

USER GUIDE

Incorporating Matrix Diffusion in the New MODFLOW Flow and Transport Models for Unstructured Grids

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List of Acronyms

1D: One-dimensional

3D: Three-dimensional

CDFTM: Coca/Delta Flow and Transport Model

DCE: cis-1,2-dichloroethylene

DPT: dual porosity transport

GMS: Aquaveo Groundwater Modeling System graphical user interface

MDT: Matrix Diffusion Transport package for MODFLOW-USG and MODFLOW-6

MODFLOW: Groundwater flow model

MODFLOW-USG: Unstructured grid version of MODFLOW

MODFLOW 6: Latest version of MODFLOW for unstructured grids

MT3DMS: Groundwater transport model that runs with MODFLOW

PCE: Tetrachloroethylene

PFAS: Per- and polyfluorinated substances

REMChlor-MD: Screening level transport and remediation model with matrix diffusion

TCE: Trichloroethylene

VC: Vinyl chloride

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ABSTRACT

The DoD has long term liability associated with contaminated groundwater at current and former military installations. The groundwater contaminants at these sites include chlorinated solvents, energetic compounds, and emerging contaminants such as PFAS and 1,4-dioxane. Some of these contaminated sites have proven to be exceedingly difficult to remediate due to the phenomenon of matrix diffusion. Matrix diffusion, also called “back diffusion,” occurs when contaminants diffuse from high permeability zones into adjacent low permeability zones during a “loading period.” During the “release period,” the contamination may be removed from the high permeability zones, but contaminants in the low permeability zones gradually diffuse back into the high permeability zones at significant levels. This process may occur in any heterogeneous setting, but it is particularly important in certain fractured bedrock sites, and in sites with silt or clay lenses and layers.

Existing groundwater plume models can only simulate matrix diffusion processes under very ideal circumstances, using computationally intensive fine grids or with crude dual porosity approaches. Groundwater transport models at most sites do not include this important plume process at all, and therefore are likely to be unreliable for making long-term predictions of plume behavior.

Objective: The purpose of this effort was to implement the semi-analytic matrix diffusion method that was recently developed for the REMChlor-MD screening model in the next generation public domain MODFLOW groundwater flow and transport codes.

Technology Description: The matrix diffusion method used in REMChlor-MD is a semi-analytical technique based on a method originally used to model transient heat conduction during enhanced oil recovery and geothermal reservoir simulation. With some modifications this method has been demonstrated to work very well for modeling matrix diffusion in both fractured and heterogeneous systems. The semi-analytic matrix diffusion method was implemented as the MDT matrix diffusion package in the MODFLOW-USG Transport and MODFLOW 6 FORTRAN codes. The Aquaveo Groundwater Modeling System (GMS) graphical user interface has been modified to run the MODFLOW-USG Transport and MODFLOW 6 codes with the MDT package. A total of seven detailed tutorials have been developed to show users how to run the MDT package using GMS v.10.7 with both MODFLOW-USG and MODFLOW 6.

Publications:

- Pham, K.T., K.M. Walton, S. Chapman, B. Parker, and R.W. Falta, 2023, Simulating matrix diffusion in discrete fracture networks using semi-analytic and dual-porosity models, submitted to *Water Resources Research*.
- Pham, K.T., 2022, Use of a Trial Function Method to Semi-analytically Simulate Matrix Diffusion in Heterogeneous and Fractured Media, Ph.D. Dissertation, Clemson University, Clemson, SC.
- Pham, K.T. and R.W. Falta, 2022, Use of semi-analytical and dual-porosity models for simulating matrix diffusion in systems with parallel fractures, *Advances in Water Resources*, V. 164.
- Falta, R.W., S. Panday, A. Lemon, and S. Farhat, MDT Matrix Diffusion Package for MODFLOW 6 and MODFLOW-USG Transport, presented at the MODFLOW and More 2022 Conference, Princeton, NJ, June 2022.
- Pham, K., and R.W. Falta, Using a Semi-Analytical Method to Simulate Matrix Diffusion in Random Discrete Fracture Systems, presented at the MODFLOW and More 2022 Conference, Princeton, NJ, June 2022.

Executive Summary

Matrix diffusion can dominate the long-term behavior of groundwater contaminants at DoD installations. Matrix diffusion occurs when contaminated water moves through a high permeability zone that is adjacent to a lower permeability zone (Figure ES-1). A concentration gradient between the two zones drives a forward diffusive mass flux that can load the lower permeability zone with the contaminant. Later, when the high permeability zone is remediated, or flushed, the concentration gradient is reversed, leading to back diffusion from the low permeability zone into the high permeability zone. Back diffusion of the contaminant may lead to exceedance of regulatory standards in the high permeability zone for decades or more.

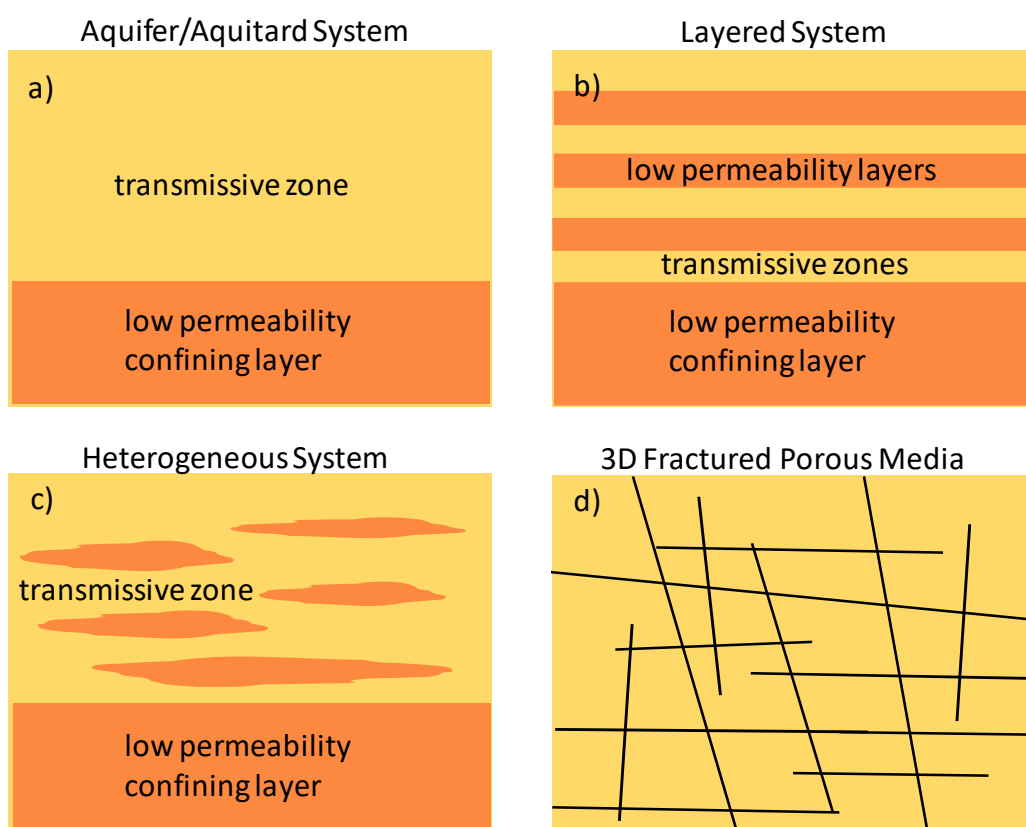


Figure ES-1. Geologic systems that contain high and low permeability zones that can result in matrix diffusion.

Modeling matrix diffusion with traditional numerical models is difficult because the matrix diffusion is typically driven by concentration gradients that occur at a scale of centimeters or less. In contrast, three-dimensional (3D) field scale numerical models of flow and transport usually have numerical gridblocks or cells that have dimensions of one to tens of meters or more. For this reason, it is most practical to simulate matrix diffusion at the sub-gridblock scale.

The classical method for simulating sub-gridblock scale mass transfer is the dual porosity method, and this method can be used in some situations to model matrix diffusion. However, the dual porosity method requires calibration of the mass transfer coefficient, the mass transfer coefficient tends to be time-dependent, and the method can fail to resolve dynamic local concentration gradients that occur during contaminant loading and unloading (Pham and Falta, 2022; Gaun et al., 2008).

In our earlier ESTCP project ER-201426, we developed an efficient semi-analytical method for simulating matrix diffusion at the sub-gridblock scale (Falta and Wang, 2017; Muskus and Falta, 2018). That method was implemented in a screening level numerical model called REMChlor-MD (Farhat et al., 2018). As a screening level model, REMChlor-MD can only consider a simple uniform groundwater flow in one direction, which limits its use at complex sites, or at sites where the flow field changes due to pumping or other stresses.

The current project implemented the sub-gridblock scale semi-analytic matrix diffusion method from REMChlor-MD into the latest versions of MODFLOW-USG (Panday, 2023) and MODFLOW 6 (Langevin et al., 2022). MODFLOW-USG and MODFLOW 6 are comprehensive 3D groundwater flow and transport models that can use unstructured numerical grids. The FORTRAN source codes for these models were modified to include a new MDT Matrix Diffusion Transport package. The MDT package is an optional package that can be selected by the user. The input parameters required by the MDT package include geometrical factors, geologic parameters, and chemical characteristics. These required parameters are identical to those used in the REMChlor-MD matrix diffusion method.

The MDT package for MODFLOW-USG and MODFLOW 6 is built into a new version of the graphical user interface by Aquaveo called the Groundwater Modeling System or GMS, version 10.7. From GMS, a groundwater flow and transport model can be developed using a conceptual model with map coverages to define boundary conditions, sources and sinks and parameter distributions. The MDT package is activated by selecting it as an optional package in MODFLOW. Figure ES-2 shows a screen shot from a GMS model using an unstructured 3D grid with MODFLOW-USG.

This example is one of seven sample problems that have been developed for use as GMS tutorials. These tutorials are listed in the Appendices of this report, and they are available online from Aquaveo at: <https://aquaveo.com/software/gms-learning-tutorials>. These tutorials recreate test problems from Falta and Wang (2017) and Muskus and Falta (2018) that involve simulations of matrix diffusion in fractured rocks and in heterogeneous unconsolidated materials. These were benchmarking problems from our previous ER-201426 project where we compared the semi-analytic matrix diffusion method to analytical solutions and laboratory experimental data.

The 3D model shown in Figure ES-2 simulates a hypothetical release of trichloroethylene (TCE) into the subsurface in a small source area. The TCE concentration is maintained at 1000 ug/L for ten years, and then it is reduced to 1 ug/L, simulating an effect source remediation effort.

Figure ES-3 shows a comparison of the simulated TCE concentrations in the aquifer 30 years after the initial release, and 20 years after source remediation. The simulation that includes matrix diffusion shows generally lower concentrations and shorter travel distances than the simulation that does not include matrix diffusion.

Concentration versus time plots of the simulated TCE concentration at two key locations are shown in Figure ES-4. The simulation that includes matrix diffusion (orange lines) predicts lower concentrations that persist for a longer time compared to the simulation that does not include matrix diffusion (blue lines).

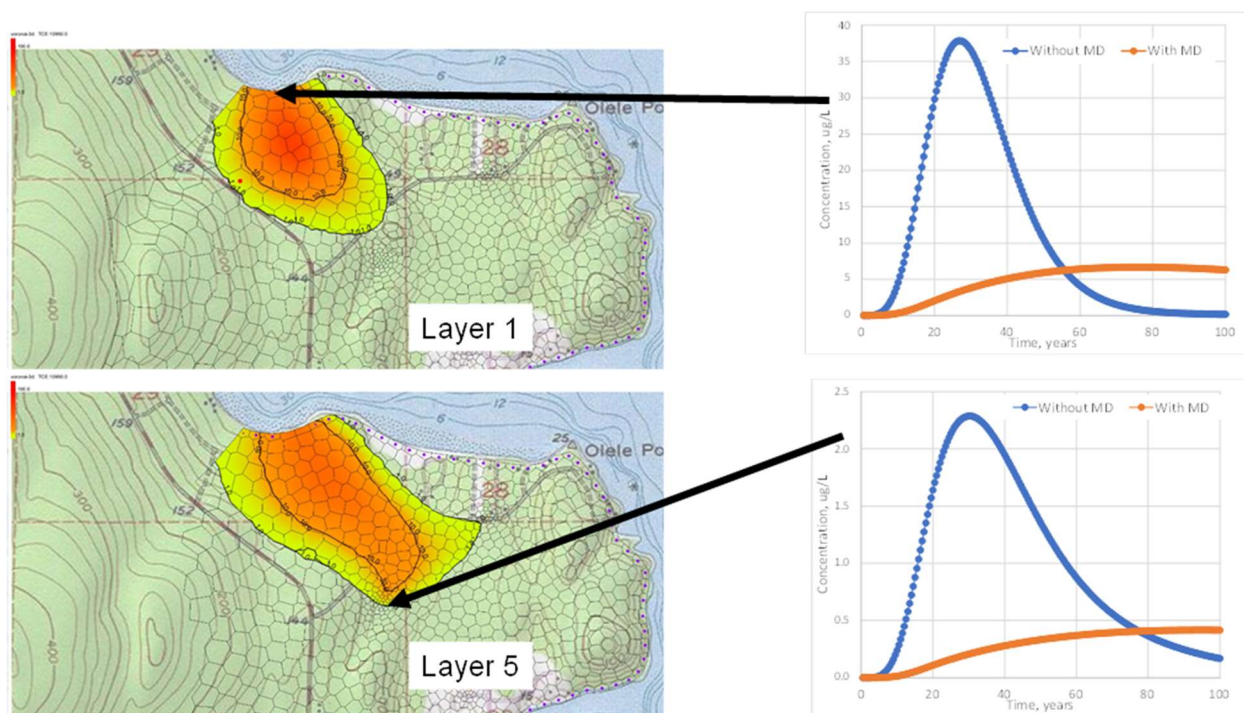


Figure ES-4. Simulated TCE concentrations with (orange) and without (blue) matrix diffusion.

The MDT package has a minimal computational burden, and the simulation that include matrix diffusion typically run nearly as quickly as transport simulations without it. The FORTRAN source codes for MODFLOW-USG and MODFLOW 6 with the MDT package are available free of charge from ESTCP, and from GSI Environmental. Aquaveo GMS v10.7 is commercially available.

Executive Summary References

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1.0 INTRODUCTION

The DoD faces long term liability associated with groundwater contaminated by chlorinated solvents and other contaminants such as per- and polyfluoroalkyl substances (PFAS). While much progress has been made over the past 20 years, significant challenges remain at some sites. These difficult sites often have large and persistent dissolved contaminant plumes that are present in complex heterogeneous or fractured media. It is now known that the process of matrix diffusion can be a primary cause of the persistence of these large dilute plumes (Parker et al., 1994; 1997; Ross and Lu, 1999; Esposito and Thompson, 1999; Reynolds and Kueper, 2001; 2002; 2004; Liu and Ball, 2002; Parker et al., 2004; Falta, 2005; Chapman and Parker, 2005; Parker et al., 2008; Sale et al., 2008, 2013)

Matrix diffusion, also called “back diffusion” occurs when contaminants diffuse from high permeability zones into adjacent low permeability zones during a “loading period.” During the “release period,” the contamination may be removed from the high permeability zones, but contaminants in the low permeability zones gradually diffuse back into the high permeability zones at significant levels relative to regulatory standards. This process may occur in any heterogeneous setting, but it is particularly important in fractured bedrock sites, and in sites with extensive clay or silt lenses or layers (Figure 1.). These types of complex site conditions lead to plumes that are long lived, requiring extensive long-term monitoring.

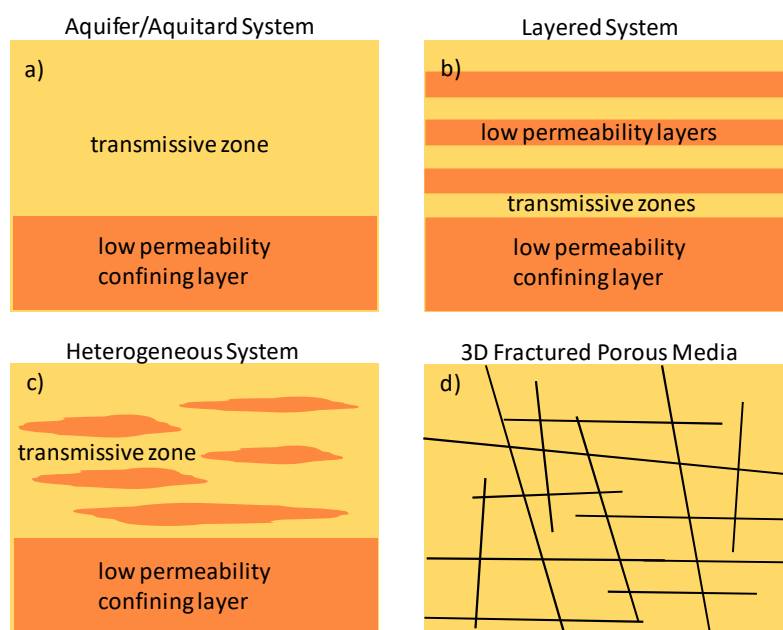


Figure 1. Typical geologic systems that can lead to strong matrix diffusion effects.

There is a need for cost-effective management tools for addressing groundwater contamination in complex fractured and heterogeneous environments where matrix diffusion effects are important. Current numerical flow and transport models are poorly suited for modeling matrix diffusion because simulation of the diffusion processes requires model resolution that is much higher than is commonly used or practical (Chapman et al., 2012). A dual porosity mass transfer modeling approach is sometimes used to simulate matrix diffusion (Feehley et al., 2000). However, the dual

porosity mass transfer model requires calibration of the mass transfer coefficient, and the first-order representation of the matrix diffusion concentration gradient is accurate only under a limited set of circumstances (Gaun et al., 2008; Pham and Falta, 2022; Pham et al., 2023).

The lack of numerical models that can accurately simulate dissolved phase contaminant transport at the end stage of remediation is a critical problem for the groundwater remediation industry. Current applications of groundwater solute transport models mean that many decision makers (regulators, site owners, consultants, and military branches) may be relying on inaccurate information to make important, multi-million dollar remediation decisions. The need for accurate groundwater solute transport models that can simulate the “long tail” at matrix diffusion dominated sites is one of the key challenges for our field.

As part of our earlier ESTCP project ER-201426 we developed a numerical method for simulating matrix diffusion in heterogeneous and fractured systems that is both practical and accurate (Falta and Wang, 2017; Muskus, 2017; Muskus and Falta, 2018). This method was extensively tested and implemented in a screening level model called REMChlor-MD (Farhat et al., 2018). The unique simulation capability in REMChlor-MD allows the user to perform transport simulations in a few seconds or minutes that are comparable in accuracy to fine-grid numerical simulations that take hours or days to run using a conventional numerical transport model (Muskus and Falta, 2018). The matrix diffusion model is based on physical parameters that can be readily measured or estimated, and little or no calibration of parameters is required.

A limitation of the REMChlor-MD model is that it assumes a one-dimensional (1D) uniform flow field. This assumption is appropriate for a screening-level model, but it restricts its use to problems involving simple flow fields without pumping wells. In the current project, we have implemented the REMChlor-MD matrix diffusion method in the three-dimensional (3D) flow and transport models MODFLOW-USG and MODFLOW 6. This is done through a new optional simulation package called the MDT matrix diffusion package.

The MODFLOW family of codes are the industry standard for modeling 3D groundwater flow. The most recent version of MODFLOW is MODFLOW 6 (Langevin et al., 2017; 2022). MODFLOW 6 incorporates the flexible unstructured grid capability developed by Panday et al., (2013) in the MODFLOW-USG code. The older 3D MODFLOW flow models are coupled with a 3D transport model such as MT3DMS (Zheng and Wang, 1999) to simulate contaminant transport. The MT3DMS transport model is restricted to regular grids, but Panday (2023) has developed a contaminant transport model for MODFLOW-USG that simulates transport in unstructured grids (<https://www.gsi-net.com/en/software/free-software/modflow-usg.html>). All these FORTRAN codes are open source, public domain models. MODFLOW 6 incorporates unstructured transport modeling capabilities similar to that of Panday (2023).

The MODFLOW FORTRAN codes are usually run using a proprietary graphical user interface such as the Groundwater Modeling System (GMS) by Aquaveo (<https://www.aquaveo.com/software/gms-groundwater-modeling-system-introduction>) Groundwater Vistas by ESI (<http://www.groundwatermodels.com/>) or Visual MODFLOW Flex by Waterloo Hydrogeologic (<https://www.waterloohydrogeologic.com/visual-modflow-flex/>) among other lesser known products. These commercial graphical user interfaces have revolutionized groundwater modeling by allowing much more rapid model construction and output visualization using geographical information system concepts and advanced 3D graphics.

In the present work, we have developed a capability in GMS version 10.7 that supports the matrix diffusion package capabilities in both MODFLOW-USG and MODFLOW 6.

1.1 MATHEMATICAL FORMULATION

The MDT matrix diffusion package that has been added to MODFLOW-USG and MODFLOW 6 is based on a semi-analytical method implemented in the screening level model REMChlor-MD (Falta et al., 2018; Farhat et al., 2018; Muskus and Falta, 2018). The method is based on an approach originally developed for simulating heat conduction in low permeability cap rocks (Vinsome and Westerveld, 1980). It was adapted to the analogous problem of dissolved solute diffusion in aquitards by Falta and Wang (2017) and extended to the case of embedded heterogeneities by Muskus and Falta (2018).

Matrix diffusion in low permeability materials can be approximated as a one-dimensional process that depends on the distance from the interface with the high permeability material, z_l . The governing partial differential equations for transient matrix diffusion assuming first order decay of a component $m-1$ that produces a daughter compound, m are:

$$R_{lm} \frac{\partial C_{lm}}{\partial t} = \tau_l D \frac{\partial^2 C_{lm}}{\partial z_l^2} + -\lambda_{lm} C_{lm} \quad \text{for } m = 1 \quad (1)$$

$$R_{lm} \frac{\partial C_{lm}}{\partial t} = \tau_l D \frac{\partial^2 C_{lm}}{\partial z_l^2} + y_{lm-1} \lambda_{lm-1} C_{lm-1} - \lambda_{lm} C_{lm} \quad \text{for } m > 1 \quad (2)$$

Here, the subscript l refers to the low permeability material. C_{lm} is the aqueous mass concentration of component m in the low permeability material, R_{lm} is the retardation factor of component m , τ_l is the tortuosity, D is the molecular diffusion coefficient, λ_{lm} is the first order decay rate of component m , and y_{m-1} is the mass yield of daughter component m from parent compound $m-1$. Equation (2) can be repeated for subsequent daughter products to form a complete decay chain. For example, at a site where tetrachloroethylene (PCE) undergoes decay to form TCE and the TCE decays to form cis-1,2-dichloroethylene (DCE) which decays to form vinyl chloride (VC), PCE would be the parent compound ($m=1$), governed by Equation (1), while TCE, DCE, and VC would be daughter compounds governed by Equation (2) with $m=2, 3$, and 4 , respectively.

