

ANALYTICAL SOLUTE & HEAT TRANSPORT MODEL

Graphical User Interface

USER MANUAL

Documentation of graphical user interface functionalities for an analytical solute and heat transport model

Tomas Perina (APTIM), Anurag Srivastava, and Fekadu Moreda (RTI International)

Version: May 2024

ASHTM v.0.0.1.24

T3D1.3.02

DRAFT

Contents

Acronym List	1
Introduction	3
Software Installation and Computer Requirements	5
Analytical Solute and Heat Transport Model (ASHTM)	7
Background	7
Graphical User Interface	9
Main Interface	9
Main Menu Options	9
Project Explorer	10
<i>Context Menu Options</i>	10
Simulation Modes	11
Forward Simulation.....	11
<i>Inputs</i>	12
<i>File Output</i>	13
<i>Graphical Output</i>	14
Inverse Simulation	17
<i>Inputs</i>	18
<i>Execution</i>	23
<i>File Output</i>	24
<i>Graphical Output</i>	24
Model Input Variables	25
Tutorials	26
Getting Started	26
Tutorial 1:.....	26
Tutorial 2:.....	32
Tutorial 3:.....	48
Tutorial 4:.....	49
Tutorial 5:.....	57
Tutorial 6:.....	64
References	78

DRAFT

Acronym List

ASHTM	Analytical Solute and Heat Transport Model
EPA	U.S. Environmental Protection Agency
GUI	Graphical User Interface
GA	Genetic Algorithm
MCMC	Markov Chain Monte Carlo
ORD	EPA's Office of Research and Development
RAC	Remedial Action Contract

DRAFT

DISCLAIMER OF LIABILITY

Regarding the ASHTM Graphical User Interface software and documentation, none of the following entities: the United States Government, RTI International, APTIM Federal LLC, or their employees, accept any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, tools, products, or processes disclosed. Moreover, the software and documentation are provided "as-is" without any explicit or implied guarantees or warranties, including but not limited to any warranties of merchantability or fitness for a particular purpose.

DISCLAIMER OF ENDORSEMENT

Mention of any commercial products, processes, or services by their trade name, trademark, manufacturer, or any other means should not be automatically construed as an endorsement, recommendation, or preference by the United States Government. The views and opinions expressed by authors in this context do not inherently represent or align with those of the U.S. Government, and they should not be utilized for advertising or promotional purposes for products. Commercial products are identified in this document for documentation purposes only.

DRAFT

Introduction

The U.S. Environmental Protection Agency (EPA) assigned APTIM Federal Services, LLC (APTIM) the task of creating an analytical model for solute transport in a three-dimensional aquifer of finite thickness, featuring uniform flow, dual porosity, sequential decay, and a source with specified time-variable concentration. This work was conducted under the Remedial Action Contract (RAC) III, contract number EP-S9-13-02. The entire process, including the development of mathematical models, coding in C++ for a portable executable, testing, and benchmark simulations, has been detailed in a standalone report (APTIM 2022). The models were subsequently published in journals (Perina 2021, 2022) and applied to analyze field tracer tests (APTIM 2023).

To create a user-friendly interface for the model, EPA's Office of Research and Development (ORD) contracted RTI International under Contract No. 68HERC21D0004/68HERC22F0031. The graphical user interface (GUI) was designed to enable users to input data, generate model input files, run the model executable, read output files, display results, and access previously saved input and output files.

The GUI for the Analytical Solute and Heat Transport Model (ASHTM), model executable, this manual, and the reports on model development and tracer tests (APTIM 2022, 2023) are all in the public domain.

This user manual documents the software installation, guidance on how to setup-the model, run the model and explore outputs. In addition, the manual presents 6 tutorials that explain the various modeling scenarios.

DRAFT

Software Installation and Computer Requirements

This software is a Windows application developed in the C# programming language using the .NET Core framework in the Microsoft Visual Studio environment.

