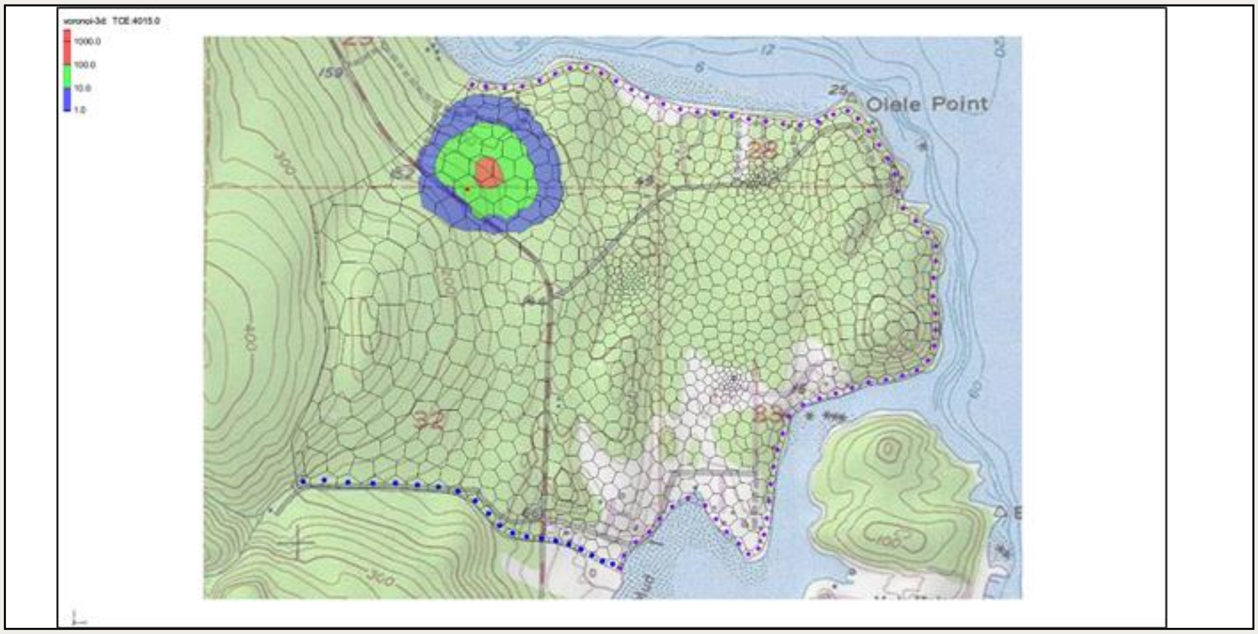
GMS 10.8

GMS 10.8 Tutorial

MODFLOW-USG Transport – MDT Package 3D Transport

Use the Matrix Diffusion Transport (MDT) package in GMS to simulate matrix diffusion in a three-dimensional model 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 three-dimensional field scale model with an unstructured grid.

Prerequisite Tutorials

- MODFLOW-USG – Complex Stratigraphy
- MODFLOW-USG Transport – Grid Approach

Required Components

- GMS Core
- MODFLOW-USG Transport

Time

- 30–40 minutes

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1 Introduction

The Matrix Diffusion Transport (MDT) package works with MODFLOW-USG Transport and 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-USG Transport simulation to simulate diffusion in a three-dimensional heterogeneous porous media system where the heterogeneity occurs at the sub-gridblock scale. This example is based on the unstructured grid flow model developed in the MODFLOW-USG – Complex

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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.*

Stratigraphy tutorial, with a hypothetical release of trichloroethylene (TCE) into the aquifer.

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].

This example uses a five-layer Voronoi UGrid from the *MODFLOW-USG Complex Stratigraphy tutorial* and adds the MODFLOW-USG BCT and MDT packages. The layers are discontinuous, and have different properties, but the properties are assumed to be constant within each layer. The conceptual model is that there are sub-gridblock scale heterogeneities such as discontinuous sand, silt, and clay layers that exist throughout the model domain. These local-scale heterogeneities give rise to strong matrix diffusion effects during contaminant transport.

With the MDT approach, the transport in the model is simulated with localized matrix diffusion into and out of the low permeability (low-K) parts of each cell using the semi-analytic method. The local low permeability zones in each cell are not specifically discretized; rather they are represented in the model in an average sense, using the volume fraction (VOLFRACMD) of higher permeability (high-K) material, and the characteristic diffusion length in the low-K material (DIFFLENMD). The conceptual model for transport is that advective flow occurs in only 20% of the overall volume (the high-K fraction) with local matrix diffusion into and out of the remaining 80% low-K fraction.