The semi-analytical method is based on the thermal conduction approximation developed by Vinsome and Westerveld (1980). Bear et al. (1994) and Falta and Wang (2017) adapted the Vinsome and Westerveld model to the problem of matrix diffusion in a semi-infinite aquitard using the mathematical analogy between transient heat conduction and transient matrix diffusion. The approach is based on the use of a fitting function to describe the concentration profile as a function of distance from the interface in the low permeability matrix:

$$C_{lm}(z_l, t) = (C_m^{t+\Delta t} + p_m z_l + q_m z_l^2) e^{-z_l/d_m} \quad (3)$$

where $C_m^{t+\Delta t}$ is the current concentration of component m at the interface between high permeability and low permeability zones and p_m and q_m are fitting parameters. The concentration $C_m^{t+\Delta t}$ is the concentration that is solved for in each gridblock of a normal numerical simulation, and it is assumed to represent the average concentration in the high permeability part of the gridblock. The concentration penetration depth, d_m , is defined by:

$$d_m = \frac{\sqrt{\kappa_{lm} t}}{2}; \quad \kappa_{lm} = \frac{\tau_l D}{R_{lm}} \quad (4)$$

The zero level of the concentrations in Equation (2) correspond to the initial (uniform) concentrations in the low permeability zone, which is usually zero. The fitting parameters p_m and q_m are determined by two conservation of mass laws. The first constraint requires the fitting function to satisfy the governing equation at the high permeability/low permeability interface:

$$R_{lm} \frac{\partial C_{lm}}{\partial t} = \tau_l D \frac{\partial^2 C_{lm}}{\partial z_l^2} \Big|_{z_l=0} + y_{lm-1} \lambda_{lm-1} C_{lm-1} \Big|_{z_l=0} - \lambda_l C_{lm} \Big|_{z_l=0} \quad (5)$$

The component production term in Equation (5) is only used for daughter products ($m > 1$).

In order to discretize the equation, a first-order finite difference approximation is applied to the time derivative. C_{lm} and C_{lm-1} are replaced with the trial functions on the right-hand side, which results in:

$$R_{lm} \left(\frac{C_m^{t+\Delta t} - C_m^t}{\Delta t} \right) = \tau_l D \left(\frac{C_m^{t+\Delta t}}{d_m^2} - \frac{2p_m}{d_m} + 2q_m \right) + y_{lm-1} \lambda_{lm-1} C_{m-1}^{t+\Delta t} - \lambda_{lm} C_m^{t+\Delta t} \quad (6)$$

The second constraint is the mass conservation of the components in the low permeability material. This requires that the rate of change of total mass in the matrix is to equal the mass flux across the interface minus the rate of decay in the matrix plus the rate of production in the matrix. For an ideal semi-infinite aquitard case, the integral of distance into low permeability areas is defined from zero to infinity (Falta and Wang, 2017). This study deals with finite embedded heterogeneities, such as low permeability lenses and layers or fractured porous media with parallel fractures. Thus, the mass conservation constraint must account for a finite diffusion distance. The characteristic average diffusion length, L corresponds to the average maximum depth or distance of diffusion into the low permeability material. The low permeability matrix mass balance constraint becomes:

$$R_{lm} \frac{\partial}{\partial t} \int_0^L C_{lm} dz_l = -\tau_l D \frac{\partial C_{lm}}{\partial z_l} \Big|_{z_l=0} + y_{lm-1} \lambda_{lm-1} \int_0^L C_{lm-1} dz_l - \lambda_{lm} \int_0^L C_{lm} dz_l \quad (7)$$

The concentration integrals in Equation (7) are directly related to the mass of the components in the low permeability material. The solution of the concentration integrals in Equation (7) using the trial functions have the form:

$$I_m(t) = \int_0^L C_{lm} dz_l = C_m(t)d_m + p_m d_m^2 + 2q_m d_m^3 - \left(C_m(t)d_m + p_m d_m L + p_m d_m^2 + q_m d_m L^2 + 2q_m d_m^2 L + 2q_m d_m^3 \right) e^{-L/d_m} \quad (8)$$

Following Pruess and Wu (1988, 1993), this integral can be written as a weighted function of $C_m(t)$, p_m , and q_m :

$$I_m(t) = \delta_m C_m(t) + \gamma_m p_m + \beta_m q_m \quad (9)$$

where

$$\delta_m = d_m - d_m e^{-L/d_m} \quad (10)$$

$$\gamma_m = d_m^2 - (d_m L + d_m^2) e^{-L/d_m} \quad (11)$$

$$\beta_m = 2d_m^3 - (L^2 d_m + 2d_m^2 L + 2d_m^3) e^{-L/d_m} \quad (12)$$

For the special case of an ideal infinite aquitard, where $L \rightarrow \infty$, $\delta_m = d_m$; $\gamma_m = d_m^2$; $\beta_m = 2d_m^3$, corresponding to the definition of $I(t)$ in Falta and Wang (2017). Replacing the derivative in Equation (7) with a finite difference approximation of the concentration integral, and substituting C_{lm} with the fitting functions in the space derivative and decay and production terms gives:

$$R_{lm} \left(\frac{\delta_m C_m^{t+\Delta t} + \gamma_m p_m + \beta_m q_m - I_m^t}{\Delta t} \right) = \tau_l D \left(\frac{C_m^{t+\Delta t}}{d_m} - p_m \right) + y_{lm-1} \lambda_{lm-1} I_{m-1}^{t+\Delta t} - \lambda_{lm} (\delta_m C_m^{t+\Delta t} + \gamma_m p_m + \beta_m q_m) \quad (13)$$

Solving the linear equations (6) and (13) by substitution provides the expressions for the fitting parameters p_m and q_m :

$$p_m = \frac{I_m^t + \frac{y_{lm-1} \lambda_{lm-1} I_{m-1}^{t+\Delta t} \Delta t}{R_{lm}} - E C_m^{t+\Delta t} - A_m \left(\frac{C_m^{t+\Delta t} - C_m^t}{2\kappa_{lm} \Delta t} - \frac{C_m^{t+\Delta t}}{2d_m^2} - \frac{y_{lm-1} \lambda_{lm-1} C_{m-1}^{t+\Delta t}}{2R_{lm} \kappa_{lm}} + \frac{\lambda_{lm} C_m^{t+\Delta t}}{2R_{lm} \kappa_{lm}} \right)}{\frac{A_m}{d_m} + B_m} \quad (14)$$

$$q_m = \frac{\frac{(C_m^{t+\Delta t} - C_m^t)d_m^2}{\kappa_{lm}\Delta t} - C_m^{t+\Delta t} + 2d_m p_m - \frac{y_{lm-1}\lambda_{lm-1}C_{m-1}^{t+\Delta t}d_m^2}{R_{lm}\kappa_{lm}} + \frac{\lambda_{lm}C_m^{t+\Delta t}d_m^2}{R_{lm}\kappa_{lm}}}{2d_m^2} \quad (15)$$

where

$$A_m = \beta_m + \frac{\lambda_{lm}\Delta t}{R_{lm}}\beta_m \quad (16)$$

$$B_m = \gamma_m + \kappa_{lm}\Delta t + \frac{\lambda_{lm}\Delta t}{R_{lm}}\gamma_m \quad (17)$$

$$E_m = \delta_m - \frac{\kappa_{lm}\Delta t}{d_m} + \frac{\lambda_{lm}\Delta t}{R_{lm}}\delta_m \quad (18)$$

Unique values of p_m and q_m are calculated in the aquifer gridblocks containing low permeability zones, and they are updated at each time step to represent the changing concentration profile in the low permeability zones. The concentration integral $I_m^{t+\Delta t}$ is recalculated at every time step in every gridblock using Equation (9) and it is stored for use in the next time step (I_m^t). For the special case of diffusion in a semi-infinite aquitard with no reactions, the formulation becomes equivalent to the original Vinsome and Westerveld (1980) method for heat conduction and to the Bear et al. (1994) method for diffusion.

The matrix diffusion mass flow entering (+) or leaving (-) the high permeability zone is described by Fick's first law of diffusion. Substituting the low permeability material concentration by the trial function:

$$\dot{m}_m = A_{md}\phi_l\tau_l D \left. \frac{\partial C_{lm}}{\partial z_l} \right|_{z_l=0} = A_{md}\phi_l\tau_l D \left(-\frac{C_m^{t+\Delta t}}{d_m} + p_m \right) \quad (19)$$

where ϕ_l is the porosity of the low permeability material and A_{md} is the matrix diffusion area, defined as the interfacial area between the high permeability and low permeability zones. The equation for p_m can be rewritten as:

$$p_m = a_m C_m^{t+\Delta t} + b_m \quad (20)$$

with

$$a_m = \frac{-E_m - \frac{A_m}{2\kappa_{lm}\Delta t} + \frac{A_m}{2d_m^2} - \frac{A_m\lambda_{lm}}{2R_{lm}\kappa_{lm}}}{\frac{A_m}{d_m} + B_m} \quad (21)$$

$$b_m^{t+\Delta t} = \frac{I_m^t + \frac{A_m C_m^t}{2\kappa_{lm}\Delta t} + \frac{A_m y_{lm-1} \lambda_{lm-1} C_{m-1}^{t+\Delta t}}{2R_{lm}\kappa_{lm}} + \frac{y_{lm-1} \lambda_{lm-1} I_{m-1}^{t+\Delta t} \Delta t}{R_{lm}}}{\frac{A_m}{d_m} + B_m} \quad (22)$$

Then the expression for the matrix diffusion mass flow rate, is:

$$\dot{m} = A_{md} \phi_l \tau_l D \left(\left(a_m - \frac{1}{d_m} \right) C_m^{t+\Delta t} + b_m^{t+\Delta t} \right) \quad (23)$$

The matrix diffusion mass flow becomes a linearly concentration dependent source/sink term added in the numerical transport model gridblocks that contain (or are adjacent to) low permeability materials. The $b_m^{t+\Delta t}$ term (Equation (22)) that appears in the gradient expression for component m does not depend on the current concentration of m , but it does depend on the previous concentration and integral of m , as well as on the current concentration and integral of the parent compound, $m-1$.

The semi-analytical approximation for matrix diffusion with a finite diffusion length does not force the concentration gradient at the symmetry boundary $z_l = L$ to be zero. This might seem to be a significant limitation of the formulation, but we have not found that to be true in practice (Muskus and Falta, 2018). It appears that it is sufficient to accurately represent the concentration gradient at the interface, and the mass balance in the low permeability material. This observation is similar to that made by Pruess and Wu (1993) in their study of heat conduction in cubic matrix blocks using a similar semi-analytic method. They tried adding a cubic term to the fitting function so that the additional free parameter could be used to force the concentration gradient to be zero at $z_l = L$, but found that this formulation gave less accurate results than the two parameter fitting function. They observed that forcing the zero-gradient condition at $z_l = L$ resulted in a less accurate representation of the gradient at the interface.

1.2 DIFFERENCES IN THE MODFLOW-USG AND MODFLOW 6 MDT PACKAGES

MODFLOW-USG and MODFLOW 6 share many similarities as state-of-the-art groundwater modeling platforms. Both codes allow for complex 3D unstructured numerical grids with a robust Newton Raphson method for stabilizing unconfined flow terms. Both models now have chemical transport packages that consider advection, dispersion, zero and first order reactions and linear and nonlinear adsorption.

The workflow for setting up a MODFLOW-USG model is similar to that used in previous versions of MODFLOW, and thus will be familiar to most groundwater modelers. MODFLOW 6 requires a few different steps to set up a flow and transport model, but these are fairly straightforward. The reader is encouraged to review the seven GMS MODFLOW-USG and MODFLOW 6 tutorials in Appendices B1-B4 and C1-C3. These GMS tutorials are also available online at: <https://aquaveo.com/software/gms-learning-tutorials>.

There is one significant difference in the MDT package implementation in MODFLOW-USG and MODFLOW 6. The MODFLOW-USG version allows for first order parent-daughter reactions to occur in the low-permeability matrix. The MODFLOW 6 MDT package only allows for the decay of a single species in the matrix, with no daughter product. This limitation to the MDT package capability is due to the formulation of the MODFLOW 6 transport code, which does not currently support coupled reactions.

1.3 3D EXAMPLE SHOWING WORKFLOW AND GMS INTERFACE

The MDT package for MODFLOW-USG and MODFLOW 6 is incorporated into the Aquaveo GMS version 10.7 graphical user interface. Adding matrix diffusion to an existing groundwater flow and transport model is straightforward, only involving a few steps and a minor amount of parameter entry. The following example was developed as a GMS tutorial, and the full tutorial is listed in Appendix B4. This example is a hypothetical release of TCE that occurs in an aquifer near the coast (Falta et al., 2022). The 3D model uses an unstructured Voronoi grid that is locally refined around 3 pumping wells (Figure 2).

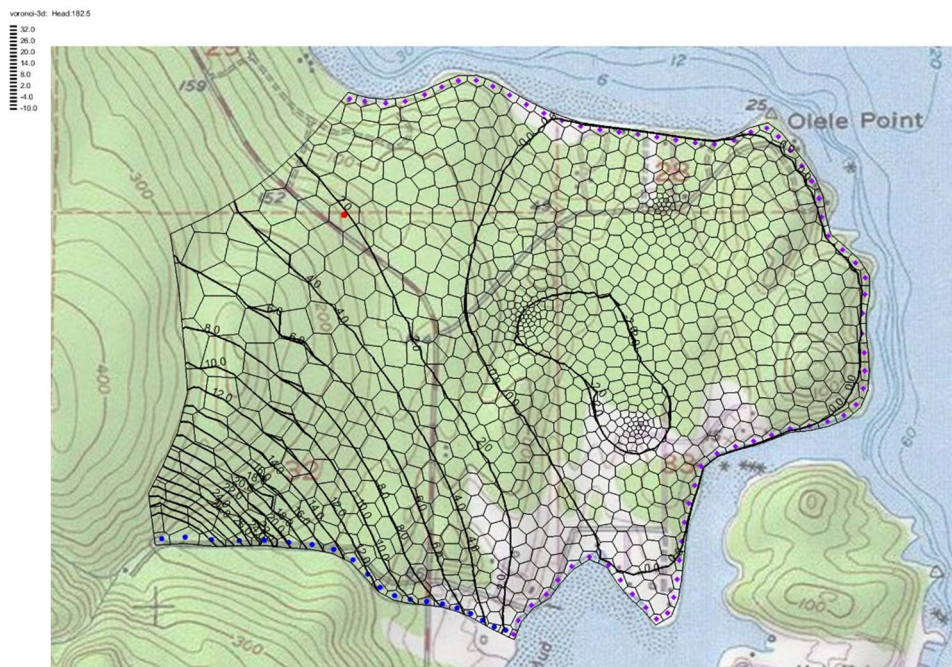


Figure 2. Unstructured grid used for 3D matrix diffusion example. Contours show hydraulic head in model layer 1.

This model has five layers, four of which are discontinuous. The upper layer represents a surficial aquifer, which is continuous across the model. Layers 2, 3, and 4 are discontinuous semi-confining layers, and layer 5 is the lower aquifer. Layer 5 pinches out towards the western side of the model. The flow and transport model was built using MODFLOW-USG in GMS with General Head (GHB) and RIVER boundaries on the north, east, and south sides, with a no-flow boundary to the west. A source of TCE is maintained in one model cell (the red dot in a cell in the upper left-hand part of Figure 2) at a concentration of 1000 ug/L for a period of 10 years, before the concentration is reduced to 1 ug/L. This step-change in concentration represents an aggressive source remediation effort that occurs 10 years after the TCE release, removing almost all of the source. Figure 3 shows the simulated TCE contours in layers 1 and 5 after 30 years (20 years after source removal) without considering matrix diffusion.

Without matrix diffusion

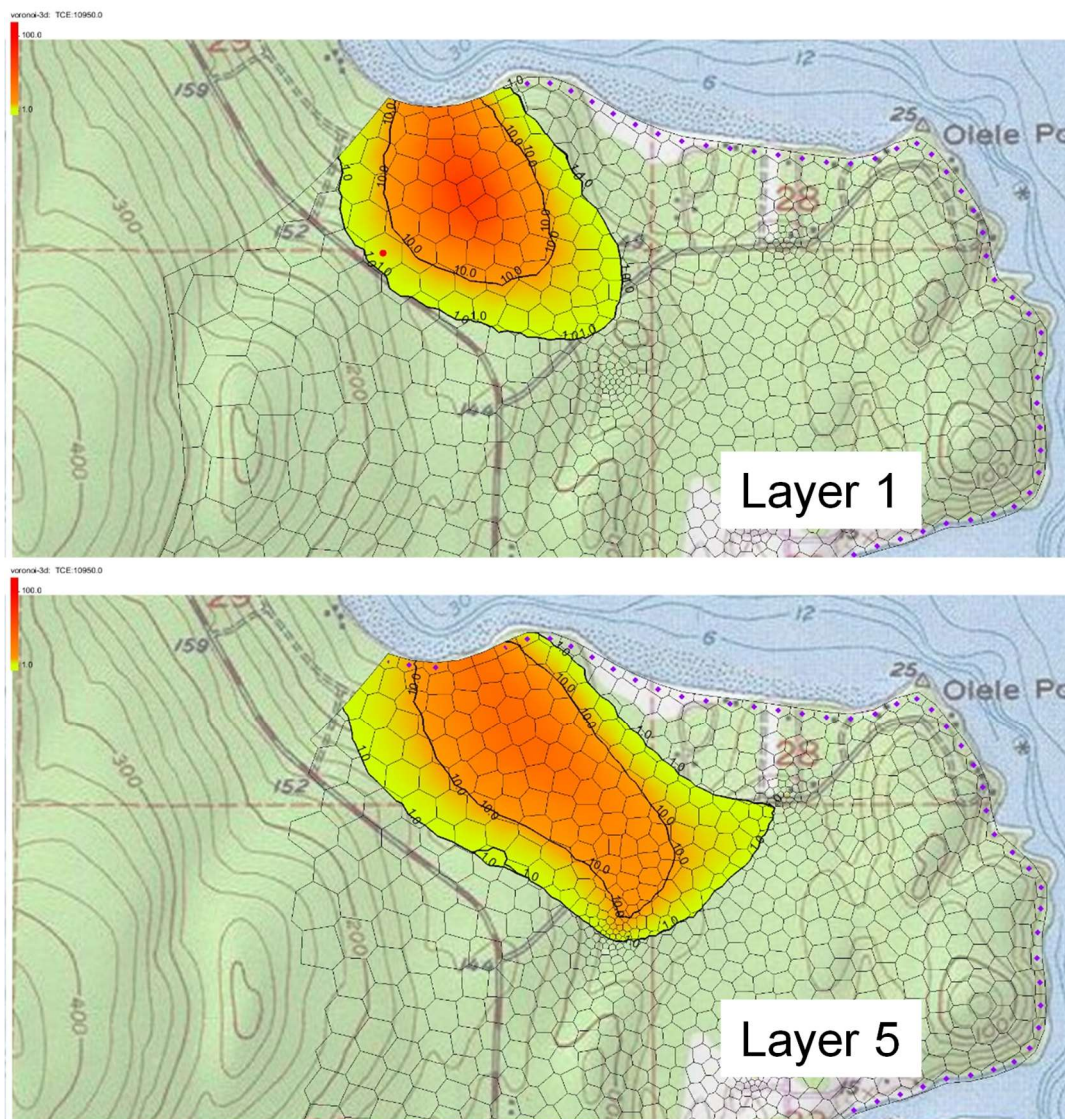


Figure 3. Simulated TCE concentrations after 30 years, 20 years after source removal.

This simulation predicts substantial TCE discharge into the water body to the north, and the plume has reached two of the 3 pumping wells in model layer 5 at 30 years.

To allow this model to include matrix diffusion, the MDT package is enabled as an optional MODFLOW package (Figure 4).

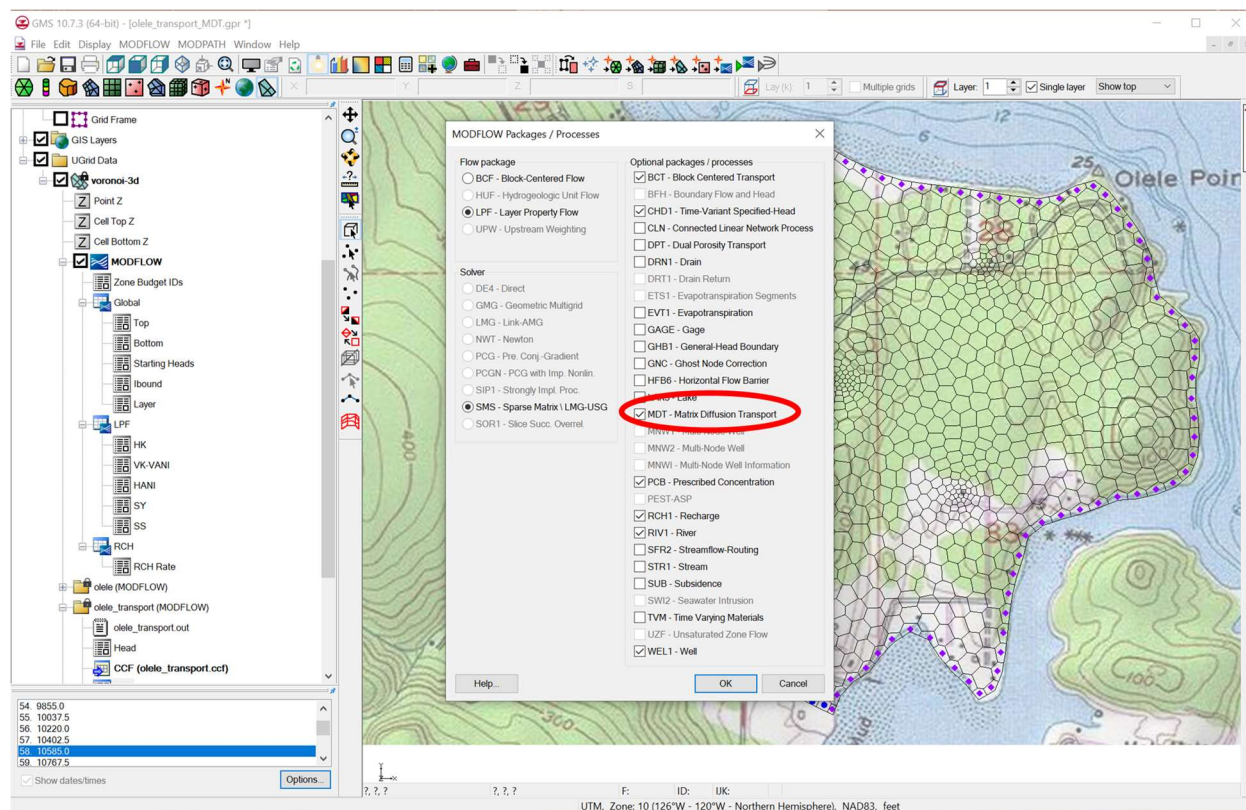


Figure 4. Screenshot from GMS V10.7 showing selection of the MDT Matrix Diffusion Transport package for MODFLOW-USG.