Computer Requirements

- Operating System: Windows 10 is the preferred edition.
- Processor: A multi-core processor, such as an Intel Core i5 or an equivalent AMD processor, is recommended for a smooth user experience.
- RAM (Memory): A minimum of 4 GB of RAM is recommended, but 8 GB or more is ideal for larger applications or complex UIs.
- Storage: Ensure you have enough disk space for the .NET Core framework and other dependencies to host the program on the machine. Sufficient space should also be available to create and store program files (the input and output files are ASCII text files of generally small size).
- Graphics: This application creates 2D and 3D graphical outputs and has been tested on an Intel (R) UHD Graphics card. Other graphics cards may also be compatible with this application.
- Screen Resolution: A monitor with a resolution of 1920x1080 or higher is recommended to handle WPF UI designs and 3D graphics rendering effectively.
- Input Devices: Standard input devices such as a keyboard, mouse, or touch screen are required for user interaction with the application.
- Internet Connection: An internet connection is necessary for downloading the application and Microsoft framework dependencies. After installation, the application can be run without requiring internet connectivity.
- .NET Core Compatibility: Ensure that your chosen Windows version is compatible with the .NET Core version you plan to use. Check the official .NET Core and WPF documentation for up-to-date compatibility information.

Installation Instructions:

To install this application on a Windows machine, follow one of the following two options:

1. Installation using the Setup Executable:
 - Run the 'setup.exe' file.
 - Select the 'Install' option on the setup screen.
 - Follow the installation instructions as they appear on the subsequent screens.

- If the installation is successful, the 'ASHTM' program will be added to the list of programs accessible via the Windows Start Menu.
2. Using the Zipped Folder:
- If you receive the program as a zipped folder, simply extract the folder to your preferred location.
 - Run 'ASHTM.exe' to start the program.

During the installation process, the user may be required to install the Microsoft .NET Core App (version 6.0) framework if it is not already installed on the Windows machine. This framework can be downloaded separately from the Microsoft website or can be installed automatically during the first-time use of the program when prompted by the application.

DRAFT

Analytical Solute and Heat Transport Model (ASHTM)

Background

Analytical solute transport models have an important role for guiding the selection of transport parameters and provide a check on accuracy for more detailed and complex numerical solute transport models. Analytical models can only represent rather simplified problem geometry and uniform flow field, but their input is simple, and their accuracy is not affected by spatial and temporal discretization and numerical dispersion. Analytical transport models are also applicable to tracer tests affecting a small portion of the aquifer. For an analytical advective-dispersive transport model to be practical in this role, it should include first-order reactions and dual porosity, its domain should be three-dimensional with finite thickness, and it should allow for a source term of flexible time-dependency.

Many analytical solutions exist for solute transport in porous media and various boundary conditions, source geometries, and dimensionality of the aquifer (Perina 2021 and 2022 provides focused review of literature on analytical solute transport models for 3D aquifers, dual porosity, and chain-decaying species). Most of the published solutions were developed to investigate a specific aspect of solute transport, such as sorption, dispersion, dual porosity, or decay of multiple species. As such, they were not intended to be used as general modeling tools. Software or executables to run these models are generally not available. A suite of new models was developed to satisfy all the requirements listed above.

The new models developed account for dual-porosity, sorption coefficients that differ in the mobile and immobile domains, decay coefficients that differ for the sorbed and dissolved mass and in the mobile and immobile domains, and two types of source term. The first source type is a vertical rectangular patch with specified concentration (as either the first type-Dirichlet or third type-Cauchy boundary condition) of arbitrary time dependency (Model 1). The second source type is a point source or volumetric source in the shape of a rectangular prism with mass generation of arbitrary time-dependence (Model 2). The model with the rectangular patch source can represent chain-decaying species with an arbitrary number of daughter products (Model 3). The volumetric source model (Model 2) can also represent an initial concentration distribution and no source.

Heat can be utilized as a tracer in addition to chemical tracers. Heat transport can be simulated with a solute transport model after a simple change of variables when local temperature equilibrium in the aquifer is assumed; see APTIM (2022) for the substitutions and conditions for local temperature equilibrium. The models developed under this project can be also used to simulate heat transport in groundwater. The variable substitutions are done internally by the model code.