This tutorial will demonstrate the following topics:

1. Opening an existing MODFLOW-USG flow simulation.
2. Activating the BCT package
3. Activating the MDT package.
4. 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 "olele.gpr".
5. Click **Open** to import the file and close the *Open* dialog.

The Graphics Window should appear as in Figure 1.

[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/

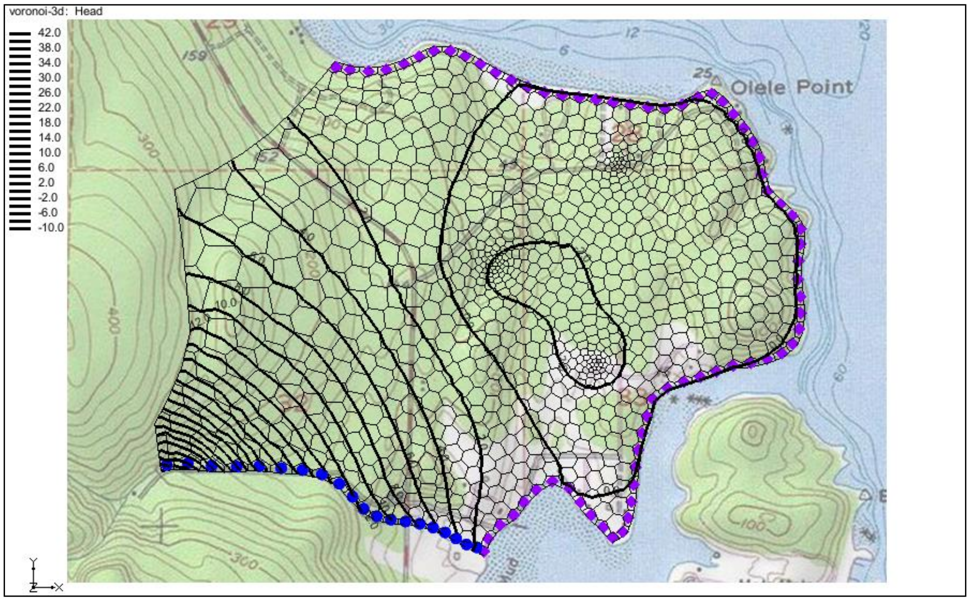


Figure 1 Imported MODFLOW-USG flow model

This model has a five-layer Voronoi UGrid with local refinement around three pumping wells. General heads have been set along the coastal boundary, and a river boundary condition exists along the lower left of the model. The no-flow boundary to the left occurs as the aquifer thins and the no-flow boundary in the upper left of the model is a parallel flow boundary.

The five model layers are discontinuous and can be viewed by turning on the *Single layer* option in the *Mini-Grid Toolbar* and changing the layer values. A total of 2627 elements are used in this 3D grid.

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 directory for this tutorial.
8. Enter “olele_transport.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 Enable MODFLOW-USG Transport

MODFLOW-USG Transport simulations use the MODFLOW-USG Transport model. To set up this model, complete the following:

1. Switch to the **UGrid** module.
2. Select *MODFLOW* **| Global Options…** to bring up the *MODFLOW Global/Basic Package* dialog.
3. Under the *MODFLOW version* section, select *USG Transport*.
4. Under the *Model type* section, select *Transient*.
5. Click the **Stress Periods** button to open the *Stress Periods* dialog*.*
6. Change the *Number of stress periods* to “2”.

7. For the first stress period, set the *Length* to “3650” days and the *Num Time Steps* to “20” time steps.
8. For the second stress period, set the *Length* to “32850” days and the *Num Time Steps* to “180” time steps.
9. Turn on the *Steady state* option for both time periods (for a steady-state flow field).
10. Click **OK** to close the *Stress Periods* dialog.

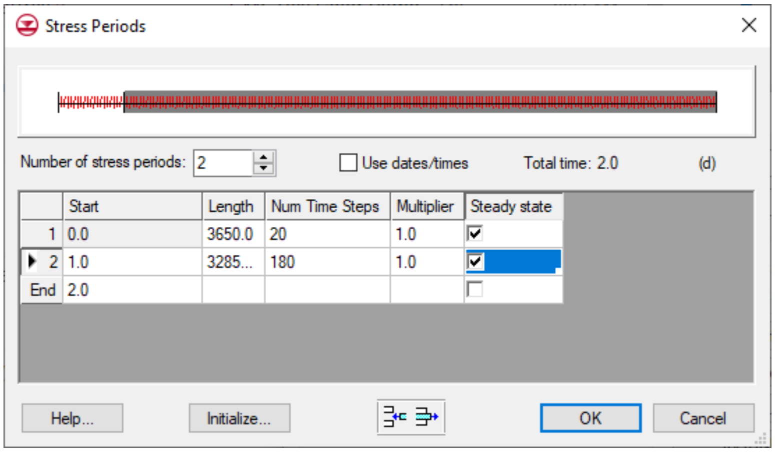


Figure 2 Stress period settings

11. Click the **Packages** button to open the *MODFLOW Packages / Processes* dialog
12. In the *Optional packages / processes* section, turn on *BCT – Block Centered Transport*, and *PCB – Prescribed Concentration.*
13. Click **OK** to exit the *MODFLOW Packages / Processes* dialog.
14. Click **OK** to exit the *MODFLOW Global/Basic Package* dialog.