With the MDT package enabled, the user then enters a GMS dialogue for parameter entry. The necessary properties are grouped into aquifer properties and chemical species properties, and each parameter can be specified as a constant value, or it may be edited on a cell-by-cell basis. Figure 5 show the MDT data entry for the aquifer and chemical species properties for MODFLOW-USG. The individual parameters in Figure 5 are defined in the next section, and also in the GMS tutorials in the Appendices.

MDT Package

Comments
Variables
Aquifer Properties
Species Properties

	Property Name	Use Constant	Constant Value	Array Editor
1	MDFLAG	☒	2.0	Edit...
2	VOLFRACMD	☒	0.2	Edit...
3	PORMD	☒	0.4	Edit...
4	RHOBMD	☒	1.6	Edit...
5	DIFFLENMD	☒	1.64	Edit...
6	TORTMD	☒	0.3	Edit...

Help... OK Cancel

MDT Package

Comments
Variables
Aquifer Properties
Species Properties

	Species ID	Property Name	Use Constant	Constant Value	Array Editor
1	1	KDMD	☒	0.25	Edit...
2	1	DECA YMD	☒	0.0	Edit...
3	1	YIELDMD	☒	0.0	Edit...
4	1	DIFFMD	☒	0.00093	Edit...
5	1	AIOLD1MD	☒	0.0	Edit...
6	1	AIOLD2MD	☒	0.0	Edit...

Help... OK Cancel

Figure 5. MDT package matrix diffusion parameters.

This example uses a high permeability zone volume fraction (VOLFRACMD) of 0.2, and a characteristic diffusion length (DIFFLENMD) of 1.64 ft (0.5m). Estimation of these geometrical parameters is discussed in Section 5.0 and also in the REMChlor-MD User's Guide (Farhat et al., 2018). The simulated TCE contours after 30 years including matrix diffusion are shown in Figure 6. The plume migration is generally slower, with lower concentrations than the simulation that did not consider matrix diffusion, however the plume is longer-lived.

With matrix diffusion, $V_f = 0.2$, $L = 0.5\text{m}$

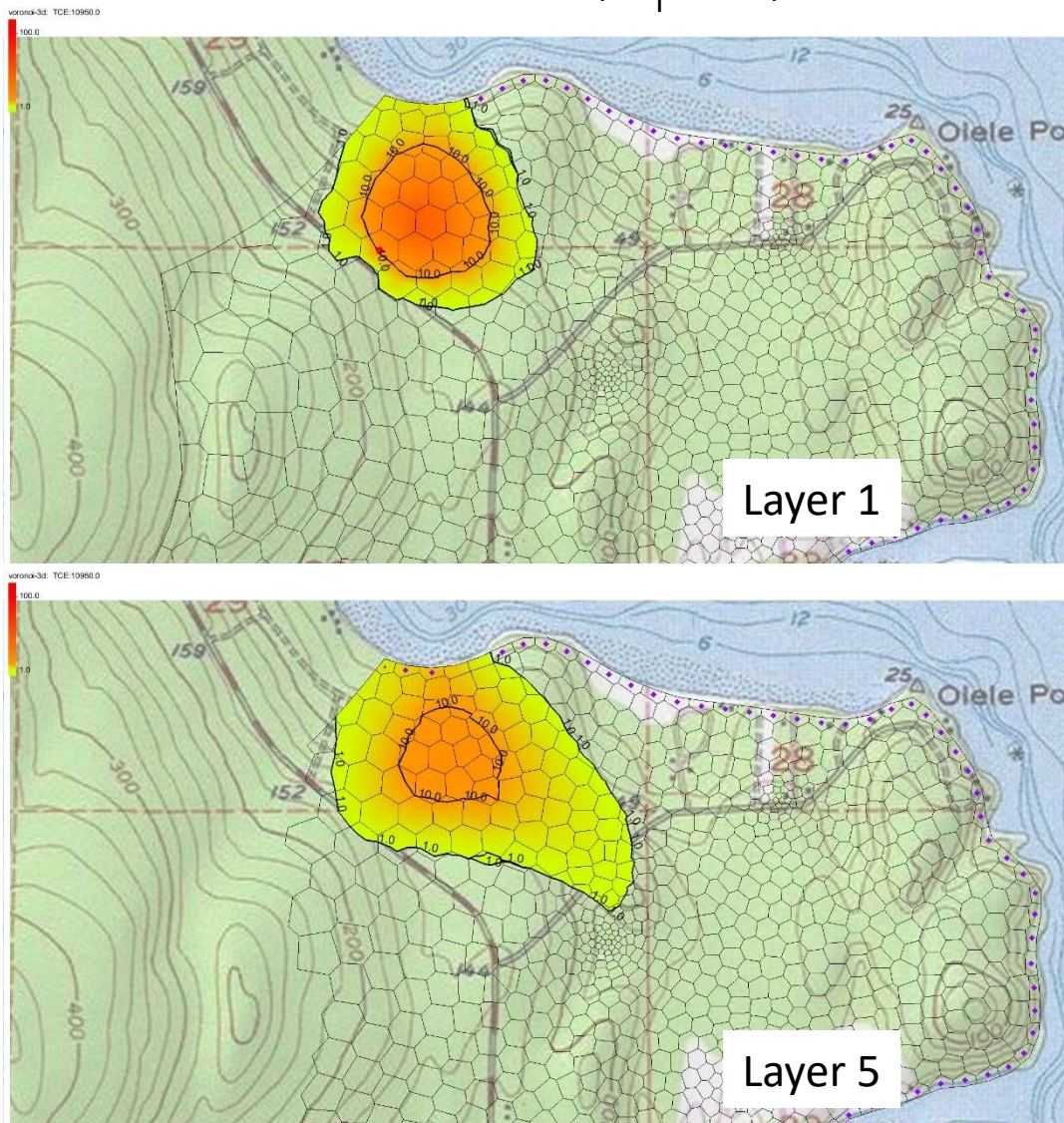


Figure 6. Simulated TCE concentrations after 30 years, considering matrix diffusion.

Figure 7 shows time-series of TCE concentration at two locations in the models; near the coast in model layer 1, where the TCE is discharging to the water body, and at a pumping well in model layer 5, where TCE has reached the well. The blue curves in these graphs are the simulated TCE concentrations without matrix diffusion. The TCE concentrations peak at about 30 years with concentrations as high as 38 ug/L discharging into the water body, and a concentration of about 2.3 ug/L near the pumping well. After 30 years, the simulated TCE concentrations decline, and reach low levels by about 100 years or less. The orange curves in Figure 7 include the effects of matrix diffusion, and indicate substantially lower concentrations at 30 years, but the plumes are persistent due to back diffusion. It is worth noting that this hypothetical example did not include any TCE decay, which could act to attenuate the plume over time.

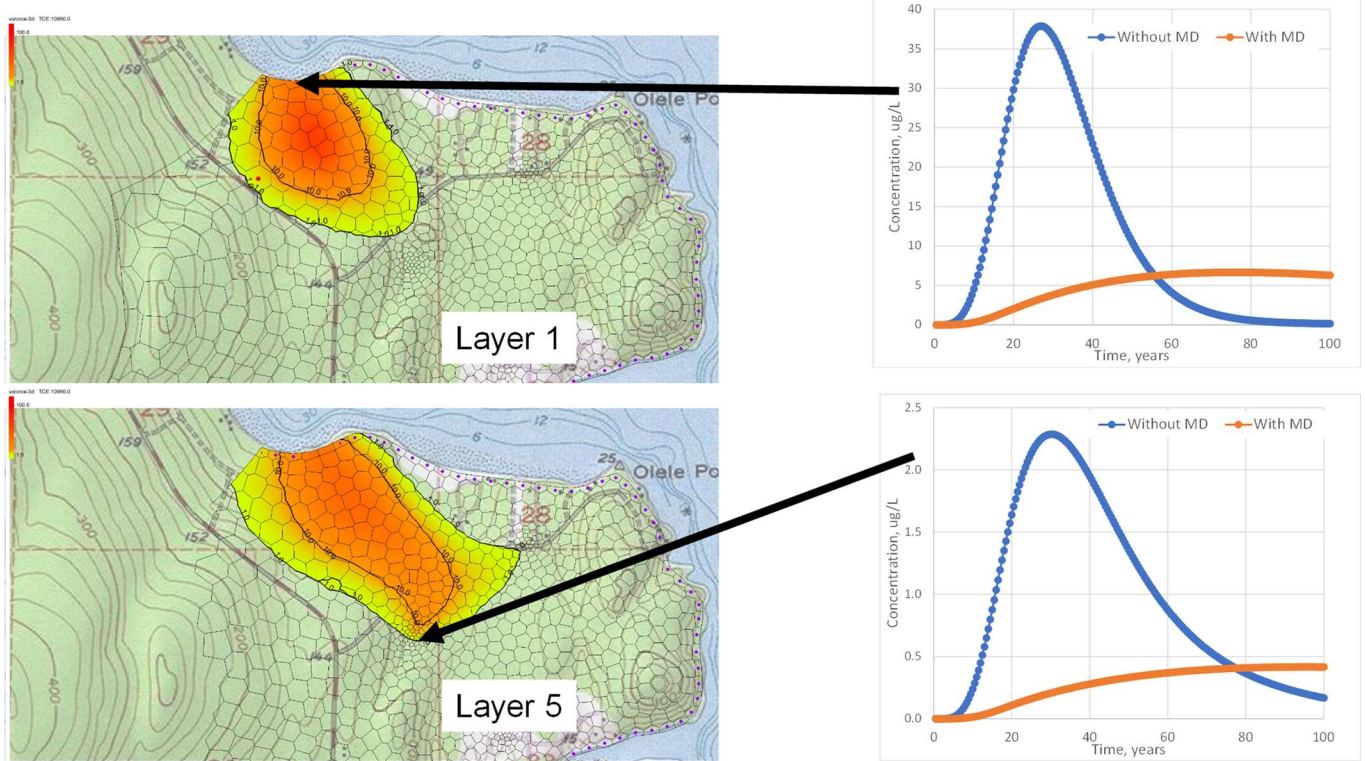


Figure 7. Comparison of simulated TCE concentrations with and without matrix diffusion.

2.0 MODFLOW-USG MDT MATRIX DIFFUSION PACKAGE

MODFLOW-USG has a chemical transport package that advection, dispersion, adsorption, and chemical reactions including chain decay with daughter product generation (Panday, 2023). The MDT matrix diffusion package is incorporated in the latest version of the code, version 2.1.0. The FORTRAN version of MODFLOW-USG Transport is supported by GSI Environmental. The source code, executable, and a complete user's guide are available for free download from the GSI website: <https://www.gsienv.com/product/modflow-usg/>. The code is also available from ESTCP.

The MODFLOW-USG Transport MDT capability has been incorporated in version 10.7 of Aquaveo's GMS graphical user interface (<https://aquaveo.com/>). Appendices B1 through B4 are four MDT package tutorials for MODFLOW-USG. These tutorials are available online at: <https://aquaveo.com/software/gms-learning-tutorials>.

2.1 NUMERICAL TREATMENT OF MDT PACKAGE

The MDT Process for MODFLOW-USG is implemented directly into the code as subroutines and modules that are called from within the main program or within the BCT solute transport program. The program design for MODFLOW-USG is expanded to include appropriate calls from the main program for allocating the required arrays, reading and preparing the information, and formulating and solving the governing transport equations. Figure 8 is a flow chart that illustrates how the MDT subroutines are implemented in the MODFLOW-USG code.

The code structure for the full chemical transport process is described in the main MODFLOW-USG user's guide (Panday, 2023).

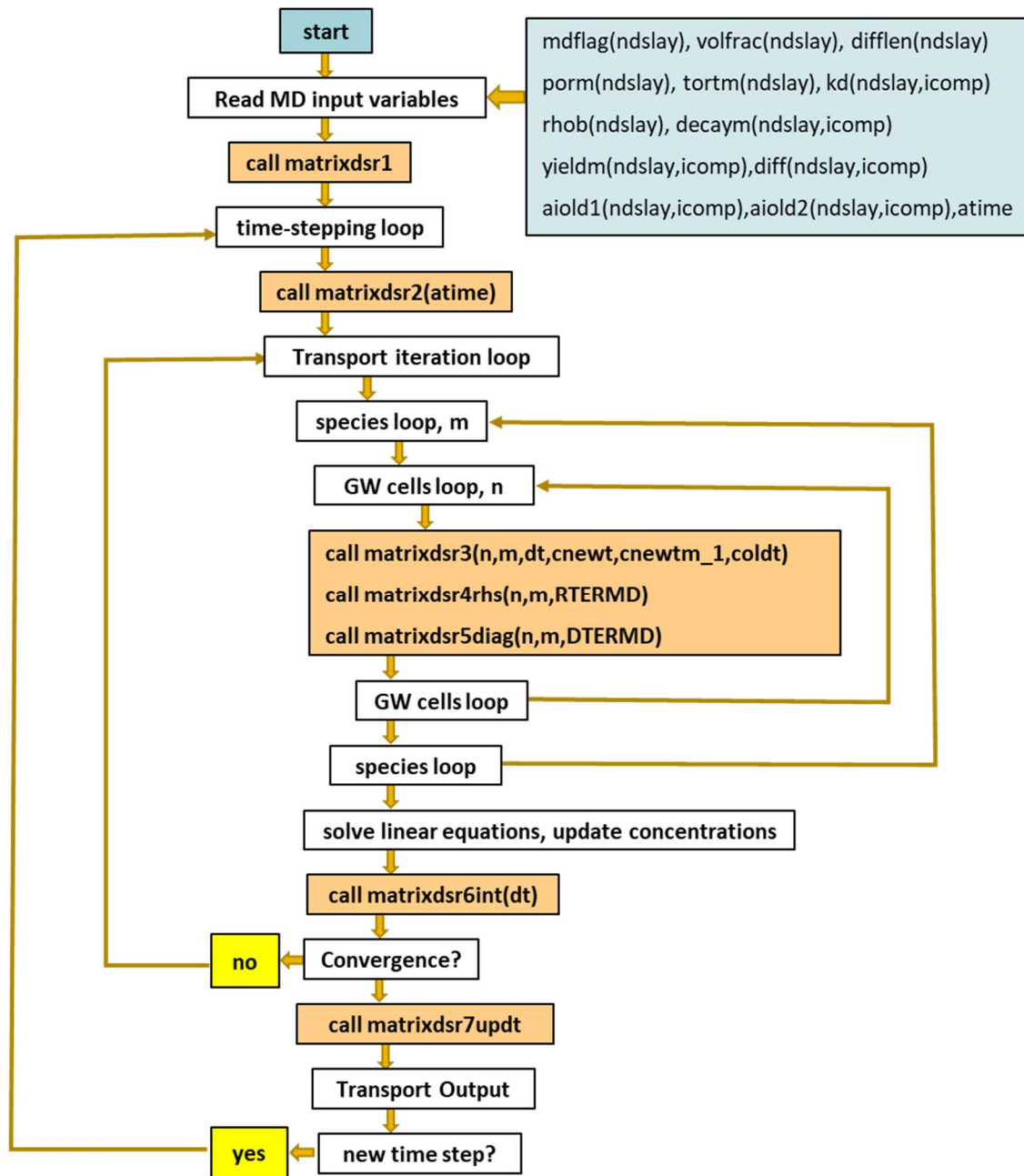


Figure 8. Flow chart showing the MDT subroutine implementation in MODFLOW-USG.

2.2 MATRIX DIFFUSION TRANSPORT PACKAGE INPUT INSTRUCTIONS

The following input instructions pertain to users running the MODFLOW-USG FORTRAN code directly. Users running the code through the GMS interface can refer to the GMS tutorials in Appendices B1 through B4 for input instructions.

Input for the Matrix Diffusion Transport (MDT) Package is read from the file that is type "MDT" in the Name File. The MDT Package input instructions include flags, indices, transport related parameters and initial conditions for solution to transport of contaminants in a steady-state or transient flow field, for the matrix domain of the dual porosity system. The MDT package functions in a similar manner to the dual porosity transport (DPT) package in that it addresses matrix diffusion in a simulation. The MDT package uses a semi-analytical solution for solute mass evolution within the matrix domain and therefore provides greater accuracy than the DPT formulation which solves for this diffusion numerically, with only one node representing the entire matrix domain. Since concentration differences in the matrix domain can be large within small distances, the DPT formulation with just one average matrix concentration may not be sufficient in many cases to accurately depict the transport of solutes where the semi-analytical solution is required. The MDT package differs from the DPT package in several other ways. Specifically, simplifications and assumptions to the semi-analytical solution are required as listed below:

- Zeroth order decay is not considered within the matrix. Only first order decay is allowed.
- Nonlinear adsorption is not considered within the matrix. Only linear adsorption is allowed.
- Branched chain decay is not considered within the matrix. Only straight chains are allowed.
- Decay is assumed to only occur in the aqueous phase; however, decay in the matrix domain can be simulated with the same decay coefficient as in water if the decay coefficient is multiplied by the matrix retardation factor for the solute.
- For transient flow conditions, the matrix is assumed to be at steady-state and there is no flow of water between the fracture domain and the matrix domain. Therefore, it is assumed that solutes move into the matrix domain by diffusion only, even in transient flow situations.
- For transient flow conditions, all the storage term is attributed to the fracture domain and none to the matrix domain. This is because of the assumption of no transfer of water between the matrix and fracture domains. In certain situations, the opposite may be the case where fractures provide the flow and little storage, while the matrix provides most of the storage of the domain with water flowing between matrix and fracture under transient flow conditions.
- The saturation of the matrix is assumed to be unity and unchanged throughout the simulation.

Matrix Diffusion Transport Package Input Instructions Note

Input for the mobile (fracture) domain is supplied with the BCT package. The input for MDT is read in a free format. Also note that only UNSRUCTURED input formats are available for the MDT package, even if the rest of the problem was set up as a STRUCTURED finite-difference system.

The flow field for transport is supplied by an associated flow simulation. The hydraulic conductivity supplied for the flow field represents the bulk (fracture plus matrix) material property

unless an option FRAKH is set, which indicates that the hydraulic conductivity supplied by the BCF or LPF packages represents the property of the fracture domain only. The MDT package cannot be used with the dual porosity flow (DPF) package, for transient flow conditions.

FOR EACH SIMULATION

1. IMDTCB IMDTCF [OPTIONS]

These variables are free format if the option “FREE” is specified in the Basic Flow Package input file; otherwise, the variables all have 10-character fields.

The rest of the file contains arrays of dual porosity transport properties. The variables needed for each cell depend on the transport options that are selected. Unneeded variables must be omitted. The required variables are read for all layers before reading the next variable. Note that there may be a different number of nodes per layer (NDSLAY) for an unstructured grid.

2. [MDFLAG(NDSLAY)] – U1DINT. Read one array for each layer.

If IDPF is zero (flow solution was not dual porosity) then read item 3.

3. [VOLFRACMD(NDSLAY)] – U1DINT. Read one array for each layer.

4. [PORMD(NDSLAY)] – U1DREL. Read one array for each layer.

5. [RHOBMD(NDSLAY)] – U1DREL. Read one array for each layer.

6. [DIFFLENMD(NDSLAY)] – U1DREL. Read one array for each layer.

7. [TORTMD(NDSLAY)] – U1DREL. Read one array for each layer.

Items 8 – 13 are read for the first component, followed by the next, till all MCOMP species components are read.

8. [KDMD(NDSLAY,ICOMP)] – U1DREL. Read one array for each layer.

9. [DECAYMD(NDSLAY,ICOMP)] – U1DREL Read one array for each layer

10. [YIELDMD(NDSLAY,ICOMP)] – U1DREL Read one array for each layer

11. [DIFFMD(NDSLAY,ICOMP)] – U1DREL. Read one array for each layer.

Items 12 – 13 (the concentration integrals AIOLD1MD and AIOLD2MD) are read only if TSHIFTMD OPTION is used. Otherwise, the coefficients are internally set to zero to denote that the concentration in the matrix domain is zero at the start of the simulation.

12. [AIOLD1MD(NDSLAY,ICOMP)] – U1DREL Read one array for each layer

13. [AIOLD2MD(NDSLAY,ICOMP)] – U1DREL. Read one array for each layer.

Explanation of Variables Read by the MDT Package:

IMDTCB—is a flag and a unit number.

If $\text{IMDTCB} > 0$, cell-by-cell mass flux terms will be written to this unit number when "SAVE BUDGET" or a nonzero value for ICBCFL is specified in Output Control. The term that is saved is the mass flux between the fracture and the matrix for every cell.

If $\text{IMDTCB} = 0$, cell-by-cell mass flux terms will not be written.

If $\text{IMDTCB} < 0$, cell-by-cell mass flux will be written in the listing file when "SAVE BUDGET" or a non-zero value for ICBCFL is specified in Output Control. The term that is written is the mass flux between the fracture and the matrix for every cell.

IMDTCF—is a flag and a unit number.

If $\text{IMDTCF} > 0$, the matrix coefficients ai1 and ai2 will be written to this unit number in a binary format when "SAVE CONC" is included (or a nonzero value of the flag ICONSV is specified) in Output Control.

If $\text{IMDTCF} = 0$, immobile domain concentrations will not be saved.

If $\text{IMDTCF} < 0$, immobile domain concentrations will be written to the listing file when the "PRINT CONC" is included (or a nonzero value of the flag ICONSV is specified) in Output Control.

OPTIONS—are optional keywords that activate options. Note that these options are required only if the flow simulation is also not dual porosity and indicates how to handle the flow simulation parameters.

FRAHK—indicates that the hydraulic conductivity and storage terms (for transient simulations) which are input are only for the fracture (mobile) domain. Otherwise, it is assumed that the hydraulic conductivity and storage input for the flow simulation are effective hydraulic conductivity and storage terms for the medium, representative of the entire volume.

FRADARCY—indicates that the Darcy flux should be computed only for the fracture domain by use of this hydraulic conductivity value. Thus, the input hydraulic conductivity is divided by the fracture volume fraction. Also, the storage terms (for transient simulations) which are input are only for the fracture (mobile) domain.

TSHIFTMD tshift —the keyword TSHIFTMD indicates that the MODFLOW start time ($t = 0$) is not the starting time of matrix diffusion, and the subsequent real variable tshift is the value of time already elapsed since matrix diffusion began. Note that if TSHIFTMD is read, then the coefficients AIOLD1MD and AIOLD2MD are also input.