A set of complimentary models (Models 4, 4.1, and 4.2). is included to simulate heat transport after instantaneous injection with greater computational efficiency than the models described above. These models also apply to mass transport in a single porosity aquifer.

Inverse simulation capability was added to the code to allow estimation of unknown transport parameters (such as Darcy velocity, effective porosity, or decay rate) from field tracer tests or from water quality monitoring records.

DRAFT

Graphical User Interface

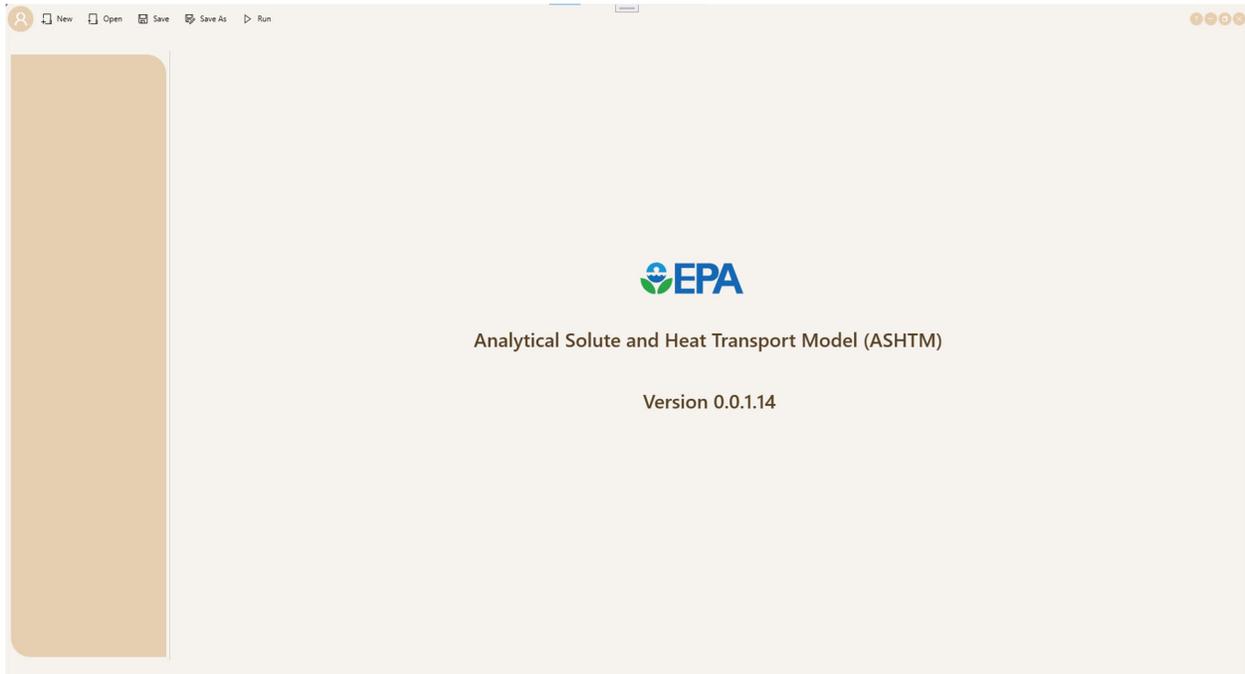


Figure 1: Snapshot of the Main Window

Main Interface

As depicted in Figure 1, the main interface comprises of three key elements:

1. The top bar, housing the main menu options along with standard window buttons that facilitate window resizing and program exit.
2. A side panel, featuring a project explorer designed to display project directories and files (with the .t3d extension).
3. The content panel, dedicated to exhibiting model inputs and outputs.

Main Menu Options

Option	Description
About	Presents a concise overview of the software's identity, encompassing its name, version, and developer information.
New	Generates a fresh, empty project (*.t3d) within the software.