A warning will appear: “Switching to USG Transport is one way. You cannot switch back to any other MODFLOW version later. Proceed?”.

15. Click **Yes** to close the warning message.

4 Defining the BCT Package

The parameters for the BCT transport package can now be defined.

1. Select *MODFLOW* | *Optional Packages* | **BCT – Block Centered Transport…** to bring up the *BCT Process* dialog.
2. In the list on the left, select *Variables*.
3. Review the options here and enter the following:
    a. *Adsorption (IADSORB)*: “Linear adsorption (1)”.
    b. *Dispersion formula (IDISP)*: “Isotropic dispersion (1)”.
4. In the list on the left, select *Aquifer Properties*.
5. Enter the following values in the *Constant Value* column:

   a. PRSITY: "0.08". This is the effective porosity used for transport. This value is based on our conceptual model where the overall porosity is 0.4, but the flow only occurs in 20% of the material (the high-K fraction).
   b. BULKD: "1.6". This is the dry bulk density value used for adsorption.
   c. DL: "20". This is the longitudinal dispersivity.
6. In the list on the left, select *Species.*
7. Enter "TCE" under *Species Name*
8. In the list on the left, select *Species Properties.*
9. Enter the following value in the *Constant Value* column:
   a. *ADSORB*: "0.05". K_d value for TCE; this value will give a retardation factor R=2.
10. Click **OK** to close the *BCT Process* dialog.
11. Select *Edit* | **Units** to open the *Units* dialog.
12. Set the *Concentration* units to "ppb".
13. Click **OK** to close the *Units* dialog.

5 Defining a Prescribed Concentration Source

Next to impose a time-dependent prescribed concentration of TCE in a single cell in grid layer 1.

1. Using the **Select Cells** tool, select cell 886 as shown in Figure 3.

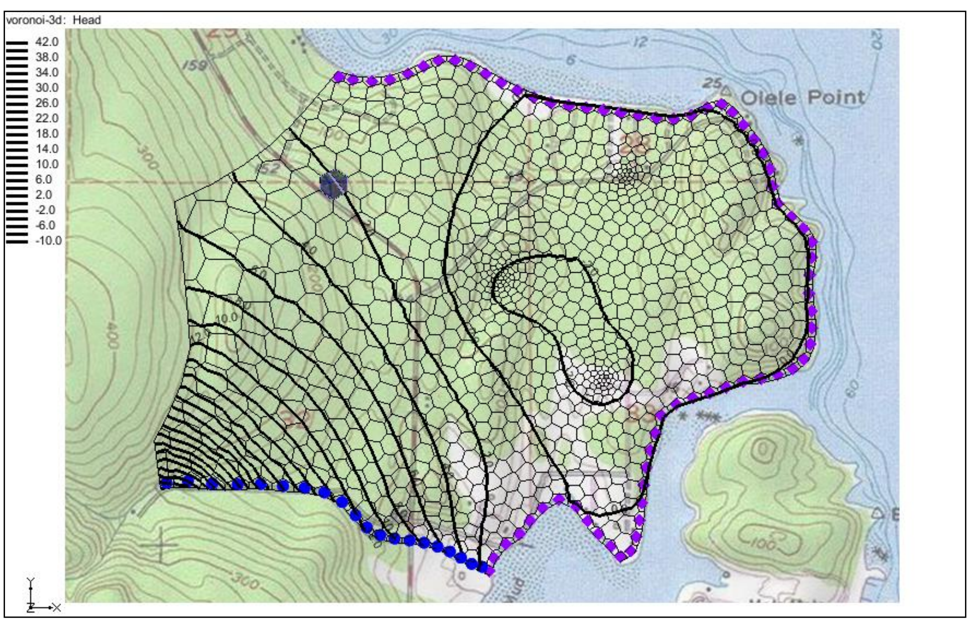
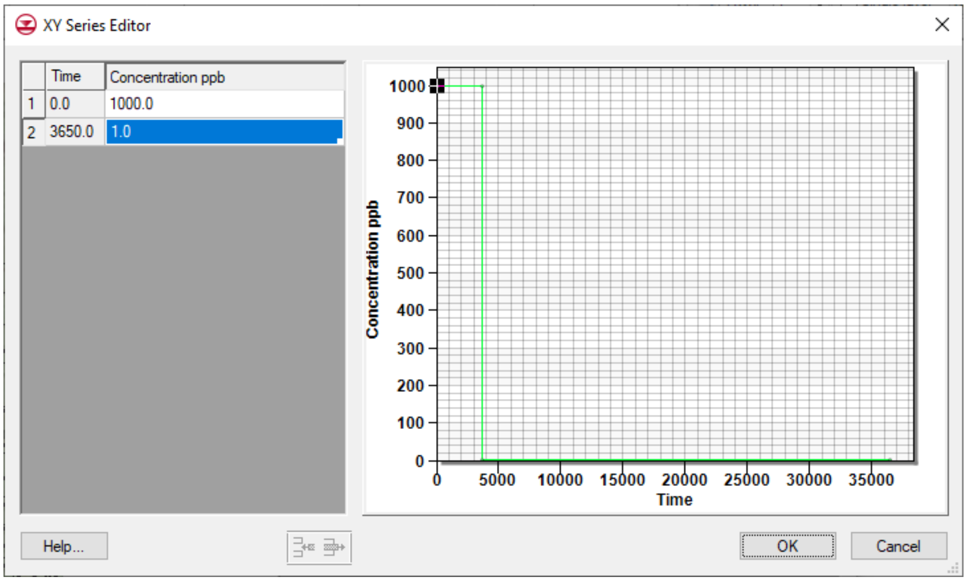