MDFLAG—is the matrix diffusion type flag at any location. This flag gives options at each cell on how the matrix diffusion is treated. One value is read for every model cell. Usually, these values are read one layer at a time; however, when the XSECTION option is specified, a single two-dimensional variable for the cross section is read.

If MDFLAG (N) = 0, cell N is inactive in the matrix domain (either the cell itself is inactive or the matrix domain does not exist at this cell).

If MDFLAG(N) = 1, cell N is active in the matrix domain with matrix diffusion occurring at the bottom of the cell.

If MDFLAG(N) = 2, cell N is active in the matrix domain with matrix diffusion occurring embedded within the cell.

If MDFLAG(N) = 3, cell N is active in the matrix domain with matrix diffusion occurring at the top of the cell.

If MDFLAG(N) = 4, cell N is active in the matrix domain with matrix diffusion occurring at both the top and bottom of the cell.

If MDFLAG(N) = 5, cell N is active in the matrix domain with matrix diffusion occurring at the bottom and embedded within the cell.

If MDFLAG(N) = 6, cell N is active in the matrix domain with matrix diffusion occurring at the top and embedded within the cell.

If MDFLAG(N) = 7, cell N is active in the matrix domain with matrix diffusion occurring at the top, bottom and embedded within the cell.

Note that MDFLAG can be inactive for active flow nodes. However, MDFLAG cannot be active for a node which is inactive for the corresponding flow and transport simulation.

VOLFRACMD—is the mobile fraction at any location, i.e., the fraction of the total space that is occupied by the fracture/high permeability domain. Note that this is the same as PHIF in DPT.

PORMD—is the effective transport porosity within the matrix domain at any location.

RHOBMD—is the dry bulk density of the porous matrix of the matrix domain at any location.

DIFFLENMD—is the diffusion length for diffusive transport within the matrix domain at any location (only used for embedded heterogeneity).

TORTMD—is the tortuosity of the matrix domain at any location.

KDMD—is the adsorption coefficient (K_d) of a contaminant species in the immobile domain at any location.

DECAYMD—is the first-order decay coefficient in water and on soil (1/time) in the matrix domain at any location.

YIELDMD—is the yield coefficient for chain decay at any location. The value indicates mass of species generated by decay of the parent component. Note that component 1 is not a daughter product for any reaction and therefore the yield coefficient should be set to zero (as it is still read for all components).

DIFFMD—is the diffusion coefficient of each species component within the matrix domain at any location.

AIOLD1MD—is the concentration integral (equation 8) of each species in an element associated with matrix diffusion into an infinite acting adjacent aquitard (MDFLAG = 1, 3, 4, 5, 6, or 7). This value is used to restart a simulation with prior matrix diffusion.

AIOLD2MD—is the concentration integral (equation 8) of each species in an element associated with matrix diffusion in low permeability zones that are embedded in the volume element (MDFLAG = 2, 5, 6, or 7). This value is used to restart a simulation with prior matrix diffusion.

Output Files from MDT Package

Concentration related data output for the MDT package is included in the MODFLOW-USG transport concentration output files. The binary output files for the MDT package include the coefficients AIOLD1MD and AIOLD2MD, which are used to compute the polynomial coefficient curves for the matrix. These coefficients are useful for restarting a simulation. These arrays are written to the binary file if the flag and unit number IMDTCF is greater than zero. The header for output is 'COEFF AI1MD' or 'COEFF AI2MD' for a single species simulation. For multiple species, the species number is appended at the end of the text (for example ('COEFF AI1MD 01', 'COEFF AI1MD 02', 'COEFF AI1MD 03', etc.).

If the flag and unit number IMDTCB is greater than zero, then the rate of mass diffusion between fracture and matrix domain are written to a binary file under the title 'MD MASS STORAGE'. For a multi-species simulation, the rate of mass transfer between matrix and fracture domain is output sequentially for each species.

Starting an MDT Run with Non-zero Matrix Concentrations

In many cases, the transport simulation may start under current site conditions and not include the historical conditions that would load solutes into the matrix domain. Since the analytical solution of matrix diffusion starts only with zero initial solute concentration in the matrix domain, it must be loaded up with solute concentration prior to running the MDT transport simulation. The analytical solution of the MDT routines uses interpolation coefficients computed from the loading mass and time of loading (AIOLD1MD and AIOLD2MD) to define the concentration profile within the matrix domain and there is no direct concentration input to initialize the matrix domain with solutes. Therefore, these coefficients need to be generated for non-zero conditions so they can be subsequently used in the transport simulation. Reasonable assumptions can be made regarding the solutes in the matrix, considering the history and solutes within the mobile domain. Specifically, the matrix domain can be appropriately loaded with solutes, given solute concentrations within the fracture domain, and a residence time over which the solutes may have bled into the matrix domain. The following steps may be used to achieve this:

Step 1: Set up initial concentrations in the mobile domain to match solute concentrations at each cell, which would load up the matrix domain, and set up a transport simulation for the historical duration required. Use the flag ITRNSP = 5 (set in the BCT package input) and run the model for the number of years required to initialize the matrix. Under this flag, the flow computations are skipped entirely, the initial concentrations of the mobile domain are set to prescribed concentrations, and transport simulation is performed for a saturated

domain with zero flow, to allow only diffusion from the mobile domain into the matrix domain to occur. The outputs from the MDT routines are AIOLD1MD and AIOLD2MD instead of concentrations within the matrix domain. These coefficients are used by the MDT routines to establish solutes within the matrix domain and may be used in a subsequent simulation of transport.

Step 2: The AIOLD1MD and AIOLD2MD arrays generated for each solute in Step 1 are extracted and inserted into the MDT input file. Note that these coefficients are zero and therefore not read when starting a simulation with zero solutes in the matrix domain. The time of loading from the previous run in Step 1 is also required to define the solute profile of the matrix domain. The ITRNSP number is changed back to the original number and the forward MDT model is run as originally designed with the matrix now being loaded up.

2.3 EXAMPLE PROBLEMS USING THE MDT MATRIX DIFFUSION PACKAGE

Several benchmark and verification simulations have been conducted with the MDT Package modules to test accuracy and performance. The code has been tested in 1-, 2-, and 3-dimensions, against analytical solutions as well as against other numerical codes; specifically, MT3DMS (Zheng and Wang, 1999). The following example problems are provided to demonstrate application of the MDT Process. It is recommended that users familiarize themselves with the different simulation options, code accuracy under various conditions, and input/output structures of the MDT Process via these test problems.

Example 1: Comparison with Semi-Analytical Solution

Matrix diffusion from a single fracture (Figure 9) is used to demonstrate the MODFLOW-USG MDT package's ability to duplicate the semi-analytical solution method detailed in Falta and Wang (2017). This combination of an extremely small fracture in a much larger unfractured surface area for diffusion represents an extreme case for matrix diffusion. In this example, tritium flows through a 100 μm fracture with a Darcy velocity of 0.1 m/day at a constant concentration for 30 years (Falta and Wang, 2017; Sudicky and Frind, 1982).

This problem is repeated in Appendix B2 using the GMS interface with MODFLOW-USG, and in Appendix C2 using the GMS interface with MODFLOW 6. These tutorials can be downloaded from <https://www.aquaveo.com/software/gms-learning-tutorials>.

The system was modeled as a one-dimension (1-D) grid along the fracture in the direction of groundwater flow with unit thickness (perpendicular to groundwater flow) representing the thickness of the fracture. To replicate Falta and Wang (2017), 61 1-m wide cells were used parallel to the groundwater flow with source concentrations assigned to the first upgradient cell. Constant head boundaries were assigned to the first and last grid cells. Model input parameters are provided in Table 1. A fracture-matrix interfacial area (A_{md}) of 2 m^2 was used in each model cell to account for matrix diffusion from both the top and bottom of the fracture. The model was run for 50 years using a time-step of 0.1 years. Similar to the Falta and Wang (2017) setup, longitudinal dispersion was not included in the model.

Table 1. Model input parameters for the simulation of matrix diffusion through a single fracture.

Parameter	Value	
	Fracture	Unfractured Media
Fracture thickness (um)	100	
Darcy velocity (m/d)	0.1	0
Tritium source concentration (mg/L)	1.0	
Tritium loading period (years)	30	
Porosity (unitless)	1	0.01
Retardation factor (unitless)	1	1
Tortuosity (unitless)	1	0.1
Diffusion coefficient (m ² /s)	1.60×10^{-9}	1.60×10^{-9}
Tritium decay rate (1/yr)	5.61×10^{-2}	5.61×10^{-2}

A comparison of the MODFLOW-USG MDT package with the semi-analytical and analytical solutions of Falta and Wang (2017) is shown in Figure 10. While the source is on, the plume continues to expand with concentrations decreasing with increasing distance from the source (year 5 and year 25 curves in Figure 10). However, once the source is removed in year 30, back diffusion of tritium from the unfractured media into the fracture is what feeds the plumes observed for years 31, 33, and 50. As stated by Falta and Wang (2017):

The semi-analytical method seems to perform quite well for this demanding case, almost perfectly matching the concentrations during the loading period. At 31 years, one year after the source is removed, the semi-analytical method is able to capture the main features of the concentration reversal near the source, and it continues to perform well as the back diffusion proceeds past 50 years.

As shown in Figure 10, the MODFLOW-USG MDT package duplicated the semi-analytical solution outputs.

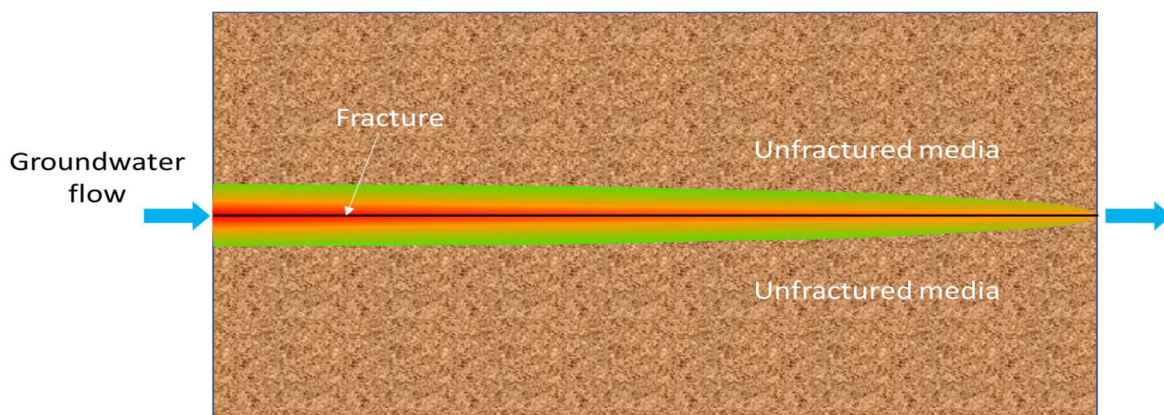


Figure 9. Simulation of matrix diffusion through a single fracture.

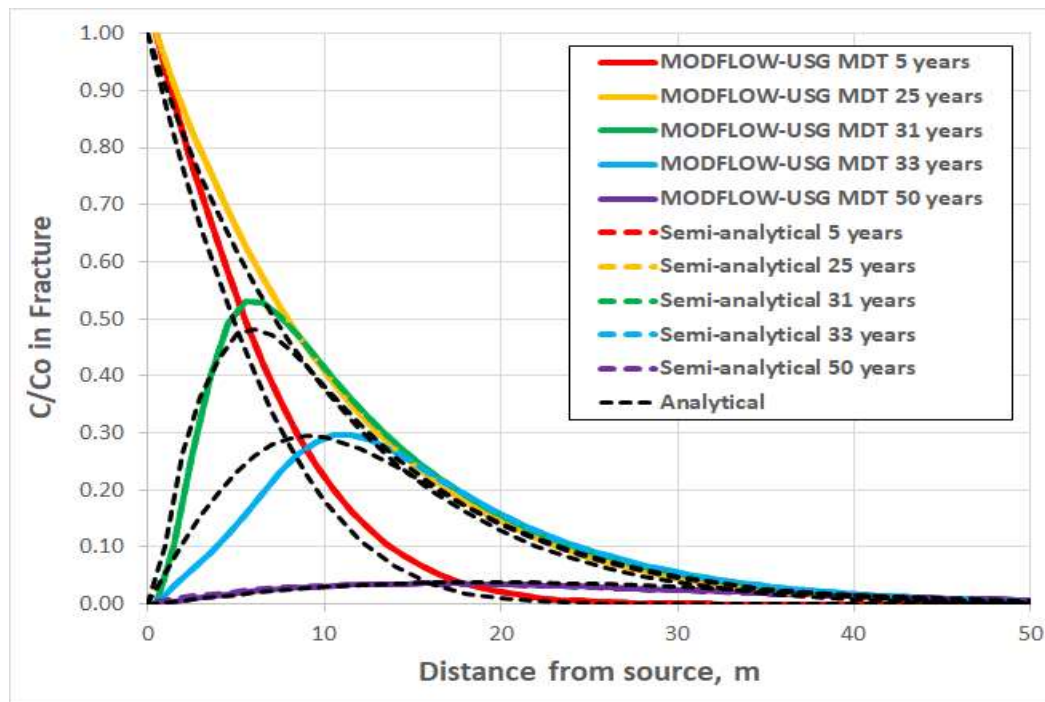


Figure 10. Comparison of MODFLOW-USG MDT package output with the REMChlor-MD semi-analytical and analytical models. Note MODFLOW-USG and the semi-analytical curves are identical.

Example 2: Comparison with Embedded Low Permeability Zones

Flow of fluorescein through a sand tank embedded with several low permeability zones is used to demonstrate the MODFLOW-USG MDT package's ability to model the effects of diffusion into and from low- k zones. The sand tank study is described in detail in Chapman et al. (2012) and a comparison with the semi-analytical solution is described in Muskus and Falta (2018). In this laboratory experiment, a tracer solution containing fluorescein and bromide was flushed through a $1.07 \times 0.03 \times 0.84$ m sand tank embedded with four clay lenses (Figure 11). Twenty-two days of tracer flushing through the system were followed by 100 days of flushing with clean water. A flow rate of 0.9 mL/min was used for the first 10 days after which a constant rate of 1.5 mL/min was employed.

This problem is repeated in Appendix B1 using the GMS interface with MODFLOW-USG, and in Appendix C1 using the GMS interface with MODFLOW 6.

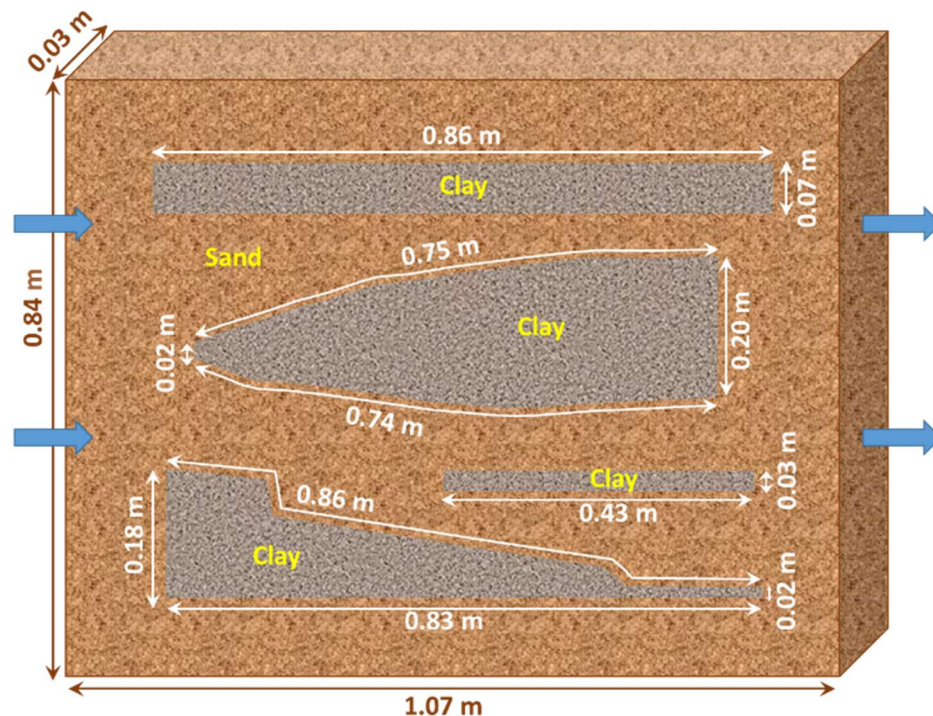


Figure 11. Sand Tank Configuration. Based on Muskus and Falta and (2018) Figure 5. Groundwater flow is from left to right (blue arrows). Not to scale.

Chapman et al. (2012) used various numerical models to simulate the tank experiment. Although their models closely matched the experimental data, they required high resolution grids with ~9,000 to 24,000 cells. Comparatively, Muskus and Falta (2018) simulated the sand tank as a 1-D model with 50 cells in the direction of groundwater flow (x direction) with the clay lenses represented as an embedded matrix diffusion area.

Developed as a 1-D model, the MODFLOW-USG MDT model contains a total of 50 cells (1 row, 50 columns, and 1 layer). Input parameters are shown in Table 2. Matrix diffusion was modeled as being from the clay lenses embedded in the transmissive zone. A total matrix diffusion area of 0.193 m^2 was obtained as the sum of the surface area (perimeter times the thickness of the sand tank) of the four clay lenses; resulting in an interfacial surface area (A_{md}) per cell of $3.85 \times 10^{-3} \text{ m}^2$ (Muskus and Falta, 2018). A volume fraction of 0.711, a characteristic diffusion length of $4.05 \times 10^{-2} \text{ m}$, and a Darcy velocity of 31.29 m/yr were also obtained from Muskus and Falta (2018). Note that while the sand tank experiment employed variable volumetric flowrates (0.9 mL/min for the first 10 days and 1.5 mL/min thereafter), Muskus and Falta (2018) selected the most prevalent flow rate (1.5 mL/min) for the entire time period for their comparison. This same methodology was applied to the MODFLOW-USG MDT model. Fluorescein source concentrations were maintained at 400 mg/L for the first 22 days, after which the tracer concentrations were set to zero.

Table 2. Model input parameters for the simulation of the sand tank.

Parameter	Value	
	Sand	Clay
Darcy velocity (m/yr)	31.29	
Porosity (unitless)	0.45	0.6
Source concentration (mg/L)	400	
Loading period (days)	22	
Retardation factor (unitless)	1.39	1
Tortuosity (unitless)	1.0	0.3
Global Parameters		
Matrix diffusion location	embedded	
Characteristic diffusion length (m)	0.0405	
Transmissive zone volume fraction (%)	71.1	
Matrix diffusion area (m ²)	0.00385	
Diffusion coefficient (m ² /yr)	0.0173	
Length along groundwater flow direction (x) (m)	1.07	
Width perpendicular to groundwater flow direction (y) (m)	0.03	
Depth (z) (m)	0.84	
Δx (m)	0.0214	
Δy (m)	0.03	
Δz (m)	0.84	
Δt (d)	0.5	

As shown on Figure 12, observed fluorescein concentrations increase over the first 22 days while the tracer is introduced into the sand tank. Once the tracer is removed on day 22, concentrations start to decrease and tail off by day 120.

Comparison of the MODFLOW-USG MDT model effluent concentrations with the experimental results is shown on Figure 12. Also shown on the figure are the simulated concentration curves reported by Muskus and Falta (2018) and Chapman et al. (2012). The MODFLOW-USG MDT package was able to reproduce the observed effluent concentrations reasonably well. The slight left shift of the leading edge of both the MODFLOW-USG MDT and semi-analytical curves compared to the observed concentrations is expected due to the difference in volumetric flowrates over the first 10 days between the simulated and experimental results.

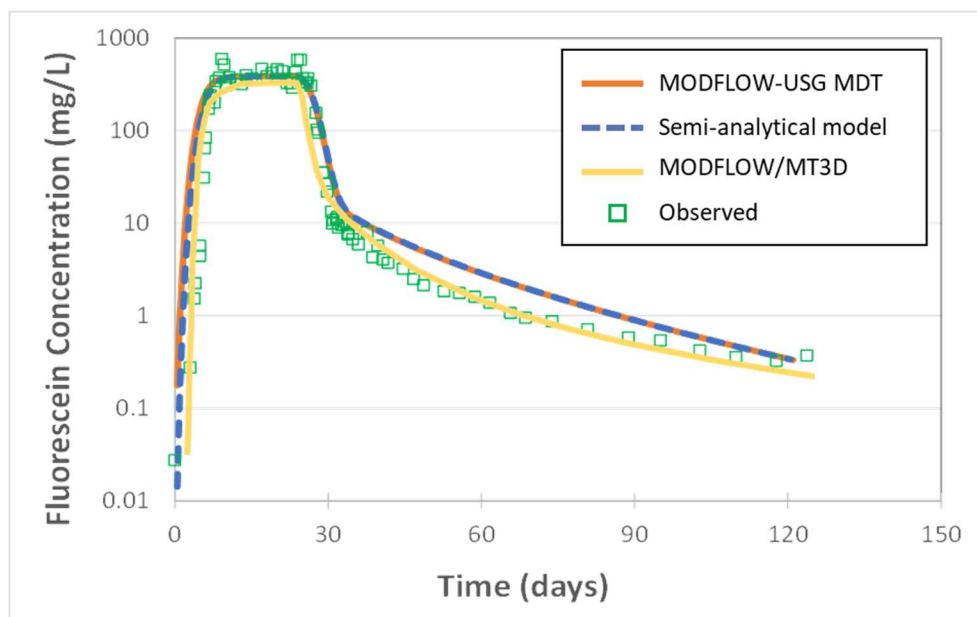


Figure 12. Comparison of MODFLOW-USG MDT model (50 model cells) output with Chapman et al. (2012) MODFLOW/MT3DMS model (8,988 model cells), semi-analytical model (50 model cells), and observed concentrations.

Example MD3: Demonstration of PCE Decay

A hypothetical site with a tetrachloroethene (PCE) release is used to demonstrate MODFLOW-USG MDT package's ability to model the effects of sequential decay in addition to diffusion into and from low- k zones (Table 3). The transmissive zone is a sandy aquifer that is interbedded with clay lenses. Hydraulic conductivity of the transmissive zone is 12,500 m/yr and the hydraulic gradient across the site is 0.002 m/m. Porosities for the sand and clay are 0.33 and 0.4, respectively. A tortuosity of 0.7 is assumed for both sand and clay. PCE is continuously released into groundwater at a concentration of 100 mg/L. The source area is 10 m perpendicular to groundwater flow and 3 m deep.