Option	Description
Open	Allows you to designate a project folder, subsequently populating the project explorer with all sub-folders and projects (.t3d files) contained within the chosen directory.
Save	Saves any pending modifications made to the chosen project, consequently overwriting the existing version of the project.
Save As	Enables you to save the current project with a new name or in an alternate location.
Run	Executes the selected project through the T3D executable, leading to the creation of model output files.

Project Explorer

The project explorer provides a tree-view presentation of parent folders and their corresponding project files (.t3d). A visual representation showcasing project files from various case studies is shown in Figure 2.

The icon associated with the project files conveys the run and output status in the following manner:

- Green: Project has been executed, and outputs are accessible for viewing.
- Hourglass: Project simulation is currently in progress.
- Gray: Project has not been executed and outputs are unavailable.
- Red: Project simulation was unsuccessful due to specific modeling or parameter errors.

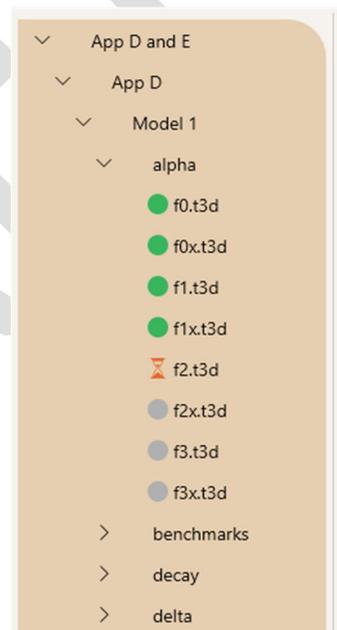


Figure 2: Illustration of Project Explorer Displaying Folder Hierarchy and Project Files

Context Menu Options

Context menu options are available after placing cursor on a simulation in the Project Explorer and clicking the right mouse button.

Note: *Hovering your mouse cursor over a folder or project file node will reveal the complete path in the tooltip.*

Level	Option	Description
Folder Level	Add Project	Introduce a new project within the chosen folder.
	Remove	Exclude the folder, along with its sub-folders and project files, from the project explorer. This action, however, does not delete the folders and files from the system.
Project File	Run	Execute simulation for the selected project.
	Cancel Run	Abort the ongoing simulation process for the currently active project.
	Remove	Exclude the project from the explorer's view.
	Delete	Delete the project (all input and output files).

Simulation Modes

Projects offer the flexibility of being configured to operate within either of two distinct execution modes:

1. **Forward Mode:** The forward, also called predictive, mode involves the computation of concentrations (with various output options) utilizing parameters assigned by the user to the analytical model.
2. **Inverse Mode:** In this mode, an optimization approach is employed to estimate unknown model inputs (parameters). This is achieved by matching the outputs of the analytical model to observations through iterative refinement that is based on an optimization algorithm.

Upon initiating a new project, users are presented with the choice of selecting one of the two simulation modes. Once a simulation mode has been chosen for the project, it cannot be changed. This restriction exists due to the divergent configuration of input between the two modes.

Forward Simulation

Following the selection of the "Forward mode" simulation for a new project, users are directed to a model configuration and input parameters page within the main content panel (Figure 2). This page prominently displays essential model configuration parameters—such as model type, transport medium, and transport type—at the upper section of the page. A menu bar containing categorized groups of parameter sets is shown below the configuration parameters.

Upon initial display, the input page provides users with a clear view of the configuration parameters alongside the menu bar. At this point, the input fields for the categorized parameter groups, depicted in Figure 2, are not visible. The menu bar controls the visibility of these parameter groups, allowing users to toggle them on or off as needed. This allows users to customize their experience by displaying the specific parameter groups they wish to access on the page. The diagram in the upper right shows the geometry for the selected model.