Figure 3 Select cell 886 in layer 1

2. Right-click and select **Sources/Sinks** to open the *MODFLOW Source/Sinks* dialog.
3. From the list on the lift, select *Concentration (PCB)*.

4. Click **Add BC** to add an entry to the table.
5. Under *Concentration ppb*, in the *886* row, click the ⋯ to open the *XY Series Editor*.
6. At *Time* 0.0 enter a value of “1000”.
7. At *Time* 3650 enter a value of “1”.

This will maintain the TCE concentration in cell 886 at a value of 1000 µg/L for 10 years, and then will switch it to a value of 1 µg/L for the remaining 90 years of the simulation. This is intended to simulate a contaminant source that is removed (mostly) after 10 years.



8. Click **OK** to exit the *XY Series Editor*.
9. Click **OK** to exit *MODFLOW Sources/Sinks* dialog.
10. Click anywhere outside the grid to unselect cell 886.

6 Output Control

To specify the output options:

1. Select *MODFLOW* | **OC – Output Control** to open the *MODFLOW Output Control* dialog.
2. Turn on the *Save concentrations to *.con file* option.
3. Click **OK** to exit the *MODFLOW Output Control* dialog.

7 Saving and Running MODFLOW-USG Transport

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.

8 Examining the Results

Next to make some adjustments to improve the appearance of the TCE contours.

1. In the Project Explorer, select the " TCE" dataset to make it active.
2. Click the **Display Options** macro to open the *Display Options* dialog.
3. Next to *Face contours* click *Options* to open the *Dataset Contour Options –UGrid – TCE* dialog.
4. Under *Contour Method* select "Color Fill and Linear" and "Use color ramp".
5. Click the **Color Ramp** button to open the *Choose color ramp* dialog.
6. Select the *Color Ramp Shader* pallette.
7. Click **OK** to close the *Choose color ramp* dialog
8. Under *Data range*, turn on *Specify a range* and enter a "1" for *Min* and "1000" for *Max*.
9. Turn off the *Fill below* and *Fill above* boxes.
10. Under *Contour interval* select "Specified Values" and enter "3".
11. Turn off the *Fill continuous color range* option.
12. In the *End Value* column, enter "10" for row *1*and enter "100" for row *2*.
13. Click **OK** to exit the *Dataset Contour Options*,
14. **OK** to exit the *Display Options* dialog.
15. In the *Time Steps* Window, select the "10,950" time step.

This is 20 years after the source has been removed. The contour plot should look similar to Figure 4 and Figure 5 for layers 1 and 5, respectively. The plume is discharging into the ocean and also migrating towards two of the extraction wells (in layer 5 where the wells are screened).