Approximately 40% of the transmissive zone comprises of clay lenses with a characteristic diffusion length of 0.5 m. Therefore, matrix diffusion was modeled as being from the clay lenses embedded in the transmissive zone. PCE is assumed to undergo reductive dechlorination to trichloroethene (TCE), then to cis-1,2-dichloroethene (cis-DCE), and finally to vinyl chloride (VC) with decay rates of 0.4 yr⁻¹ (PCE), 0.15 yr⁻¹ (TCE), 0.1 yr⁻¹ (cis-DCE), and 0.2 yr⁻¹ (VC) (Wiedemeier et al., 1999; Aziz et al., 2000). Retardation factors assigned to each of the constituents are shown in Table 3.

The MODFLOW-USG MDT model contains 5 layers, 20 rows, and 100 columns. Input parameters are shown in Table 3. Comparison of the MODFLOW-USG MDT model concentrations with the semi-analytical model results over various years is shown on Figure 13. As shown in the figure, the MODFLOW-USG MDT package was able to reproduce the constituent concentrations reasonably well for all constituents.

Table 3. Model input parameters for the simulation of sequential decay.

Parameter	Value	
	Sand	Clay
Hydraulic Conductivity (m/yr)	12,500	
Hydraulic gradient (m/m)	0.002	
Porosity (unitless)	0.33	0.4
Source concentration (mg/L)	100	
Retardation factor (unitless)		
PCE	1.94	1.78
TCE	1.57	1.47
Cis-DCE	1.18	1.15
VC	1.07	1.05
First order degradation rates (per year)		
PCE	0.40	0.40
TCE	0.15	0.15
Cis-DCE	0.10	0.10
VC	0.20	0.20
Distribution coefficient (mL/g)		
PCE	0.194	0.194
TCE	0.117	0.117
Cis-DCE	0.0363	0.0363
VC	0.0137	0.0137
Tortuosity (unitless)	0.7	0.7
Bulk density (g/mL)	1.6	1.6
Global Parameters		
Matrix diffusion location	Embedded	
Characteristic diffusion length (m)	0.50	
Transmissive zone volume fraction (%)	40	
Matrix diffusion area (m ²)	360	
Diffusion coefficient (m ² /yr)	0.0316	
Source width perpendicular to groundwater flow direction (m)	10	
Source depth (m)	3	
Model length along groundwater flow direction (x) (m)	2000	
Model width perpendicular to groundwater flow direction (y) (m)	100	
Model depth (z) (m)	15	
Yield of Component 2 from Component 1	0.795	
Yield of Component 3 from Component 2	0.737	
Yield of Component 4 from Component 3	0.64	
Δx (m)	20	
Δy (m)	5	
Δz (m)	3	
Δt (d)	1	

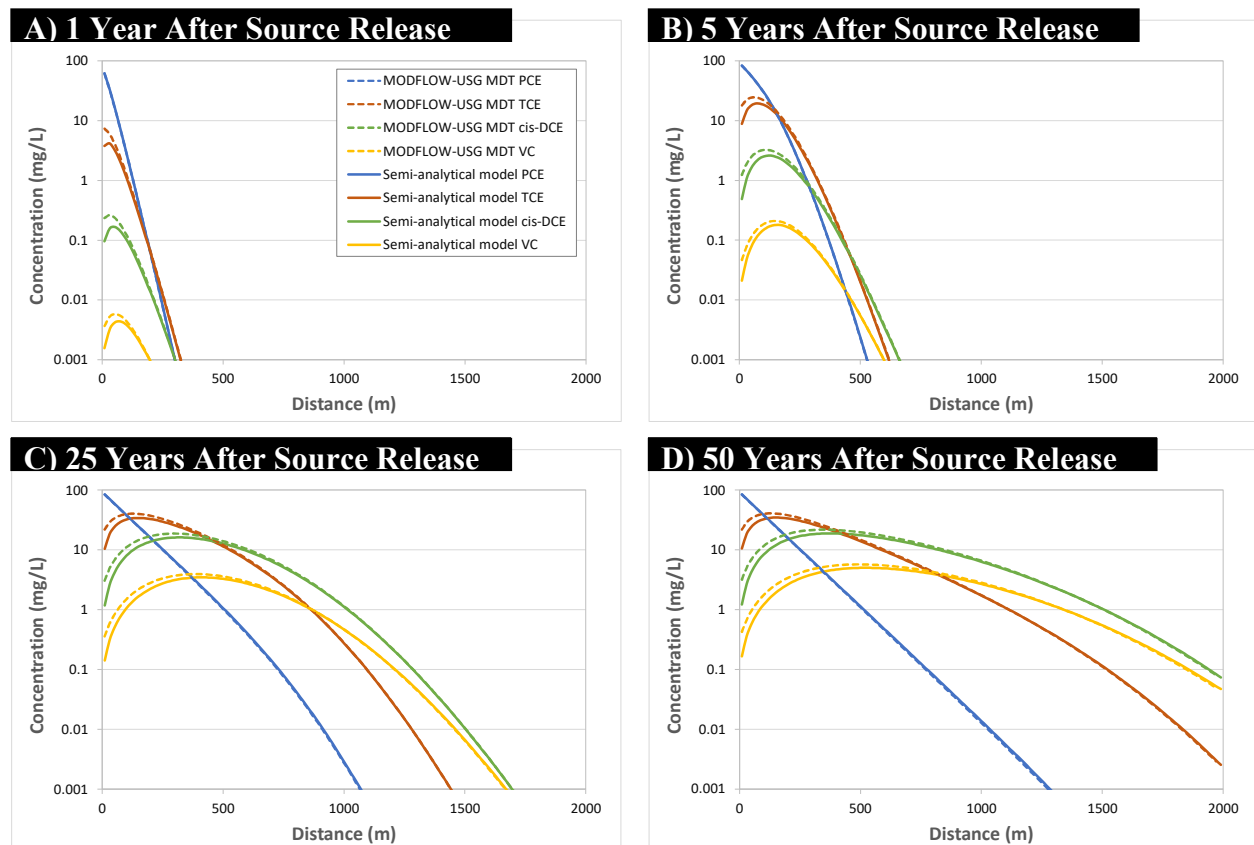


Figure 13. Comparison of MODFLOW-USG MDT model output with REMChlor-MD model for PCE degradation example.

3.0 MODFLOW 6 MDT MATRIX DIFFUSION PACKAGE

MODFLOW 6 now has a chemical transport package that advection, dispersion, adsorption, and chemical reactions (Langevin et al., 2022). The MDT matrix diffusion package is incorporated in a recent version of the code. The numerical formulation and implementation of the MDT package in MODFLOW 6 is very similar to the implementation in MODFLOW-USG, which was described in the previous section. The MODFLOW 6 source code and executable are available from GSI Environmental and from ESTCP.

The MODFLOW 6 MDT capability has been incorporated in version 10.7 of Aquaveo's GMS graphical user interface (<https://aquaveo.com/>). Appendices C1 through C3 are three MDT package tutorials for MODFLOW 6. These tutorials are available online at: <https://aquaveo.com/software/gms-learning-tutorials>.

3.1 MDT PACKAGE INPUT INSTRUCTIONS

The following input instructions pertain to users running the MODFLOW 6 FORTRAN code directly. Users running the code through the GMS interface can refer to the GMS tutorials in Appendices C1 through C3 for input instructions.

Input for the Matrix Diffusion Transport (MDT) Package is read from the file that is specified by "MDT6" as the file type. Any number of MDT Packages can be specified for a single GWT model. This allows the user to specify triple porosity systems, or systems with as many matrix-diffusion immobile domains as necessary. MDT and IST Packages can also be specified for a single GWT model to define separate immobile domain systems.

The MDT Package input instructions include options, transport related parameters and initial conditions for solution to transport of contaminants in a steady-state or transient flow field, for the matrix domain of the dual porosity system. The MDT package functions in a similar manner to the IST package in that it addresses matrix diffusion in a simulation. The MDT package uses a semi-analytical solution for solute mass evolution within the matrix domain and therefore provides greater accuracy than the IST formulation which solves for this diffusion numerically, with only one node representing the entire matrix domain. Since concentration differences in the matrix domain can be large within small distances, the IST formulation with just one average matrix concentration may not be sufficient in many cases to accurately depict the transport of solutes where the semi-analytical solution is required. The MDT package differs from the IST package in several other ways. Specifically, simplifications and assumptions to the semi-analytical solution are required as listed below:

- Zeroth order decay is not considered within the matrix. Only first order decay is allowed.
- Nonlinear adsorption is not considered within the matrix. Only linear adsorption is allowed.
- Decay is allowed but generation of a component due to decay of another is not allowed. This is a significant difference from the MODFLOW USG MDT package, and the REMChlor-MD codes, which allow the production of daughter products (chain decay).

- Decay is assumed to only occur in the aqueous phase and not on adsorbed solutes in the matrix domain; however, decay of adsorbed solutes in the matrix domain can be simulated with the same decay coefficient as in water if the decay coefficient is multiplied by the matrix retardation factor for the solute.
- For transient flow conditions, the matrix is assumed to be at steady-state and there is no flow of water between the fracture domain and the matrix domain. Therefore, it is assumed that solutes move into the matrix domain by diffusion only, even in transient flow situations.
- For transient flow conditions, all the storage term is attributed to the fracture domain and none to the matrix domain. This is because of the assumption of no transfer of water between the matrix and fracture domains. In certain situations, the opposite may be the case where fractures provide the flow and little storage, while the matrix provides most of the storage of the domain with water flowing between matrix and fracture under transient flow conditions.
- The saturation of the matrix is assumed to be unity and unchanged throughout the simulation.

Matrix Diffusion Transport Package Input Instructions Note

Input for the mobile (fracture) domain is supplied with the other transport packages of MODFLOW 6. Input for the MDT domain is provided here. The MDT package input parameters use consistent units.

Structure of Blocks

```

BEGIN OPTIONS
  [SAVE_FLOWS]
  [PRINT_FLOWS]
  [SORPTION]
  [FIRST_ORDER_DECAY]
  [TSHIFTMD <tshift>]
  [MD_FILEOUT <coeff_filename>]
END OPTIONS
BEGIN GRIDDATA
  MD_TYPE_FLAG
    <md_type_flag(nodes)> -- READARRAY
  MD_FRACTION
    <md_fraction(nodes)> -- READARRAY
  MD_POROSITY
    <md_porosity(nodes)> -- READARRAY
  BULK_DENSITY
    <bulk_density(nodes)> -- READARRAY
  MD_DIFF_LENGTH
    <md_diff_length(nodes)> -- READARRAY
  MD_TORTUOSITY
    <md_tortuosity(nodes)> -- READARRAY
  MD_DIST_COEFF

```

```

      <md_dist_coeff(nodes)> -- READARRAY
MD_DECAY
      <md_decay(nodes)> -- READARRAY
MD_DIFF_COEFF
      <md_type_flag(nodes)> -- READARRAY
AIOLD1MD
      <aiold1md(nodes)> -- READARRAY
AIOLD2MD
      <aiold2md(nodes)> -- READARRAY
END GRIDDATA

```

Explanation of Variables Read by the MDT Package:

Block: OPTIONS

SAVE FLOWS—keyword to indicate that MDT flow terms will be written to the file specified with “BUDGET FILEOUT” in Output Control.

PRINT FLOWS—keyword to indicate that the list of constant concentration flow rates will be printed to the listing file for every stress period time step in which “BUDGET PRINT” is specified in Output Control. If there is no Output Control option and “PRINT FLOWS” is specified, then flow rates are printed for the last time step of each stress period.

SORPTION—is a text keyword to indicate that sorption will be activated. Use of this keyword requires that BULK DENSITY and DISTCOEF are specified in the GRIDDATA block.

FIRST ORDER DECAY—is a text keyword to indicate that first-order decay will occur. Use of this keyword requires that DECAY and DECAY SORBED (if sorbtion is active) are specified in the GRIDDATA block.

ZERO ORDER DECAY—is a text keyword to indicate that zero-order decay will occur. Use of this keyword requires that DECAY and DECAY SORBED (if sorbtion is active) are specified in the GRIDDATA block.

TSHIFTMD tshift —the keyword TSHIFTMD indicates that the MODFLOW start time ($t = 0$) is not the starting time of matrix diffusion, and the subsequent real variable tshift is the value of time already elapsed since matrix diffusion began. Note that if TSHIFTMD is read, then the coefficients AIOLD1MD and AIOLD2MD are also input in the GRIDDATA block.

MD—keyword to specify that record corresponds to ai1 and ai2 matrix coefficients.

FILEOUT—keyword to specify that an output filename is expected next.

coeff_filename—name of the binary output file to write ai1 and ai2 matrix coefficients.

Block: GRIDDATA

MD_TYPE_FLAG—is the matrix diffusion type flag at any location. This flag gives options at each cell on how the matrix diffusion is treated. One value is read for every model cell. Usually, these values are read one layer at a time; however, when the XSECTION option is specified, a single two-dimensional variable for the cross section is read.

If MD_TYPE_FLAG(N) = 0, cell N is inactive in the matrix domain (either the cell itself is inactive or the matrix domain does not exist at this cell).

If MD_TYPE_FLAG (N) = 1, cell N is active in the matrix domain with matrix diffusion occurring at the bottom of the cell.

If MD_TYPE_FLAG (N) = 2, cell N is active in the matrix domain with matrix diffusion occurring embedded within the cell.

If MD_TYPE_FLAG (N) = 3, cell N is active in the matrix domain with matrix diffusion occurring at the top of the cell.

If MD_TYPE_FLAG (N) = 4, cell N is active in the matrix domain with matrix diffusion occurring at both the top and bottom of the cell.

If MD_TYPE_FLAG (N) = 5, cell N is active in the matrix domain with matrix diffusion occurring at the bottom and embedded within the cell.

If MD_TYPE_FLAG (N) = 6, cell N is active in the matrix domain with matrix diffusion occurring at the top and embedded within the cell.

If MD_TYPE_FLAG (N) = 7, cell N is active in the matrix domain with matrix diffusion occurring at the top, bottom and embedded within the cell.

Note that MD_TYPE_FLAG can be inactive for active flow nodes. However, MD_TYPE_FLAG cannot be active for a node which is inactive for the corresponding flow and transport simulation.

MD_FRACTION—is the immobile fraction at any location, i.e., the fraction of the total space that is occupied by the matrix/low permeability domain. Note that in the USG-Transport version of MDT, the mobile fraction is input. Input of immobile fraction in MODFLOW 6 version of MDT is required because MODFLOW 6 allows for more than one MDT domain and each MDT domain will have its own VOLFRACMD.

MD_POROSITY—is the effective transport porosity within the matrix domain at any location.

BULK_DENSITY—is the dry bulk density of the porous matrix of the matrix domain at any location.

MD_DIFF_LENGTH—is the diffusion length for diffusive transport within the matrix domain at any location (only used for embedded heterogeneity).

MD_TORTUOSITY—is the tortuosity of the matrix domain at any location.

MD_DIST_COEFF—is the adsorption coefficient (K_d) of a contaminant species in the immobile domain at any location.

MD_DECAY—is the first-order decay coefficient in water and on soil (1/time) in the matrix domain at any location.

MD_DIFF_COEFF—is the diffusion coefficient of each species component within the matrix domain at any location.

AIOLD1MD—is the concentration integral (equation 8) of each species in an element associated with matrix diffusion into an infinite acting adjacent aquitard (MD_TYPE_FLAG = 1, 3, 4, 5, 6, or 7). This value is used to restart a simulation with prior matrix diffusion.

AIOLD2MD—is the concentration integral (equation 8) of each species in an element associated with matrix diffusion in low permeability zones that are embedded in the volume element (MD_TYPE_FLAG = 2, 5, 6, or 7). This value is used to restart a simulation with prior matrix diffusion.

Example Input file from MDT Package

```
# MODFLOW6 MST Package
BEGIN OPTIONS
  SAVE_FLOWS
  PRINT_FLOWS
  SORPTION
END OPTIONS

BEGIN GRIDDATA
  MD_TYPE_FLAG
  CONSTANT 2
  FRACT_FRACTION
  CONSTANT 7.110000e-001
  MD_POROSITY
  CONSTANT 0.600000e+000
  BULK_DENSITY
  CONSTANT 1.600000e+000
  MD_DIFF_LENGTH
  CONSTANT 4.052000e-002
  MD_TORTUOSITY
  CONSTANT 0.300000e+000
  MD_DIST_COEFF
  CONSTANT 9.330000e-009
  MD_DECAY
  CONSTANT 0.000000e+000
  MD_DIFF_COEFF
  CONSTANT 0.017300e+000
  AIOLD1MD
  CONSTANT 0.000000e+000
  AIOLD2MD
  CONSTANT 0.000000e+000
END GRIDDATA
```

Output files from MDT Package

Concentration related data output for the MDT package is included in the MODFLOW 6 transport concentration output files. The binary output file for the MDT package when the MD option is specified includes the coefficients AIOLD1MD and AIOLD2MD, which are used to compute the polynomial coefficient curves for the matrix. These coefficients are useful for restarting a simulation. These arrays are written to the binary file if the flag and unit number IMDTCF is greater than zero. The header for output is 'COEFF AI1MD' or 'COEFF AI2MD'.

If the SAVE FLOWS option is activated, then the rate of mass diffusion between fracture and matrix domain are written to a binary file under the title 'MD MASS STORAGE'. For a multi-species simulation, MODFLOW 6 treats each species as a separate transport simulation and all output for each species is treated as a separate simulation with separate output files.

4.0 CASE STUDY: SANTA SUSANA FIELD LABORATORY, VENTURA COUNTY, CA

The National Aeronautics and Space Administration (NASA) worked with groundwater modelers at Jacobs Engineering Group, Inc. (Jacobs) to develop a groundwater flow and transport model for the Coca/Delta Area of Impacted Groundwater at the Santa Susana Field Laboratory (SSFL) in Ventura County, California. This site was formerly used for development and testing of liquid-fueled rocket engines, which led to groundwater impacts by TCE. The subsurface at the SSFL is characterized as a fractured sandstone with interbedded shale, siltstone, and conglomerate. The numerical model was developed using USG-Transport (Panday, 2023), because it had the capability to handle the complex hydrogeology as well as the matrix-diffusion process via its Matrix Diffusion Transport (MDT) Process module.

The MDT process in the USG-Transport code was beta tested by the Jacobs groundwater modeling team, including Peter Lawson, Nate Brown, Darren Meadows, Craig Cooledge, and Heather Perry. Different conceptualizations were evaluated to assess the ability of the model to represent the complex geology, simulate the complex flow field, and develop reasonable initial conditions for TCE in the matrix domain for the projection transport simulations.

The Coca/Delta Flow and Transport Model (CDFTM) was built using an unstructured numerical grid. Voronoi tessellation was used in the horizontal dimension with 6,952 cells per model layer. The model was subdivided vertically into 37 layers that conform to hydrostratigraphic units at the site (NASA, 2022). Figure 14 shows three-dimensional views of the numerical grid from several directions. The Voronoi cells have horizontal dimensions ranging from 8 to 120 feet, whereas the model layer thicknesses are variable across the model, ranging from a minimum of 0.3 feet thick to approximately 2,000 feet thick. Groundwater flow in the fractured rock is simulated using an equivalent porous medium approximation, and the calibrated bulk hydraulic conductivity for the sandstone units ranges from 0.0028 to 0.28 feet per day (1×10^{-6} to 1×10^{-4} centimeters per second).

TCE transport at this site is believed to be strongly affected by matrix diffusion. The solute transport modeling approach used the ESTCP MDT matrix-diffusion package in MODFLOW-USG. In the MDT package, the fracture volume fraction was set to 0.0001, with a rock matrix porosity of 0.14, and a characteristic diffusion length of 1.25 feet (i.e., one-half of the measured average fracture spacing observed in boreholes).

Historical loading of dissolved TCE in the rock matrix was simulated by specifying time-dependent TCE concentrations in the fracture domain in selected zones in the model and allowing the model to run for a historical period with matrix diffusion being the only transport process (advection was shut off for the TCE loading period). This process sought to establish TCE “present-day” concentrations in the matrix domain, based on the historical load of TCE mass in the fracture domain (NASA, 2022). These TCE concentrations were used as a basis for the initial TCE conditions in the matrix for the projection transport simulations. Figure 15 shows past measured concentrations of TCE in selected monitoring wells with future projections calculated by the CDFTM. In most cases, the projected concentration trends are consistent with the historical data.

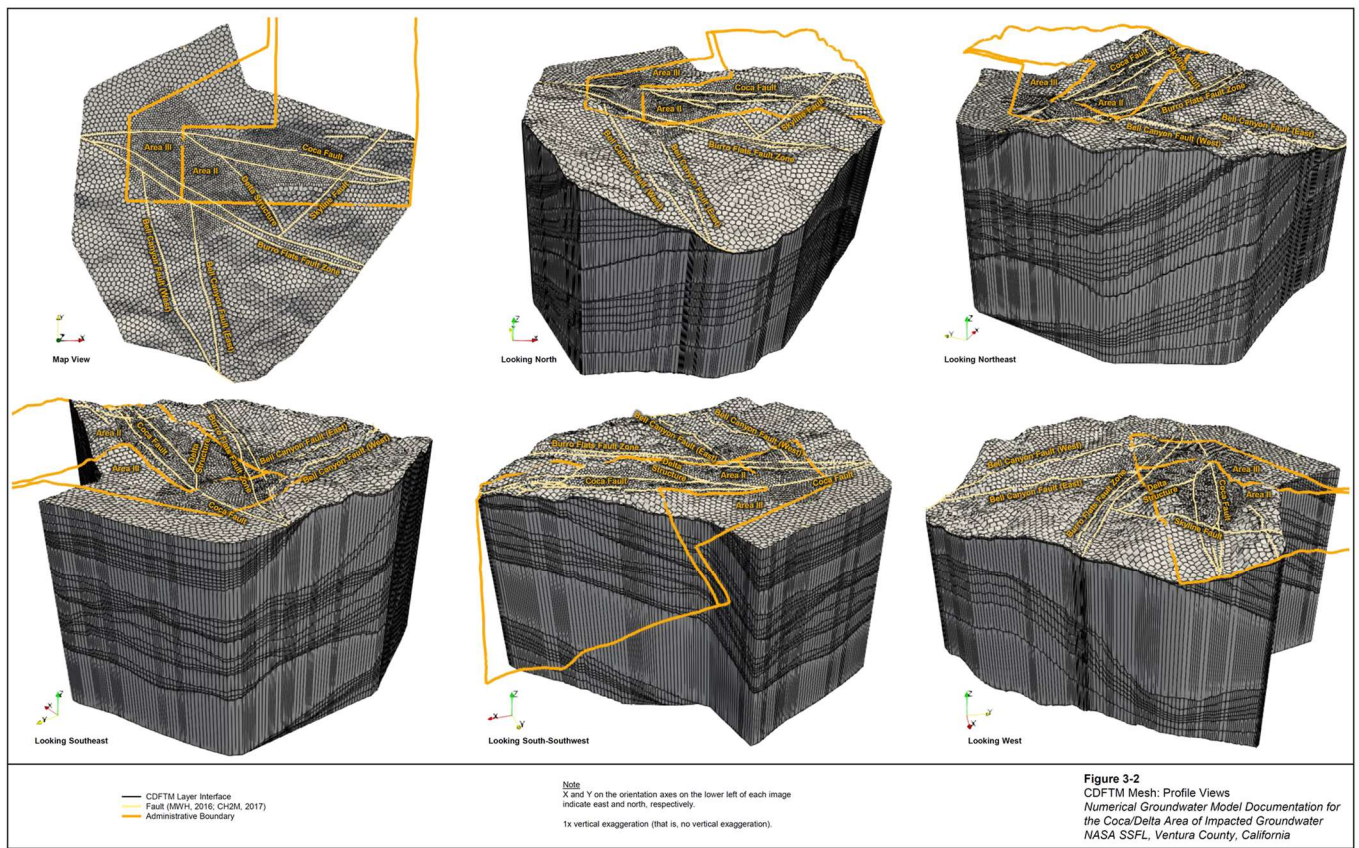


Figure 14. Unstructured numerical mesh used in the NASA Coca/Delta MODFLOW-USG Flow and Transport Model (NASA, 2022).

