialog.

7 Adding a GWF-GWT Exchange

A GWF-GWT exchange creates a relationship where the GWF Model provides the flow data that informs the GWT Model. To create this exchange, do the following:

1. Right-click on " sand_tank" and select *New Package* | **GWF-GWT**.
2. Double-click on " sand_tank" to open the *Simulation Options* dialog.
3. Under *Sections*, turn on *EXCHANGES.*
4. In the *EXCHANGES* table, click the blank cell under the *EXGMNAMEA* column to bring up the *Select Model* dialog.
5. Select the "flow_model" model and click **OK** to close the *Select Model* dialog.
6. Click the blank cell under the *EXGMNAMEB* column to bring up the *Select Model* dialog.
7. Select the "trans" model and click **OK** to close the *Select Model* dialog.
8. Under *Sections*, turn on *SOLUTIONGROUPS.*
9. In the *SOLUTIONGROUPS* table, click the blank cell on the second row under the *SLNMNAMES* column to open the *Select Model(s)* dialog.
10. Select the "trans" model and click **OK** to close the *Select Model(s)* dialog.
11. Click **OK** to close the *Simulation Options* dialog.

8 Saving and Running the Simulation

Now save and run the simulation:

1. Right-click on " sand_tank" 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*.

9 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 " sand_tank (MODFLOW 6)" folder.
3. Using the **Select Cells** tool, select cell 50 (the last cell on the right).
4. Click the **Plot Wizard** macro to open the *Plot Wizard* dialog.
5. Under *Plot Type*, select "Active Dataset Time Series".

 © Aquaveo 2024

6. Click **Finish** to close the *Plot Wizard* and generate the plot.

The generated plot should appear similar to Figure 2.

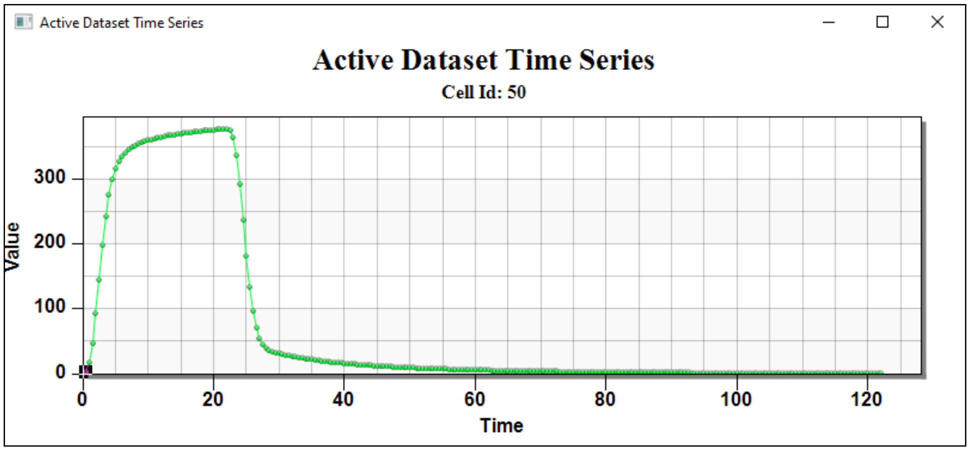


Figure 2 The active dataset time series plot

10 Conclusion

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

- Creating a MODFLOW 6 transport model.
- Adding the MDT Package to MODFLOW 6.
- Running MODFLOW 6.
- Reviewing the MODFLOW 6 solution.

 © Aquaveo 2024