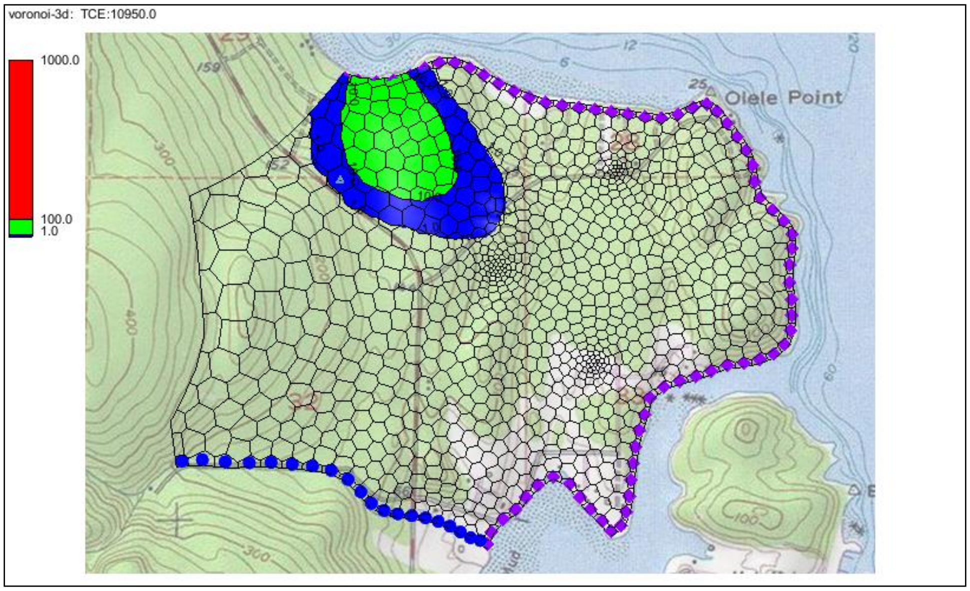


Figure 4 Simulated TCE plume in layer 1 after 10,950 days without matrix diffusion

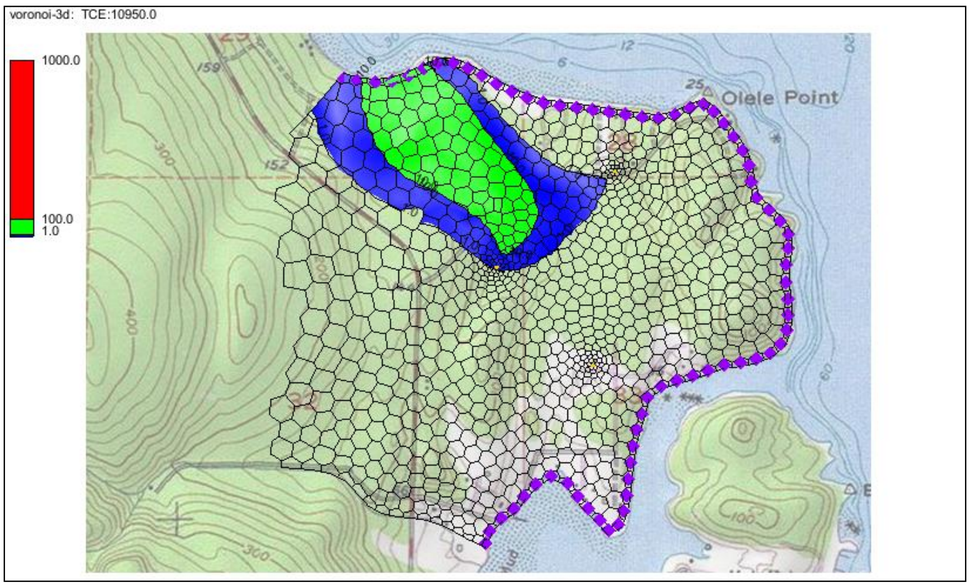


Figure 5 Simulated TCE plume in layer 5 after 10,950 days without matrix diffusion