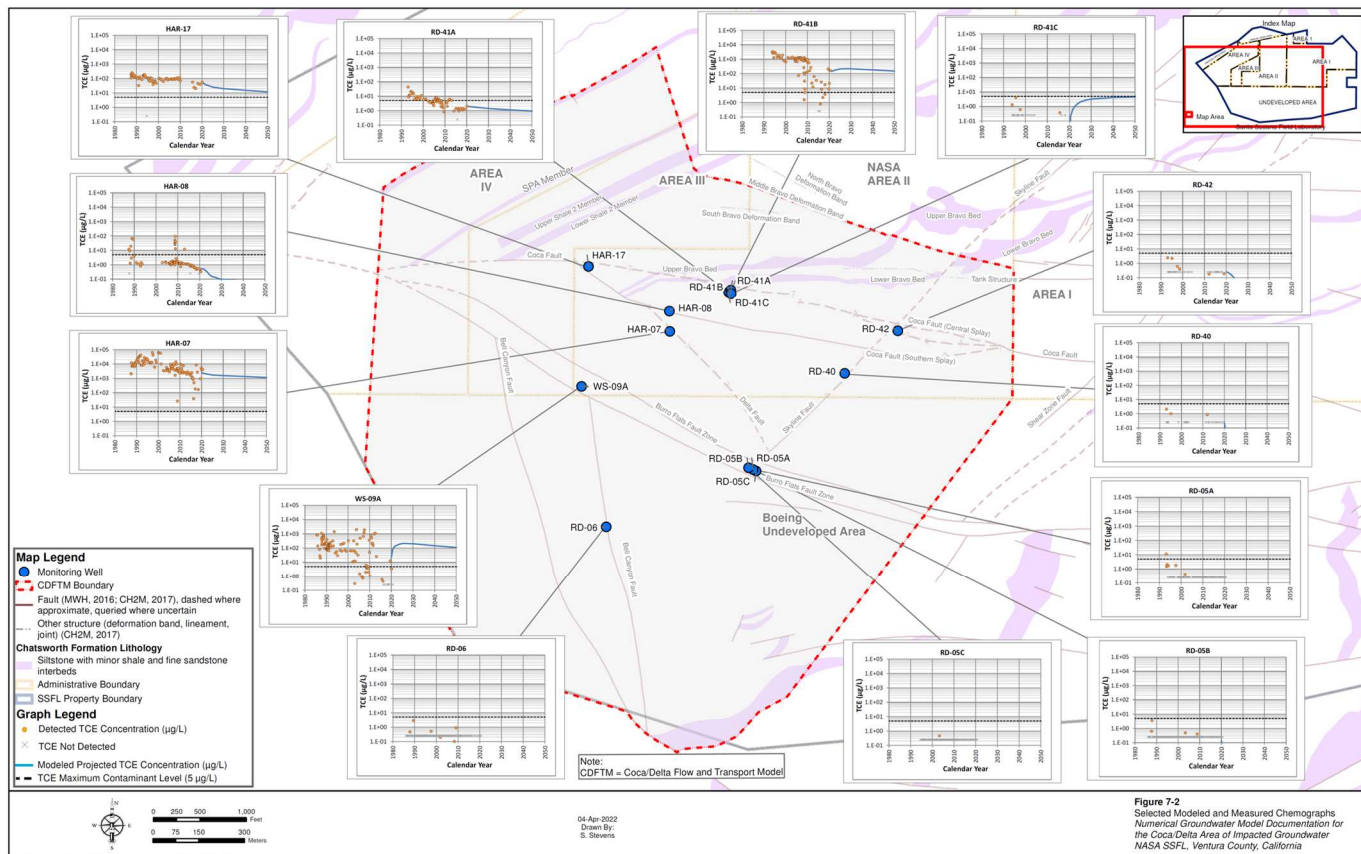


Figure 15. Selected simulated and measured TCE concentrations in wells at the Coca/Delta Area of Impacted Groundwater (NASA, 2022).

5.0 ESTIMATION OF MDT PACKAGE MATRIX DIFFUSION GEOMETRIC AND TRANSPORT PARAMETERS

The MDT matrix diffusion package that has been implemented in MODFLOW-USG and MODFLOW 6 is based on the semi-analytic method used in REMChlor-MD. The user's manual for REMChlor-Md (Farhat et al., 2018) contains a comprehensive guide to estimating the necessary matrix diffusion parameters, including chemical parameter and geologic parameter databases.

The key geometrical parameters that are needed in the MDT package are the volume fraction of high permeability material in a numerical element, V_f , the characteristic average diffusion length, L , and the interfacial area between the high and low permeability media in an element, A_{md} . From a volume balance on the low permeability material, Muskus and Falta (2018) showed that the three geometrical parameters can be related to each other:

$$V_n(1 - V_f) = A_{md}L \quad (24)$$

where V_n is the volume of element n . Using this relationship, it is only necessary to estimate the volume fraction and characteristic diffusion length. For heterogeneous systems, Muskus (2017) and Muskus and Falta (2018) showed that borehole data could be used to estimate the volume fraction and the characteristic diffusion length. This methodology is also used in the REMChlor-MD toolkit (Farhat et al., 2018).

Using N boring logs from a site, the volume fraction V_f is estimated from:

$$V_f = \frac{\sum_{i=1}^N (b_i - bl_i) / N}{\sum_{i=1}^N b_i / N} \quad (25)$$

where b_i is the plume thickness in the i^{th} boring log, and bl_i is the total thickness of low permeability units lying within the plume. The characteristic diffusion length can be estimated from a volume-weighted average of the low permeability layer thicknesses:

$$L = \frac{\sum_{i=1}^N 0.5 \times \left(\frac{\sum_{j=1}^n (bl_{ij})^2}{\sum_{j=1}^n bl_{ij}} \right)}{N} \quad (26)$$

where bl_{ij} is the thickness of the j^{th} low permeability unit lying within the plume, in the i^{th} boring log. The REMChlor-MD model interface contains a heterogeneity calculator that can be used with data from up to 100 boring logs.

In a fractured rock system with parallel fractures, the volume fraction is equal to the fracture aperture, b divided by the fracture spacing, a :

$$V_f = b/a \quad (27)$$

The average diffusion length is then

$$L = (a - b)/2 \quad (28)$$

Pham (2023) and Pham et al. (2023) provide a method for estimating the volume fraction and characteristic diffusion length of more complex 3D fracture systems with variable fracture spacing. In each case, once the volume fraction and diffusion lengths are known, the interfacial area is calculated using Equation (24).

6.0 CONCLUSIONS

The semi-analytical matrix diffusion method used in REMChlor-MD has been added to MODFLOW USG and MODFLOW 6 in the form of MDT (matrix diffusion) packages. This allows for consideration of matrix diffusion in fractured or heterogeneous materials with complex, time-dependent flow fields. The FORTRAN source codes for the two models are available free of charge from GSI Environmental (see sections 2.0 and 3.0).

The MODFLOW USG and MODFLOW 6 MDT packages have been incorporated into the Aquaveo GMS version 10.7 graphical user interface (<https://www.aquaveo.com/>). Seven detailed tutorials showing application of the MDT package have been developed (Appendices B1-B4 and C1-C3). These tutorials are available for free download from <https://www.aquaveo.com/software/gms-learning-tutorials>.

The MODFLOW USG MDT package allows for the production of daughter products during first order decay in the matrix, but the MODFLOW 6 MDT package does not. This is a limitation of the current implementation of the MDT package in MODFLOW 6. It would be valuable, in the future, to add this capability to MODFLOW 6 once the MODFLOW 6 transport code allows coupled reactions.

7.0 REFERENCES

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APPENDICES

Appendix A: Points of Contact

POINT OF CONTACT Name	ORGANIZATION Name Address	Phone Fax E-mail	Role in Project
Ron Faltar	Clemson University Brackett Hall Room 336, Clemson University, SC 29634	864-656-0125 faltar@clemson.edu	Principal Investigator
Sorab Panday	GSI Environmental, 626 Grant Street, Suite C, Herndon, VA 20170	703-991-8665 sp@gsi-net.com	Co-Investigator
Alan Lemon	Aquaveo 3210 N. Canyon Road Suite 300 Provo, UT 84604	801-691-5534 alemon@aquaveo.com	Co-Investigator

Appendix B: GMS Tutorials for the MDT Package in MODFLOW-USG

These tutorials are available online at: <https://aquaveo.com/software/gms-learning-tutorials>

B1: Heterogeneous sand/clay system

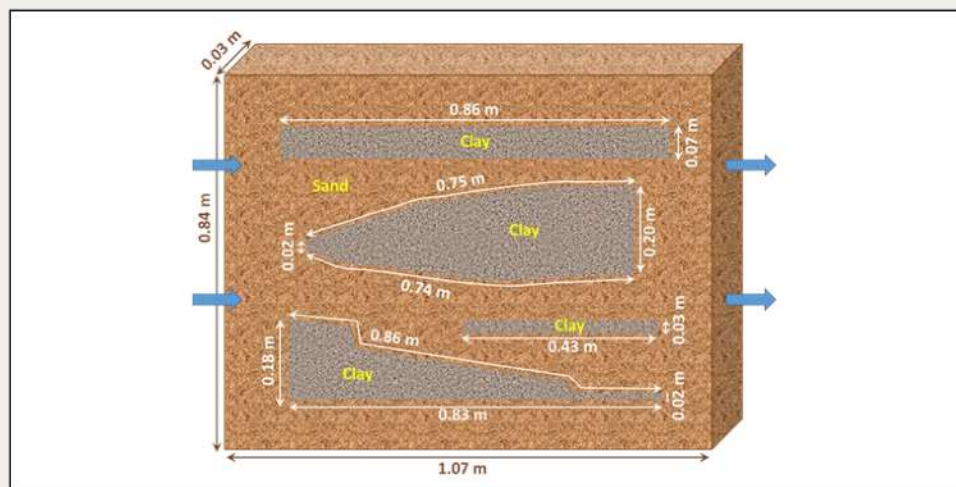


GMS 10.7

GMS 10.7 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

Required Components

- GMS Core
- MODFLOW-USG Transport

Time

- 30–40 minutes

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2	Getting Started.....	4
3	Activating the MDT Package.....	5
4	Defining the MDT Package.....	5
5	Saving and Running MODFLOW.....	6
6	Examining the Results.....	6
7	Conclusion.....	8

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 guide¹ 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 Guide⁴.

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, *Journal 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/>

For this example, a simulation of the Doner⁵ (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. Chapman⁶ 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 Falta³. Additional model parameters are given in Table 1.

Table 1. Input parameters used to simulate Doner⁵ (2008) experiment

Parameter	Value
Darcy velocity, v_x (m/yr)	31.29
Sand porosity, ϕ	0.45
Matrix porosity, ϕ_i	0.6
Sand retardation (fl), R	1.39
Matrix retardation, R_i	1
Matrix tortuosity, τ_i	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.

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

⁶Chapman, 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.

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.

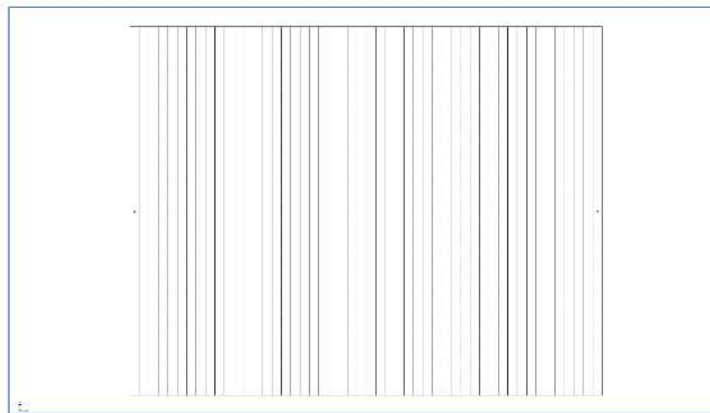


Figure 1 Imported MODFLOW-USG Transport model

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.

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 volume³.
 - 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 lenses³ of 0.193 m². Given the total tank volume (V) of 0.027 m³ and the sand volume fraction (V_f) of 0.711, the characteristic diffusion length (L) can be estimated from a volume balance on the clay³: $(1 - V_f) = A_{md}L$.
 - 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, m²/yr.

- Click **OK** to close the *MDT Package* dialog.

5 Saving and Running MODFLOW

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

- Click **Save**  to save the project.
- Click the **Run MODFLOW**  macro in the toolbar to bring up the *MODFLOW* model wrapper dialog.
- When MODFLOW finishes, check the *Read solution on exit* and *Turn on contours (if not on already)* boxes.
- Click **Close** to close the *MODFLOW* model wrapper dialog.
- 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.

- In the Project Explorer, select the "Species 1" dataset to make it active.
- Click the **Plot Wizard**  macro to open the *Plot Wizard* dialog.
- Under *Plot Type*, select the *Active Dataset Time Series* option.
- Click **Finish** to close the *Plot Wizard* dialog and generate the plot.
- 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.

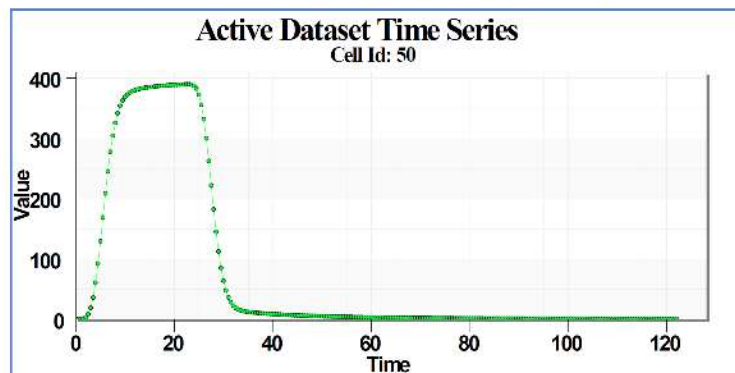


Figure 2 The *Active Dataset Time Series* for the last cell

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

7. Select the *Axis* tab.
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.

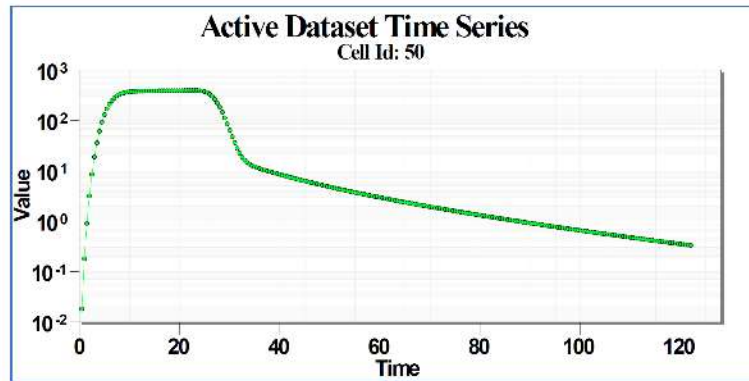


Figure 3 The Active Dataset Time Series with applied log scale

The results calculated using the MDT Package in MODFLOW-USG Transport⁴ 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 Chapman⁶ et al. (2012) are shown as the yellow line.

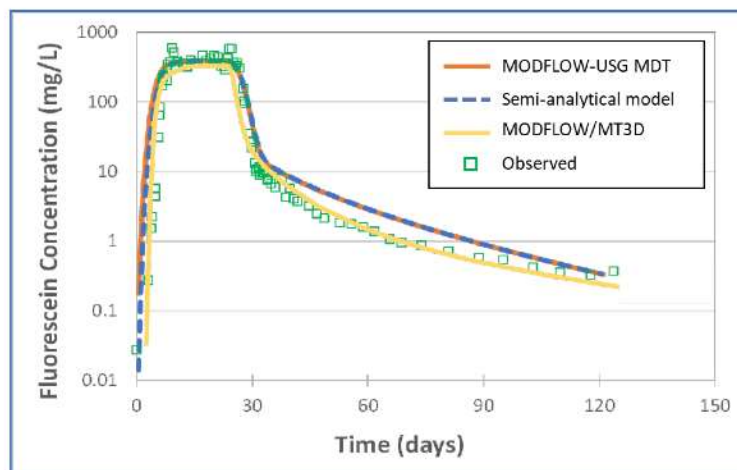


Figure 4 Comparison of MODFLOW-USG MDT model (50 model cells) output with Chapman et al. (2012) MODFLOW/MT3DMS model (8,988 model cells), REMChlor-MD (semi-analytic) model (50 model cells), and observed concentrations

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.

B2: Single discrete fracture

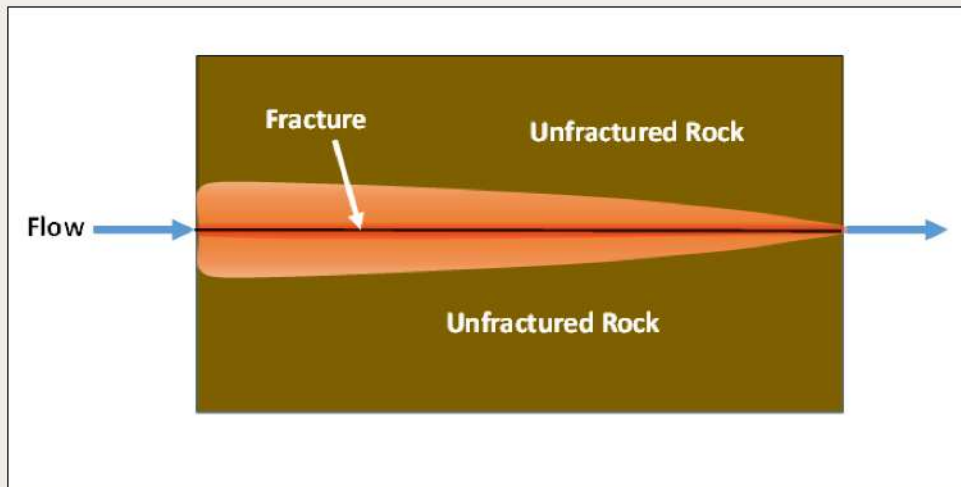


GMS 10.7

GMS 10.7 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

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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 guide¹ 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 Guide⁴.

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, *Journal 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 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 Wang² where water containing tritium is injected into a 100 μm 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.

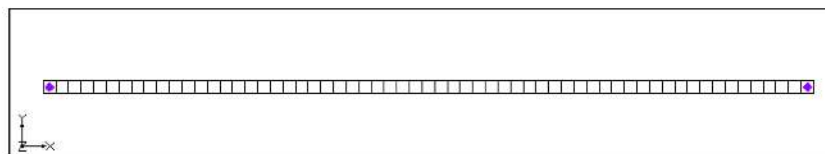


Figure 1 Imported MODFLOW-USG Transport model

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, m²/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.

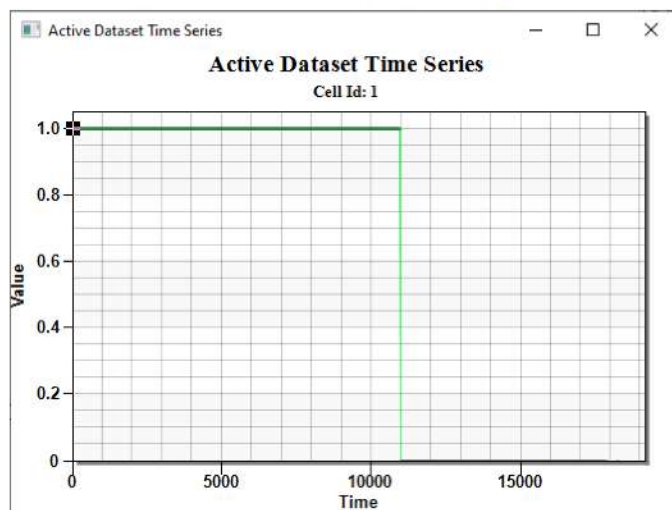


Figure 2 The Active Dataset Time Series for the first cell

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.

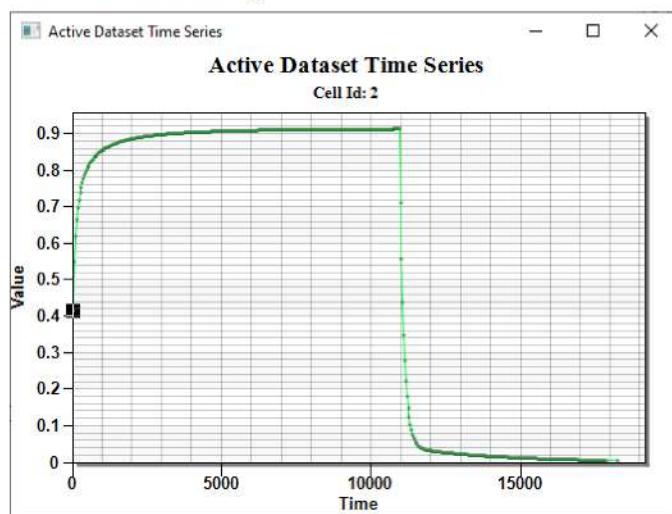


Figure 3 The Active Dataset Time Series for the second cell

The results calculated using the MDT Package in MODFLOW-USG Transport⁴ 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.