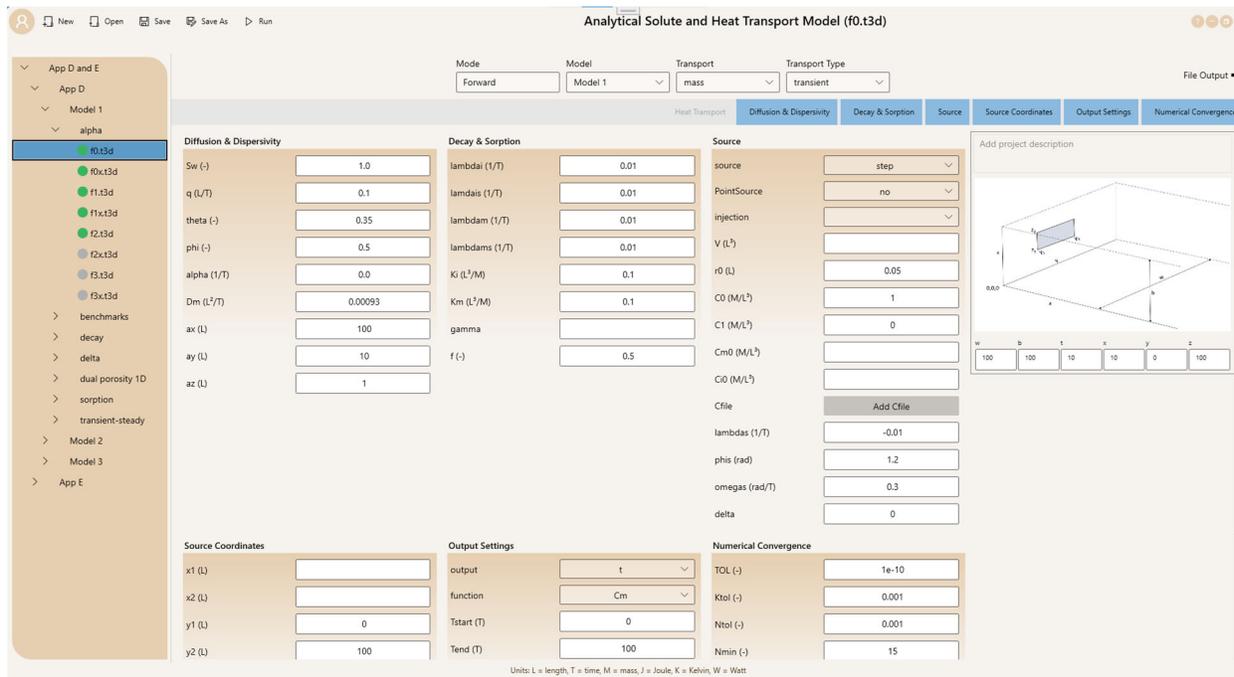


Figure 2: Snapshot of Input Parameters Page for Forward Simulation

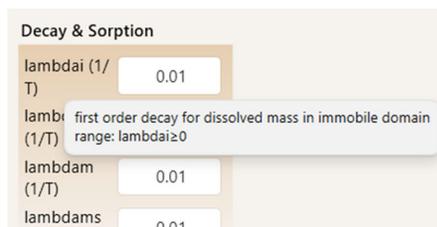
When selecting an existing "Forward mode" simulation project, users are immediately directed to the corresponding input page, upon selecting the desired project file in the project explorer panel.

Inputs

When initiating a new project, users must initially define the model configuration parameters. These parameters dictate the parameter groups and their individual components. Only pertinent parameter groups and parameters are activated based on the configuration parameter selections. For instance, the 'Heat Transport' parameter group becomes active solely when the 'Transport' is designated as 'heat,' while the 'Decay & Sorption' group is exclusively activated for the 'mass' transport. The variables below the model geometry diagram define the dimensions of the model domain and coordinates for a point at which output is computed (unless superseded by Output settings).

To allocate inputs to a parameter group, users should first choose the desired group from the menu bar. Subsequently, input values are entered within the displayed input block. Some of the parameter fields include default values that can be user adjusted.