16. Using the **Select Cells** tool, select cell 840 in layer 1 as in Figure 6.

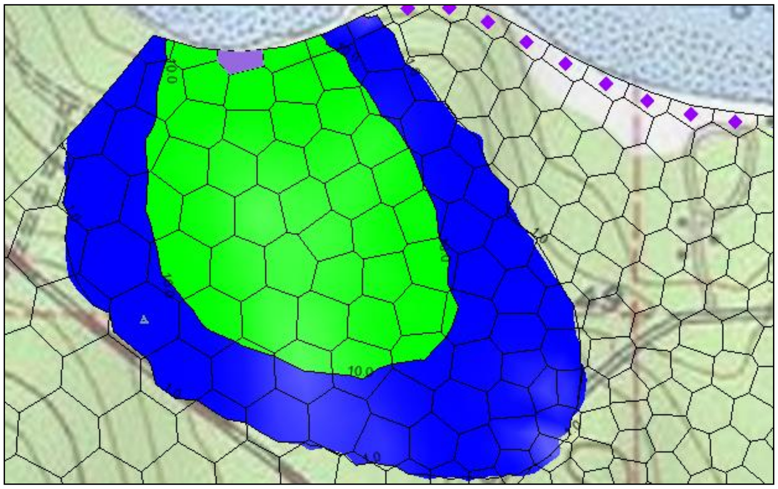


Figure 6 Select cell 840 in layer 1

17. Click the **Plot Wizard** macro to open the *Plot Wizard* dialog.
18. Under *Plot Type*, select the *Active Dataset Time Series* option.
19. Click **Finish** to close the *Plot Wizard* dialog and generate the plot.

The *Active Dataset Time Series* plot should appear similar to Figure 7.

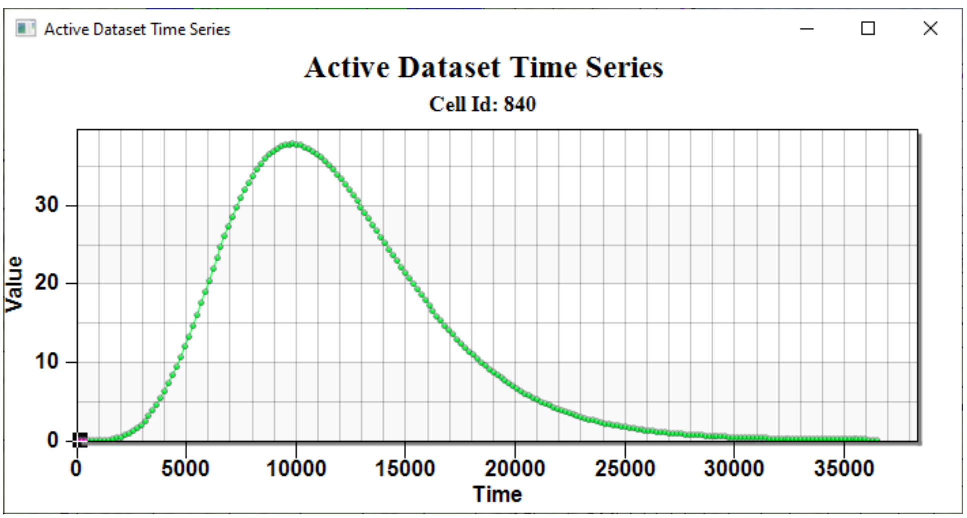


Figure 7 The Active Dataset Time Series for cell 840

9 Activating the MDT Package

Before continuing, save the project.

1. Click **Save** to save the project.

To activate the MDT package:

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.

10 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 in 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 low permeability zones with a finite diffusion length.
    a. *VOLFRACMD*: "0.2". This is the volume fraction of high-K material in each cell.
    b. *PORMD*: "0.4". This is the porosity of the low-K material.
    c. *RHOBMD*: "1.6". Dry bulk density of the low-K material.
    d. *DIFFLENMD*: "1.64". This is the characteristic diffusion length in the low-K material in each cell. The value here was chosen to be 0.5m, but since the dimensions of this model are in feet, the value is converted to units of feet. More information on the estimation of the diffusion length is available in the REMChlor-MD User's Guide[1].
    e. *TORTMD*: "0.3". Tortuosity of the low-K material in each cell.
5. In the list on the left, select *Species Properties*.
6. Enter the following *Constant Values*:
    f. *KDMD*: "0.25". K_d value for the low-K material, selected to give a retardation factor R=2.
    g. *DIFFMD*: "9.3e-4". The TCE diffusion coefficient, ft^2/d due to the choice of units in this model.
7. Click **OK** to close the *MDT Package* dialog.

11 Adjusting Values in the BCT Package to Fit Conceptual Model

The transport properties of the high-K part of each cell are defined in the BCT package.With the MDT VOLFRACMD parameter set to 0.2, the high-K material is assumed to only occupy 20% of the cell. In case, adjust the corresponding porosity and

Kd values in the BCT package so that this simulation is consistent with the previous one without matrix diffusion.

1. Select *MODFLOW* | *Optional Packages* | **BCT – Block Centered Transport…** to bring up the *BCT Process* dialog.
2. In the list on the left, select *Aquifer Properties*.
3. Enter the following value:
    a. *PRSITY*: “0.4”. This is the porosity of the high-K material in each cell. Since the volume fraction of high-K material (VOLFRACMD) is 20%, this is equivalent to the effective porosity value of 0.08 used in the previous simulation without matrix diffusion.
4. In the list on the left, select *Species Properties.*
5. Enter the following value:
    a. *ADSORB*: “0.25”. K_d value for TCE; this value will give a retardation factor R=2 for the porosity value of 0.4. This is consistent with the previous simulation without matrix diffusion.
6. Click **OK** to close the *BCT Process* dialog.