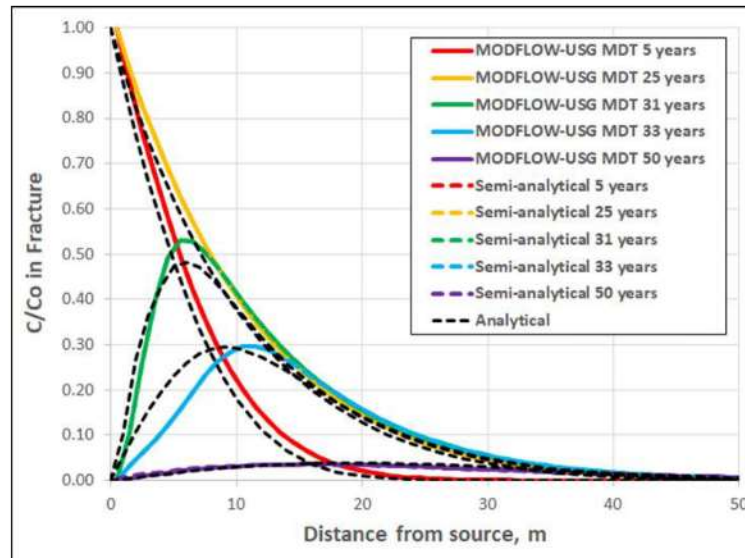


Figure 4 Comparison of MODFLOW-USG MDT Package output with REMChlor-MD (semi-analytical) and the analytical solution.

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.

B3: Parallel fractures with equivalent porous media

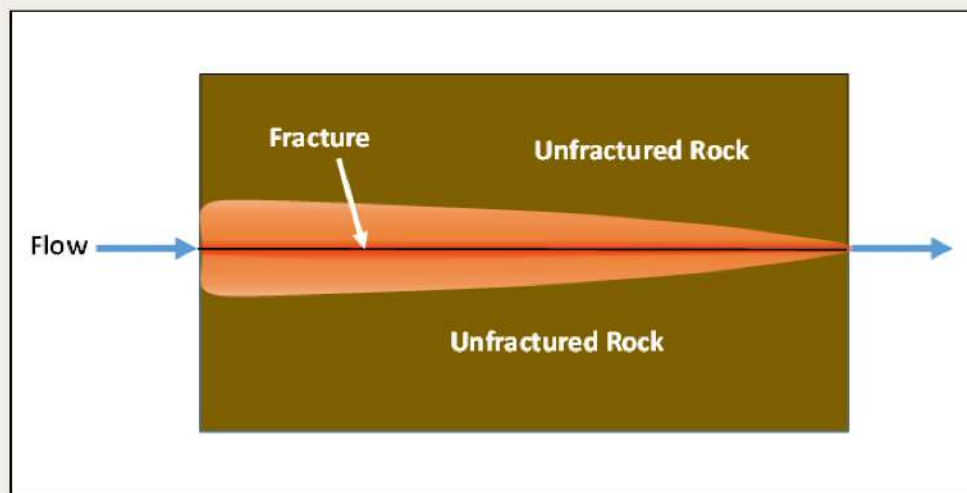


GMS 10.7

GMS 10.7 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

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3	Activating the MDT Package.....	4
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6	Conclusion	6

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 guide¹ 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 Guide⁴.

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.

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, *Journal 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.

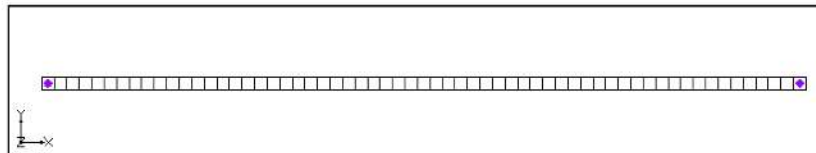


Figure 1 Imported MODFLOW-USG Transport model

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 Falta³. 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 Falta² 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 Falta³, the pore velocity in the fractures is 100 m/yr. The volume fraction of the fractures is $0.0001\text{m}/0.5\text{m} = 0.0002$. 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_L , (years)	50	

Before continuing, save the project with a new name.

1. Select **File | Save As...** to bring up the Save As dialog.
2. Enter "model-mdt_parallel.gpr" as the *File name*.
3. Select "Project Files (*.gpr)" from the *Save as type* drop-down.
4. 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.

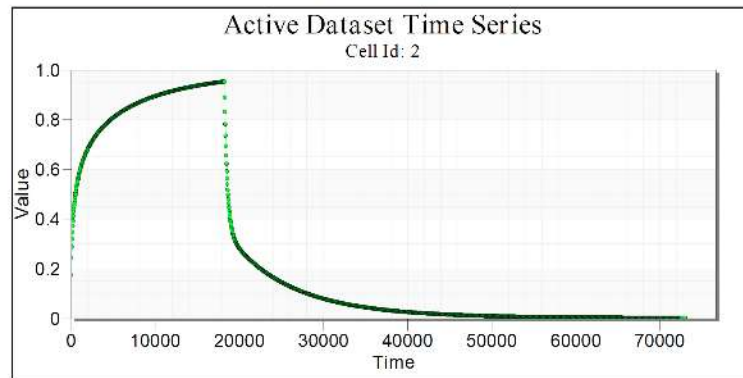


Figure 2 The Active Dataset Time Series for the second cell

6 Conclusion

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

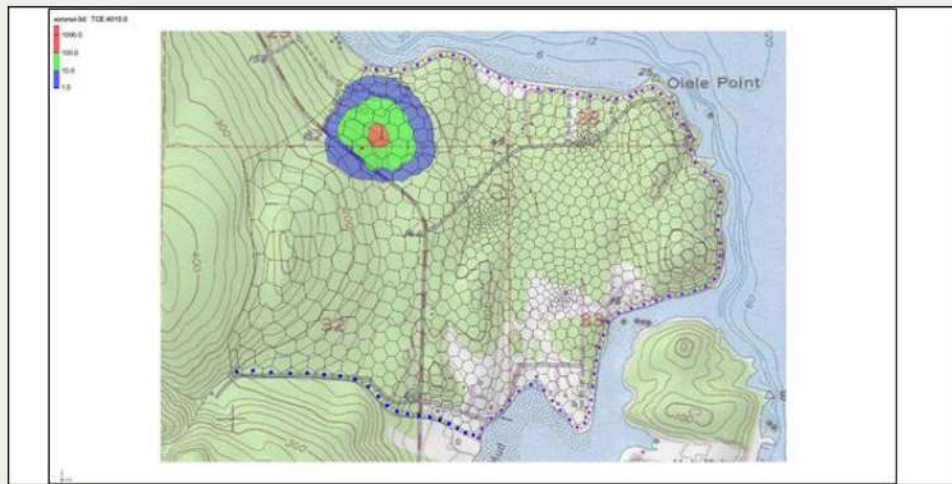
- The MODFLOW-USG Transport MDT package can be used to simulate matrix diffusion from multiple fractures in fractured porous materials.
- The MDT package allows an equivalent porous media approach where normal grid elements are used with embedded matrix diffusion occurring over a finite distance in the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



GMS 10.7 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 Stratigraphy tutorial, with a hypothetical release of trichloroethylene (TCE) into the aquifer.

¹Farhat, 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, *Journal 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.

For a more detailed description of the semi-analytic method used in the MDT package, please refer to the REMChlor-MD user's guide¹ 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 Guide⁴.

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/>

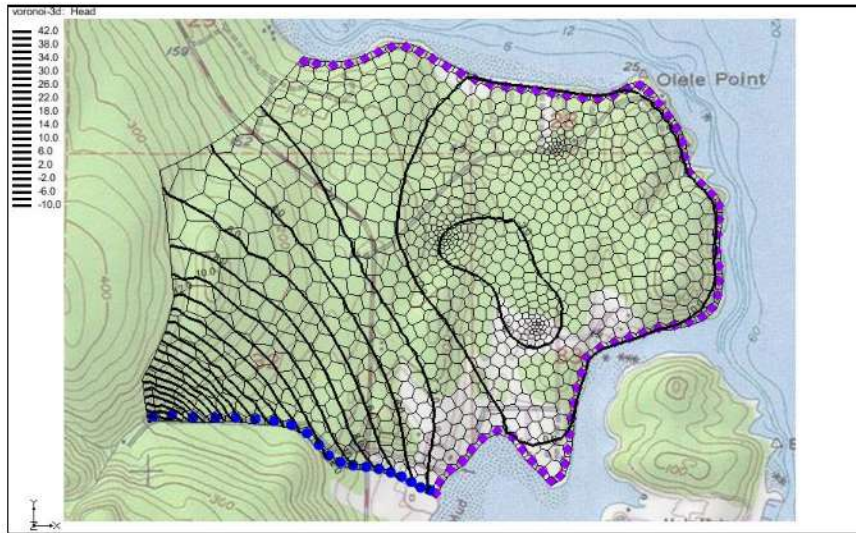


Figure 1 Imported MODFLOW-USG flow model

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.

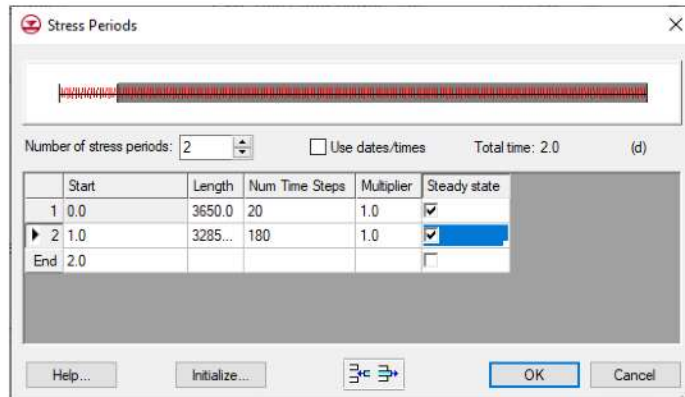


Figure 2 Stress period settings

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.

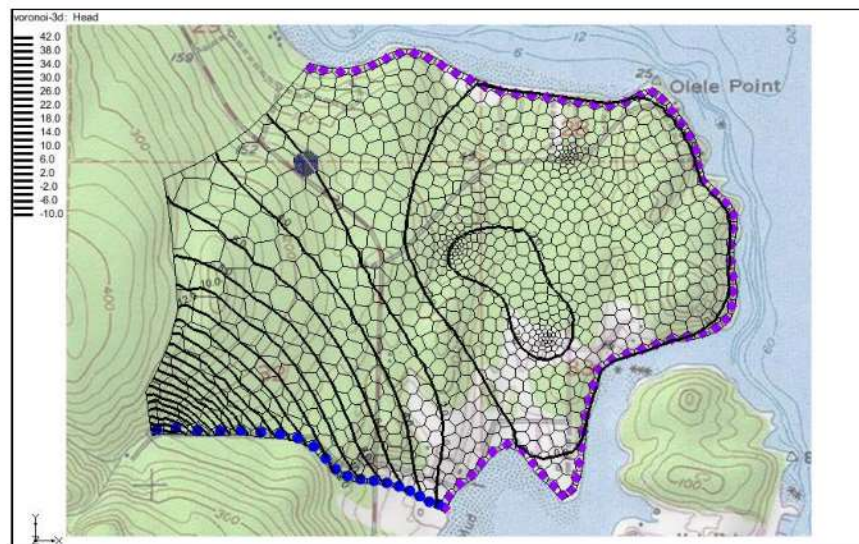
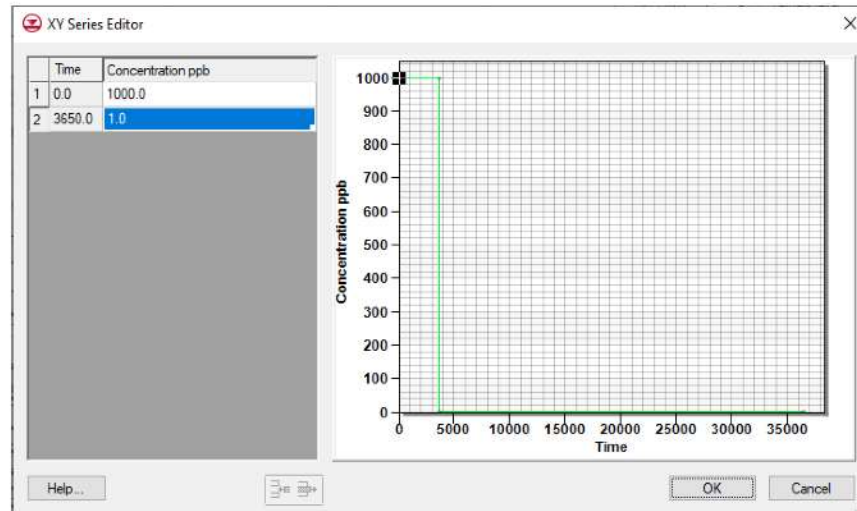


Figure 3 Select cell 886 in layer 1

2. Right-click and select **Sources/Sinks** to open the *MODFLOW Source/Sinks* dialog.
3. From the list on the left, 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 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 *Color Options* dialog.
6. Select **Reverse** in the *Palette preview* section.
7. Click **OK** to close the *Color Options* 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 "3.0".
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).

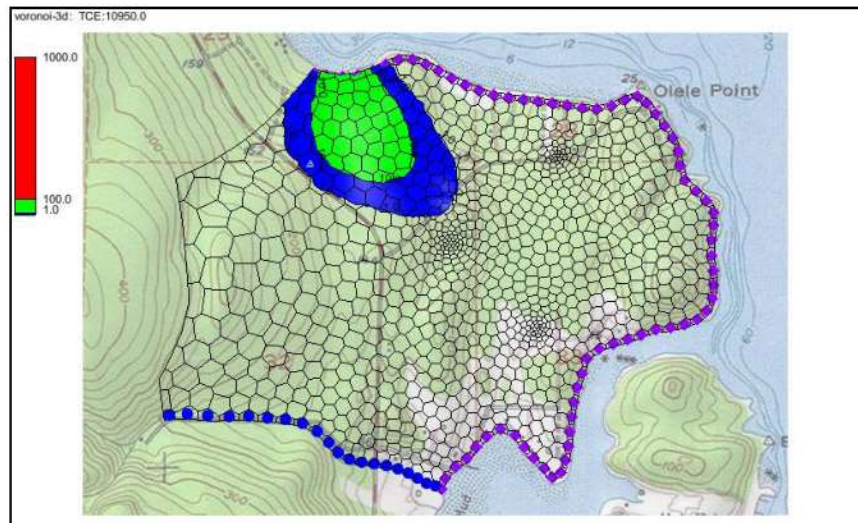


Figure 4 Simulated TCE plume in layer 1 after 10,950 days without matrix diffusion

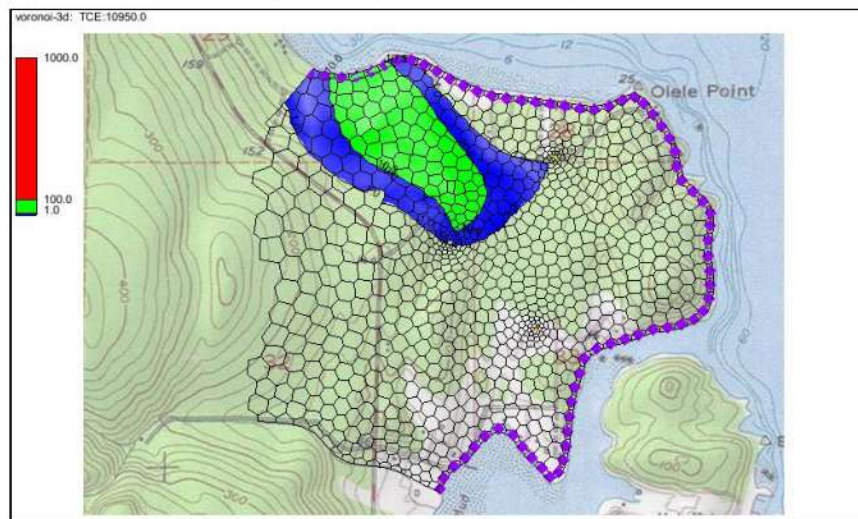


Figure 5 Simulated TCE plume in layer 5 after 10,950 days without matrix diffusion

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

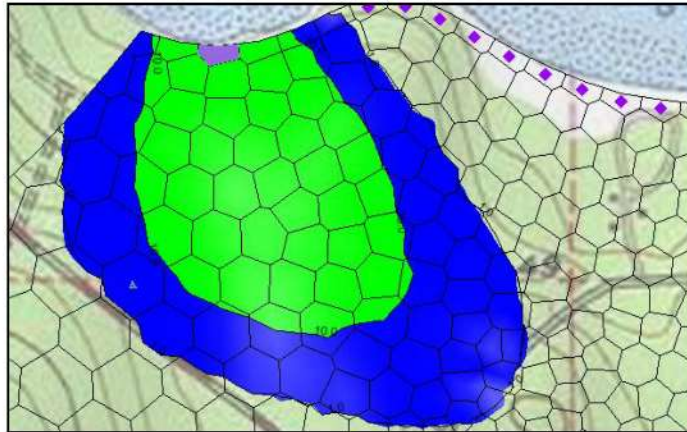


Figure 6 Select cell 840 in layer 1

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.

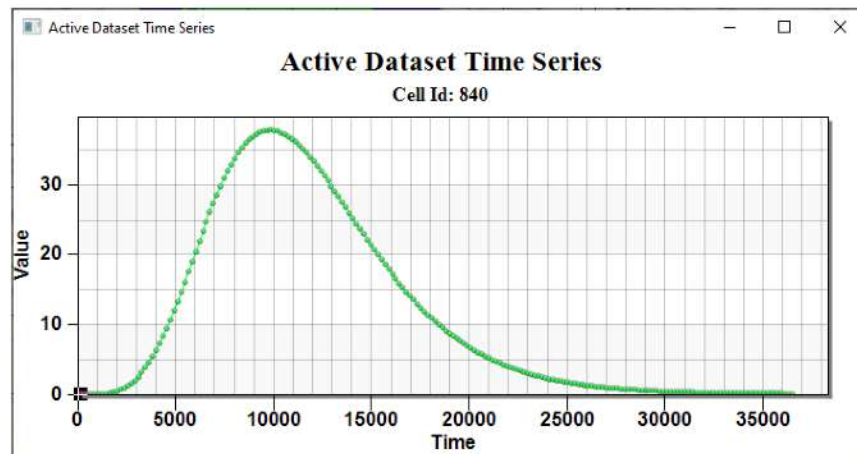


Figure 7 The Active Dataset Time Series for cell 840

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 Guide¹.
 - 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 K_d 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 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).

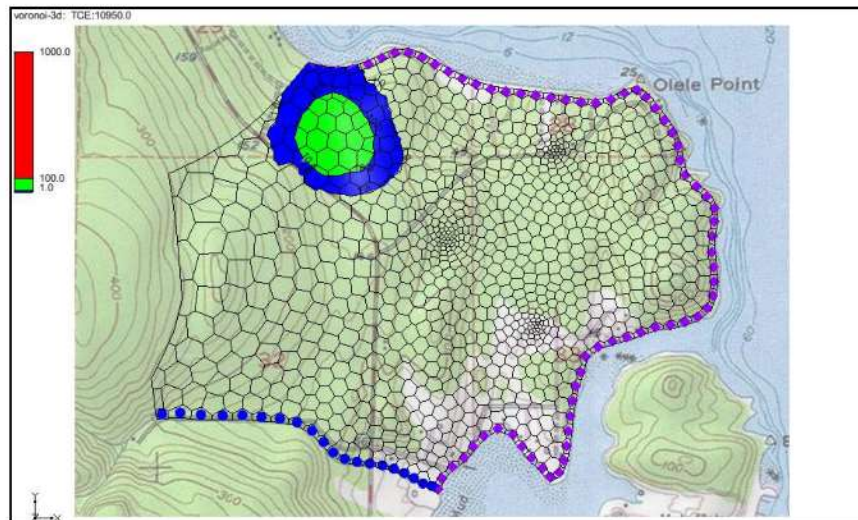


Figure 8 Simulated TCE plume in layer 1 after 10,950 days with matrix diffusion

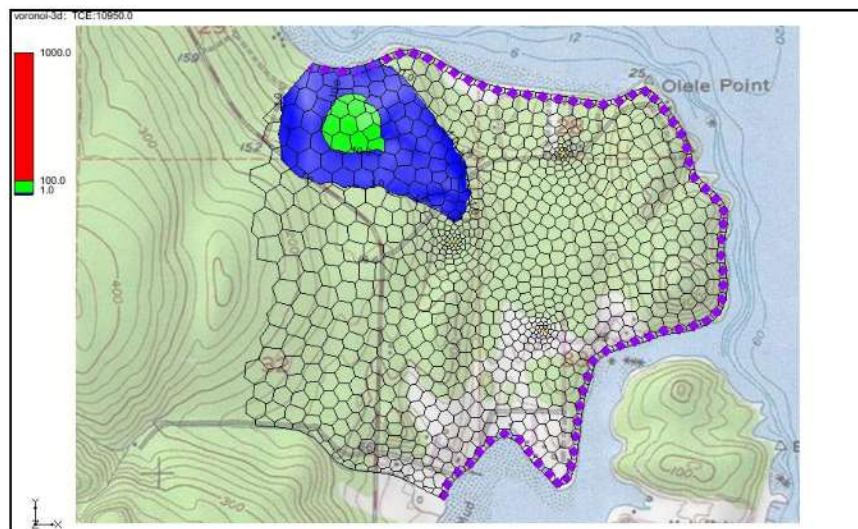


Figure 9 Simulated TCE plume in layer 5 after 10,950 days with matrix diffusion

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

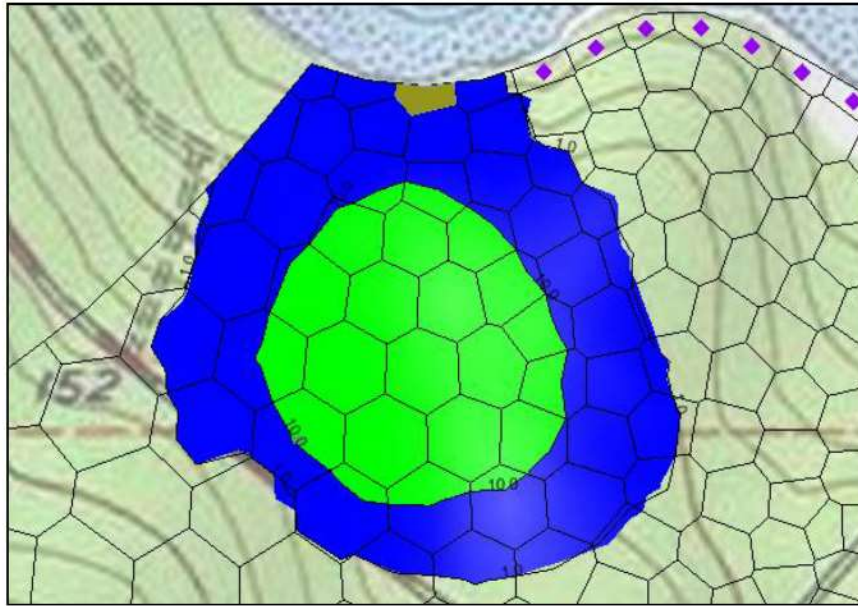


Figure 10 Select cell 840 in layer 1

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.