The input variable names follow the symbols used in the derivation of the mathematical model. Hovering the cursor above the variable name shows brief explanation of the variable and its input value range; the example below shows explanation for the first variable “lambdai”:



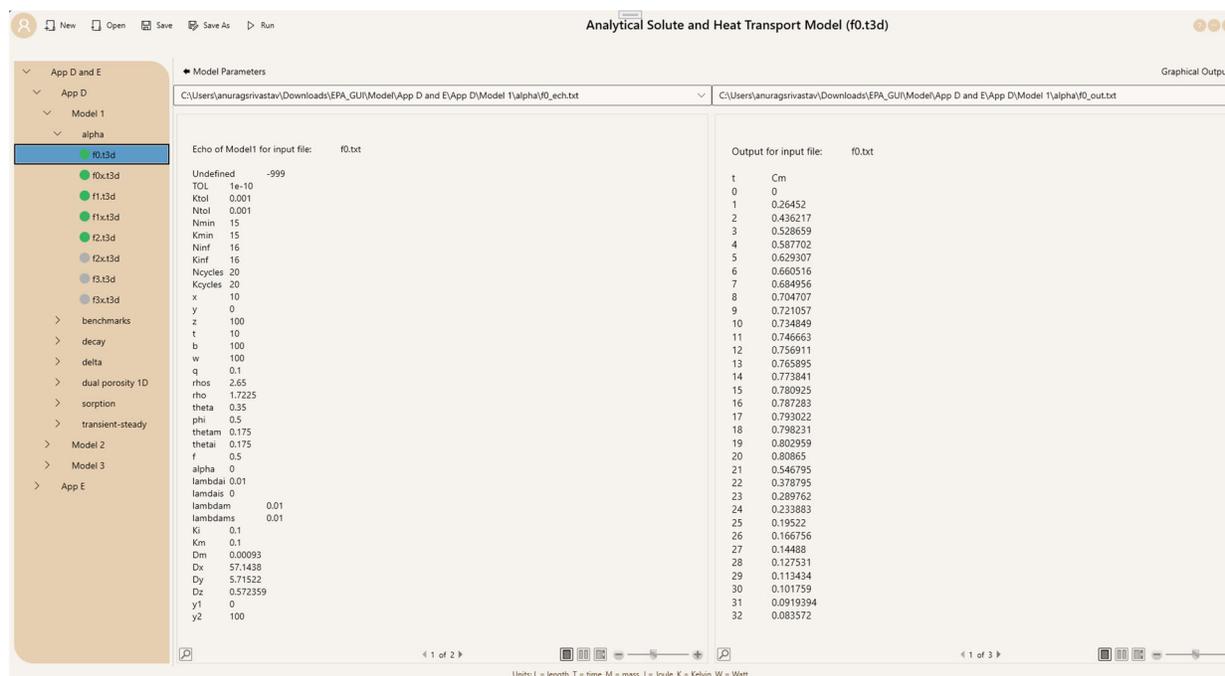


Figure 3: Snapshot of File Output Page for an Example Forward Simulation

The units are shown in parenthesis after the variable name as L (length), T (time), and M (mass) with additional units for heat transport. All input and output must be in consistent units.

While the software performs checks on certain parameter inputs and assesses their validity within acceptable ranges, users bear the responsibility of assigning all necessary parameters for the model simulation. For comprehensive insights into the modeling process and the requisite parameters, users should consult the technical manual.

File Output

Once all necessary parameter inputs have been assigned, the subsequent stage involves saving the project and commencing the simulation using the executable for the analytical model (T3D.exe). To save the project, users should ensure the project node remains selected in the project explorer and then access the 'Save' option from the top menu within the main window.

Users have a couple of options for executing the model simulation. Firstly, they can opt to click on the 'Run' selection from the main menu while keeping the project node highlighted in the project explorer. Alternatively, they can utilize the context menu's (right-click the project to display the context menu) 'Run' option specific to the project node.

While the simulation is in progress, an hourglass icon is exhibited alongside the project node in the project explorer. Upon the completion of the simulation, this icon transforms into a green circular symbol, indicating that the execution has finished and the model outputs are now ready for user review.

Note: If a parameter input is invalid, the background of the input box will turn red. Despite this, users can still save or execute the model simulation. However, it's important to rectify any invalid entries before proceeding with the saving and execution of the model simulation.