With the revised transport parameter values, this transport model will exactly match the previous model without matrix diffusion if the diffusion coefficient in MDT is set to a very small (but non-zero) number.

12 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.

13 Examining the Results

To examine the results, complete the following:

1. In the Project Explorer, select the “ TCE” dataset to make it active.
2. In the *Time Steps* Window, select the “10,950” time step.

This is 20 years after the source has been removed. The contour plots should look similar to Figure 8 and Figure 9 for layers 1 and 5, respectively. The plume is discharging into the ocean and also migrating towards two of the extraction wells (in layer 5 where the wells are screened).

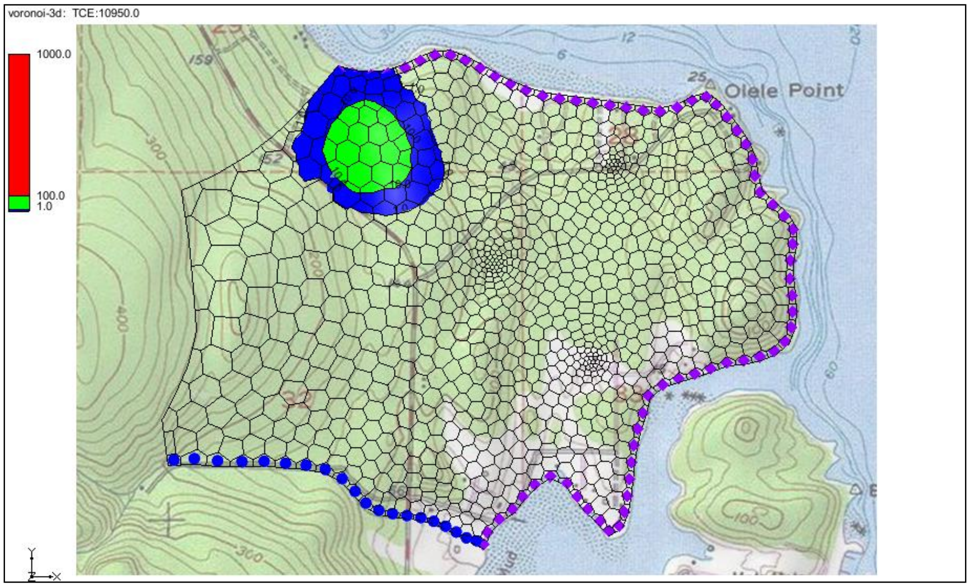


Figure 8 Simulated TCE plume in layer 1 after 10,950 days with matrix diffusion