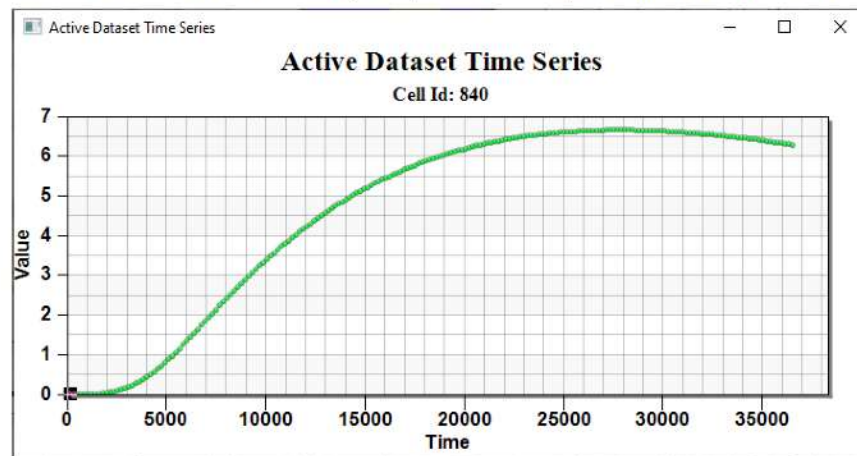


Figure 11 The Active Dataset Time Series for cell 840

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.

Appendix C: GMS Tutorials for the MDT Package in MODFLOW 6

These tutorials are available online at: <https://aquaveo.com/software/gms-learning-tutorials>

C1: Heterogeneous sand/clay system

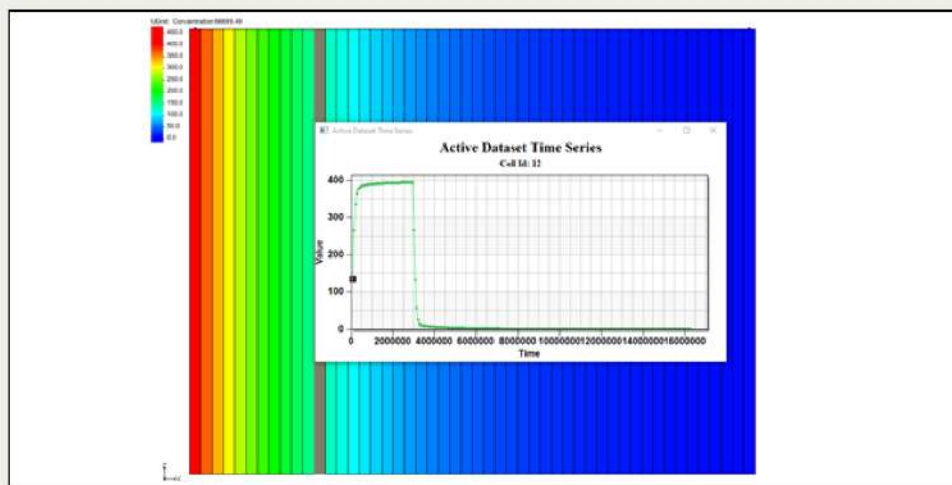


GMS 10.7

GMS 10.7 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

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2	Opening a MODFLOW 6 Simulation.....	4
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8	Saving and Running the Simulation	8
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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, *Journal 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.

description of the semi-analytic method used in the MDT package, please refer to the REMChlor-MD user's guide¹ 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 Guide⁴.

For this example, a simulation of the Doner⁵ (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. Chapman⁶ 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 Falta³. Additional model parameters are given in Table 1.

Table 1. Input parameters used to simulate Doner⁵ (2008) experiment.

Parameter	Value
Darcy velocity, v_x (m/yr)	31.29
Sand porosity, ϕ	0.45
Matrix porosity, ϕ_i	0.6
Sand retardation (fl), R	1.39
Matrix retardation, R_i	1
Matrix tortuosity, τ_i	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:

⁴Panday, 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/>

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

⁶Chapman, 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.

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.

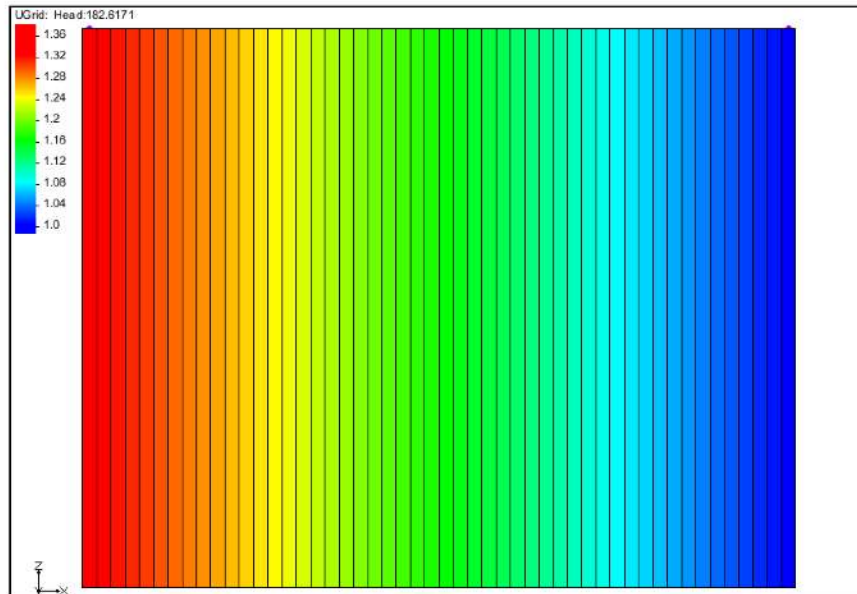


Figure 1 Initial project for the MODFLOW 6 model

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.

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.

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.

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*.

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”.

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

The generated plot should appear similar to Figure 2.

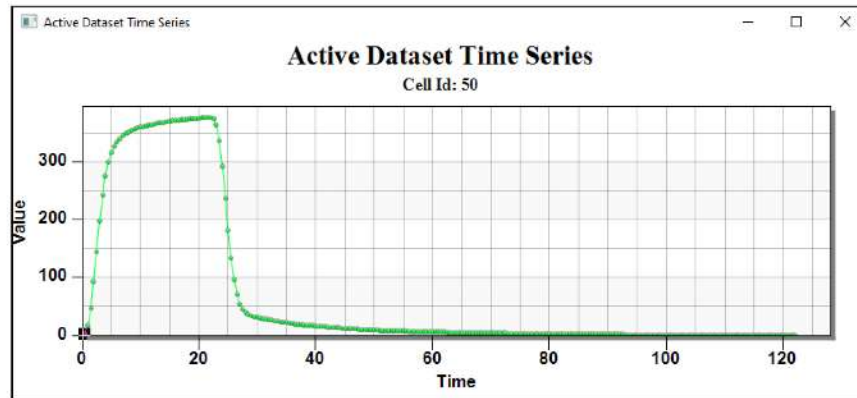


Figure 2 The active dataset time series plot

10 Conclusion

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

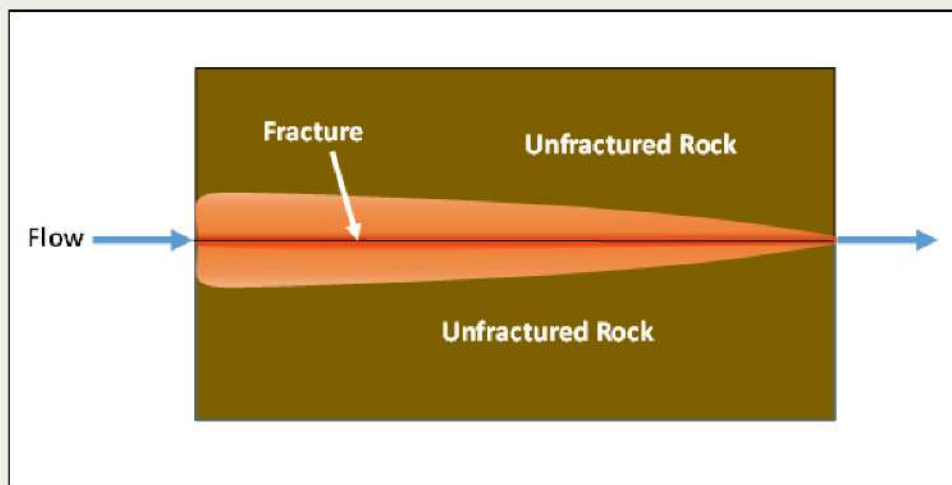
- Creating a MODFLOW 6 transport model.
- Adding the MDT Package to MODFLOW 6.
- Running MODFLOW 6.
- Reviewing the MODFLOW 6 solution.



GMS 10.7 Tutorial

MODFLOW 6 – MDT Discrete Fracture

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



Objectives

Learn how to use the Matrix Diffusion Transport package (MDT) with MODFLOW 6 to simulate diffusion from a single fracture.

Prerequisite Tutorials

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

Required Components

- GMS Core
- MODFLOW Interface

Time

- 20–30 minutes

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4	Defining the MDT Package.....	4
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6	Examining the Solution.....	5
7	Conclusion.....	6

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 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 guide¹ and related journal papers^{2, 3}.

The problems in this tutorial consist of a single layer, one-dimensional unstructured grid (UGrid) with a MODFLOW 6 simulation. The head values have been set for the grid.

For 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 Wang² 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

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, *Journal 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.

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_f , (years)	30	

This tutorial will demonstrate the following topics:

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_discrete* 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).

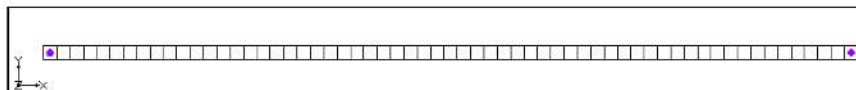


Figure 1 Initial project for the MODFLOW 6 model

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

Before continuing, save the project with a new name.

8. Select *File* | **Save As...** to bring up the Save As dialog.
9. Browse to the *Tutorials\MODFLOW 6\mf6_mdt_discrete* directory.
10. Enter "discrete_fracture.gpr" as the *File name*.
11. Select "Project Files (*.gpr)" from the *Save as type* drop-down.
12. Click **Save** to save the project file and close the Save As dialog.

3 Adding the MDT Package

The MODFLOW 6 simulation has been setup without the MDT package. Both a groundwater flow model and a groundwater transport model have been added. The MDT package can be added by doing the following:

1. Right-click on " trans" and select *New Package* | **MDT** to add the package.

Notice the " MDT" package is now shown in the Project Explorer under the groundwater transport model. Make certain the package is not locked before continuing.

2. In the Project Explorer, right-click on " model-mdt" and select **Unlock All**.

4 Defining the MDT Package

The MDT package can be defined during the process of setting up the GWT model or after the GWT model has been created as in this case. To define the MDT package, do the following:

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 "4". 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.
3. On the *MD_FRACTION* tab, set the *Constant* value to "0". This is the volume fraction of low permeability material in the element. Since this example is only modeling the fracture, the value is zero.

Note: this convention is different from that used in REMChlor-MD and in the MODFLOW-USG MDT package where the MDT volume fraction is the fraction of high permeability material in the element.

4. On the *MD_POROSITY* tab, set the *Constant* value to "0.01". This is the porosity of the unfractured rock.
5. On the *BULK_DENSITY* tab, set the *Constant* value to "2.0". This is the dry bulk density of the rock, which is not used in this simulation of tritium transport.
6. On the *MD_DIFF_LENGTH* tab, set the *Constant* value to "1e-10". The characteristic diffusion length is used with other *MD_TYPE_FLAG* options, but is not needed for *MD_TYPE_FLAG*-4. Nonetheless, a small non-zero value has been added.

7. On the *MD_TORTUOSITY* tab, set the *Constant* value to "0.1". This is the tortuosity in the rock matrix
8. On the *MD_DIST_COEFF* tab, set the *Constant* value to "0.0". This is the adsorption distribution coefficient, which is not used in this example.
9. On the *MD_DECAY* tab, set the *Constant* value to "0.0561". This is the tritium decay rate, 1/yr.
10. On the *MD_DIFF_COEFF* tab, set the *Constant* value to "0.05046". This is the tritium molecular diffusion coefficient, m²/yr.
11. Click **OK** to close the *Matrix Diffusion Transport (MDT) Package* dialog.

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

5 Saving and Running the Simulation

Save and run the simulation by doing the following:

1. Right-click on " model-mdt" 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*.

6 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 "model-mdt (MODFLOW 6)" folder.
3. Using the **Select Cells**  tool, select cell 2 (the second cell on the left).
4. Click the **Plot Wizard**  macro to open the *Plot Wizard* dialog.
5. Under *Plot Type*, select "Active Dataset Time Series".
6. Click **Finish** to close the *Plot Wizard* and generate the plot.

The generated plot should appear similar to Figure 2.

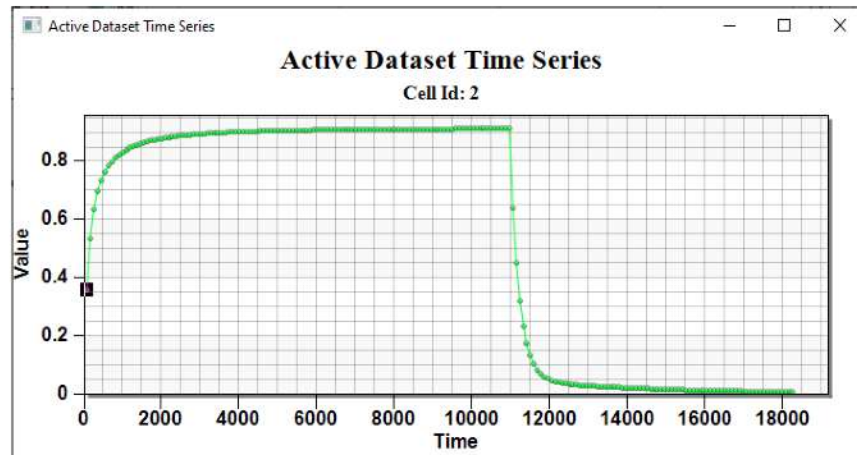


Figure 2 The active dataset time series plot

7 Conclusion

This concludes the “MODFLOW 6 – MDT Discrete Fracture” tutorial. The following topics were discussed and demonstrated:

- Adding the MDT Package to MODFLOW 6.
- Defining the MDT Package.
- Running MODFLOW 6.
- Reviewing the MODFLOW 6 solution.

C3: Parallel fractures with equivalent porous media

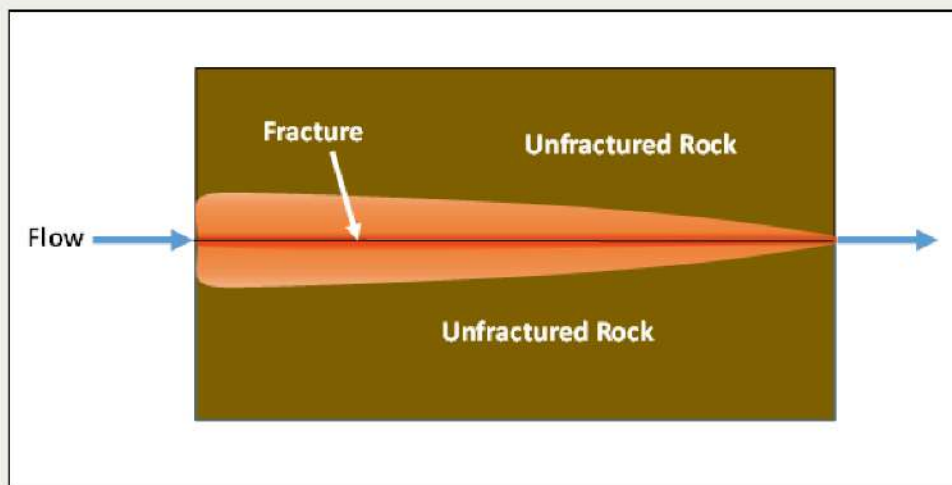


GMS 10.7

GMS 10.7 Tutorial

MODFLOW 6 – MDT Equivalent Porous

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



Objectives

Learn how to use the Matrix Diffusion Transport package (MDT) with MODFLOW 6 to simulate diffusion from a set of parallel fractures.

Prerequisite Tutorials

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

Required Components

- GMS Core
- MODFLOW Interface

Time

- 20–30 minutes

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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 with collaboration 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 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 guide¹ and related journal papers^{2, 3}.

The problems in this tutorial consist of a single layer, one-dimensional unstructured grid (UGrid) with a MODFLOW 6 simulation. The head values have been set for the grid.

This tutorial will demonstrate the following topics:

1. Opening an existing MODFLOW 6 simulation.
2. Activating the MDT package.
3. Running the simulation and examining the results.

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, *Journal 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

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_equivalent_porous* 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).

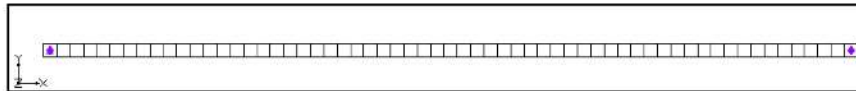


Figure 1 Initial project for the MODFLOW 6 model

This model has a single layer UGrid. Specified heads (CHD) have been set at each end. A total of 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.

A general simulation 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 Falta³. 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. In REMChlor-MD and in the MODFLOW-USG MDT package, this is the VOLFRACMD variable. In the MODFLOW 6 MDT package, a different convention is used, and the volume fraction of the low permeability is specified as the MD_FRACTION variable, where $MD_FRACTION = 1 - VOLFRACMD$. The characteristic diffusion length used in the MDT package, MD_DIFF_LENGTH 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 Falta² 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 Falta³, the pore velocity in the fractures is 100 m/yr. The volume fraction of the fractures is $0.0001\text{m}/0.5\text{m} = 0.0002$. Then the bulk Darcy velocity is 0.02 m/yr. With our previous

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 1.

Table 1. Parameters used in the fractured rock matrix diffusion comparison.

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.

8. Select **File** | **Save As...** to bring up the *Save As* dialog.
9. Browse to the *Tutorials\MODFLOW 6\mf6_mdt_equivalent_porous* directory.
10. Enter "equivalent_porous.gpr" as the *File name*.
11. Select "Project Files (*.gpr)" from the *Save as type* drop-down.
12. Click **Save** to save the project file and close the *Save As* dialog.

3 Adding the MDT Package

The MODFLOW 6 simulation has been setup without the MDT package. Both a groundwater flow model and a groundwater transport model have been added. The MDT package can be added by doing the following:

1. Right-click on  *trans* and select **New Package** | **MDT** to add the package.

Notice the  *MDT* package is now shown in the Project Explorer under the groundwater transport model. Make certain the package is not locked before continuing.

2. In the Project Explorer, right-click on  *model_mdt_parallel* and select **Unlock All**.

4 Defining the MDT Package

The MDT package can be defined during the process of setting up the GWT model or after the GWT model has been created as in this case. To define the MDT package, do the following:

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". 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.

3. On the *MD_FRACTION* tab, set the *Constant* value to “0.9998”. This is the volume fraction of the low permeability material.
Note: that this definition is different from the *VOLFRACMD* variable that is used in REMChlor-MD and the MODFLOW USG MDT package. *MD_FRACTION* = 1 – *VOLFRACMD*.
4. On the *MD_POROSITY* tab, set the *Constant* value to “0.1”. This is the porosity of the unfractured rock.
5. On the *BULK_DENSITY* tab, set the *Constant* value to “2.0”. This is the dry bulk density of the unfractured rock.
6. On the *MD_DIFF_LENGTH* tab, set the *Constant* value to “0.25”. This is the characteristic diffusion length, which is one-half of the fracture spacing.
7. On the *MD_TORTUOSITY* tab, set the *Constant* value to “0.1”.
8. On the *MD_DIST_COEFF* tab, set the *Constant* value to “0.05”. This is the rock/water distribution coefficient for the chemical. This value, combined with the bulk density of 2.0 and porosity of 0.1 gives a retardation factor of 2.
9. On the *MD_DECAY* tab, set the *Constant* value to “0.0”. The solute is not undergoing decay.
10. On the *MD_DIFF_COEFF* tab, set the *Constant* value to “0.03159”. This is the molecular diffusion coefficient, m²/yr.
11. Click **OK** to close the *Matrix Diffusion Transport (MDT) Package* dialog.

The MDT Package is now set up for the parallel fracture system and ready for the simulation run.

5 Saving and Running the Simulation

Save and run the simulation by doing the following:

1. Right-click on “ model_mdt_parallel” 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*.

6 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 “ model_mdt_parallel (MODFLOW 6)” folder.
3. Using the **Select Cells**  tool, select cell 2 (the second cell on the left).
4. Click the **Plot Wizard**  macro to open the *Plot Wizard* dialog.
5. Under *Plot Type*, select “Active Dataset Time Series”.
6. Click **Finish** to close the *Plot Wizard* and generate the plot.

The generated plot should appear similar to Figure 2.

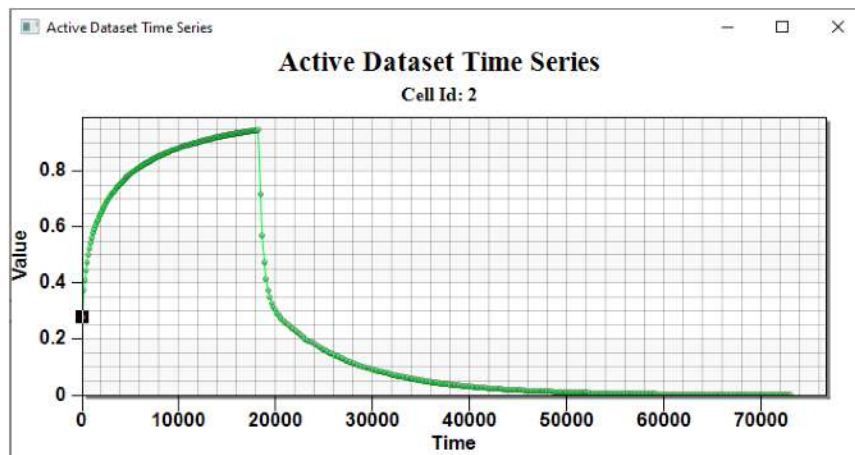


Figure 2 The active dataset time series plot

7 Conclusion

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

- The MODFLOW 6 MDT package can be used to simulate matrix diffusion from multiple fractures in fractured porous materials.
- The MDT package allows for an equivalent porous media approach to be used for fractured systems where normal grid elements are used with embedded matrix diffusion occurring over a finite distance in the matrix material in each element.