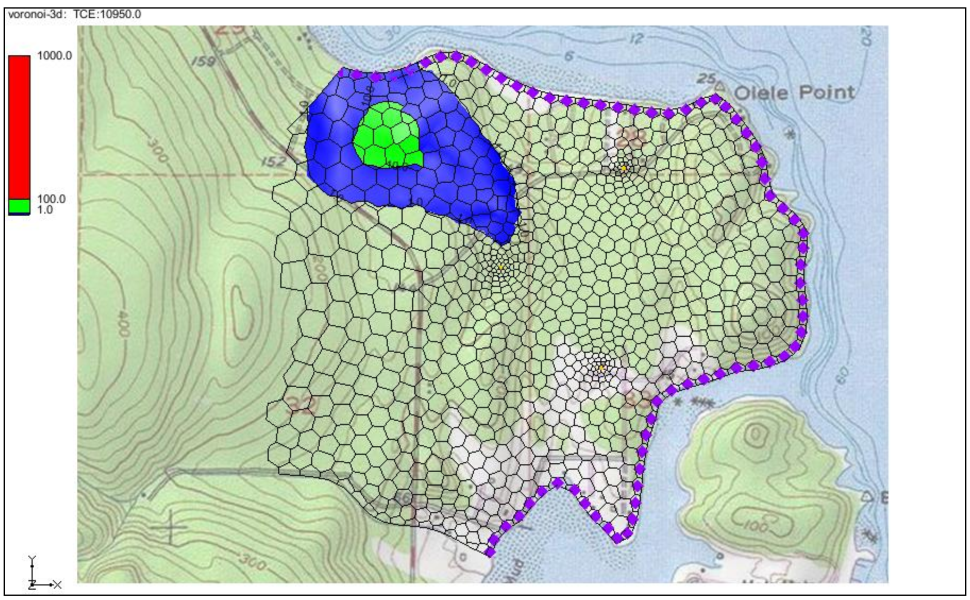


Figure 9 Simulated TCE plume in layer 5 after 10,950 days with matrix diffusion

3. Using the **Select Cells** tool, select cell 840 in layer 1 as in Figure 10.

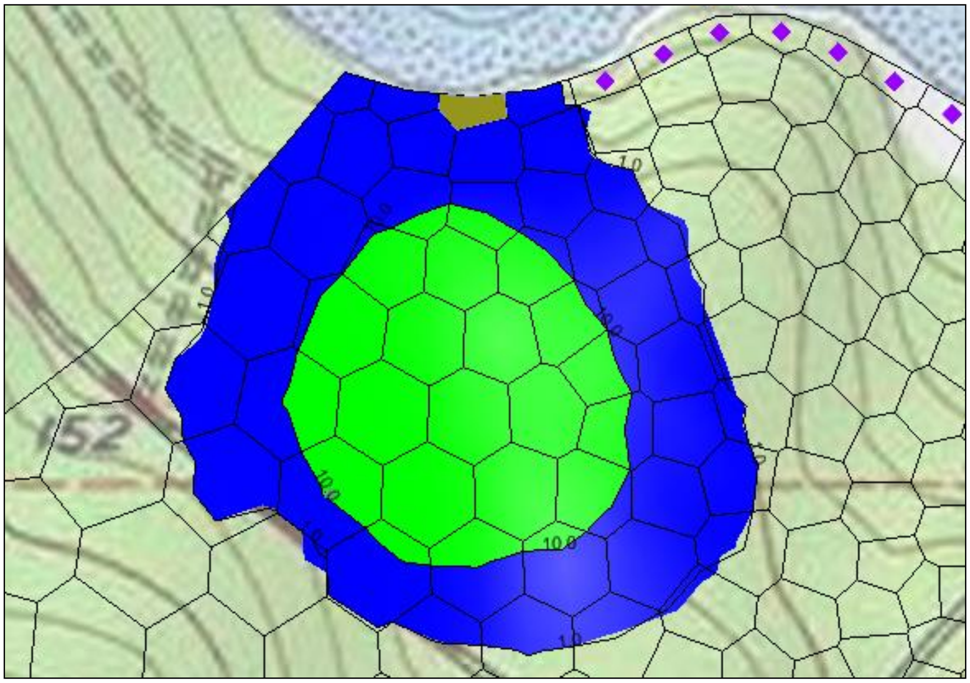


Figure 10 Select cell 840 in layer 1

4. Click the **Plot Wizard** macro to open the *Plot Wizard* dialog.
5. Under *Plot Type*, select the *Active Dataset Time Series* option.
6. Click **Finish** to close the *Plot Wizard* dialog and generate the plot.

The *Active Dataset Time Series* plot should appear similar to Figure 11. Note the significant difference of this time series with Figure 7, which was computed without matrix diffusion.

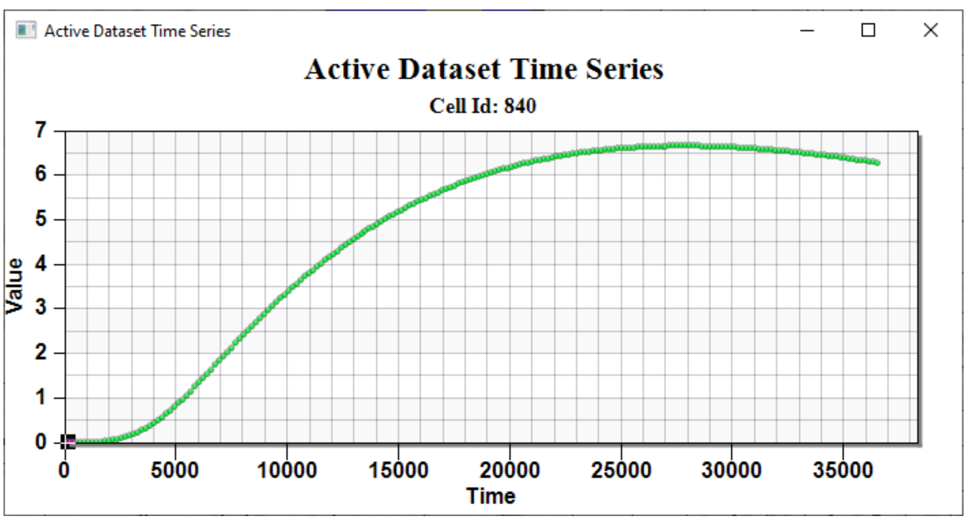


Figure 11 The Active Dataset Time Series for cell 840

14 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.