To stop the simulation in progress, right-click the running project in the project explorer and select "Cancel Run."

Upon successful completion of the forward model simulation, two output files are generated:

1. An "echo" file containing the parameter inputs as read by the analytical model executable. It also lists any error messages arising from input errors that stop the model's execution.
2. An output file that presents concentration profiles, depending on output options selected. This file is not generated if errors are listed in the echo file.

To access these output files, users can navigate to the 'File Output' page (Figure 3) via the navigation menu positioned on the upper right corner of the input page. This page features two panels designed for side-by-side viewing of the output files. To examine an output file, users simply select the desired file from the dropdown list provided atop each panel.

Graphical Output

Located in the uppermost section of the 'File Output' page, there are two distinct navigation menus: one labeled "Model Parameters" on the left and the other titled "Graphical Output" on the right. To return to the input page dedicated to the model parameters, use the 'Model Parameters' navigation option. Conversely, if you're interested in generating visual graphical depictions of the model's output, transition to the 'Graphical Output' page by selecting the corresponding navigation menu option.

DRAFT

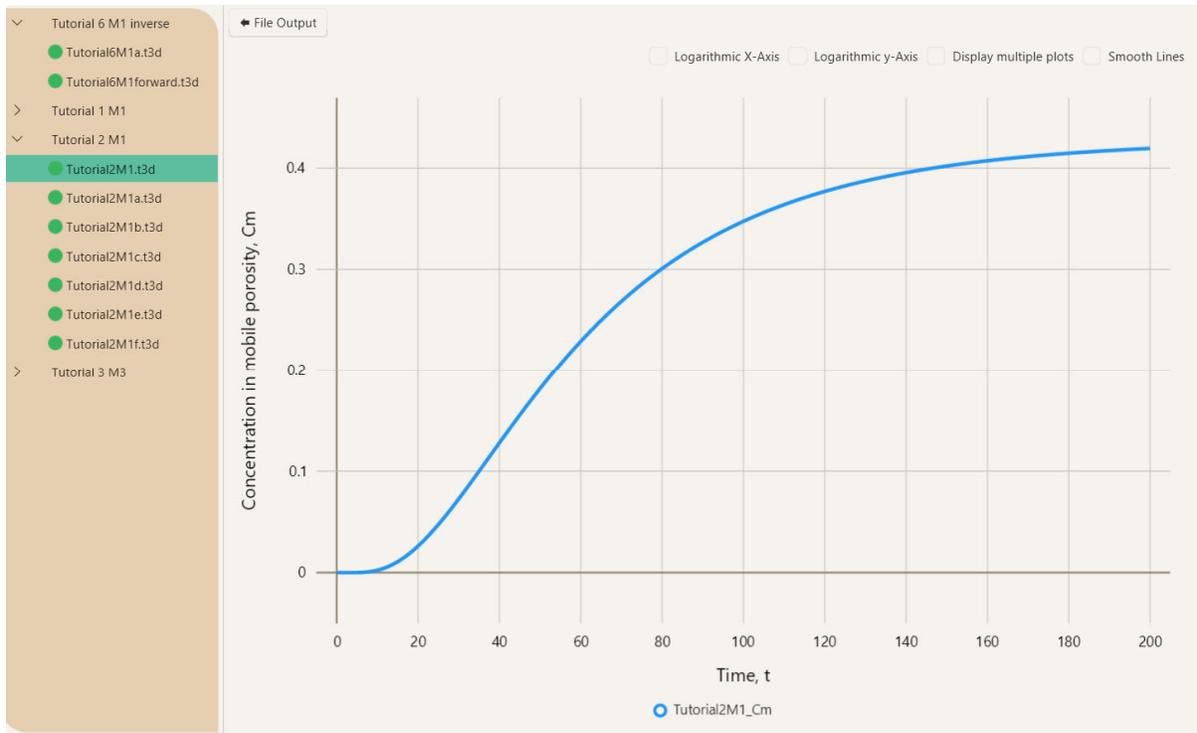


Figure 4: An Example Graphical Display of Model 1 Output – concentration vs time

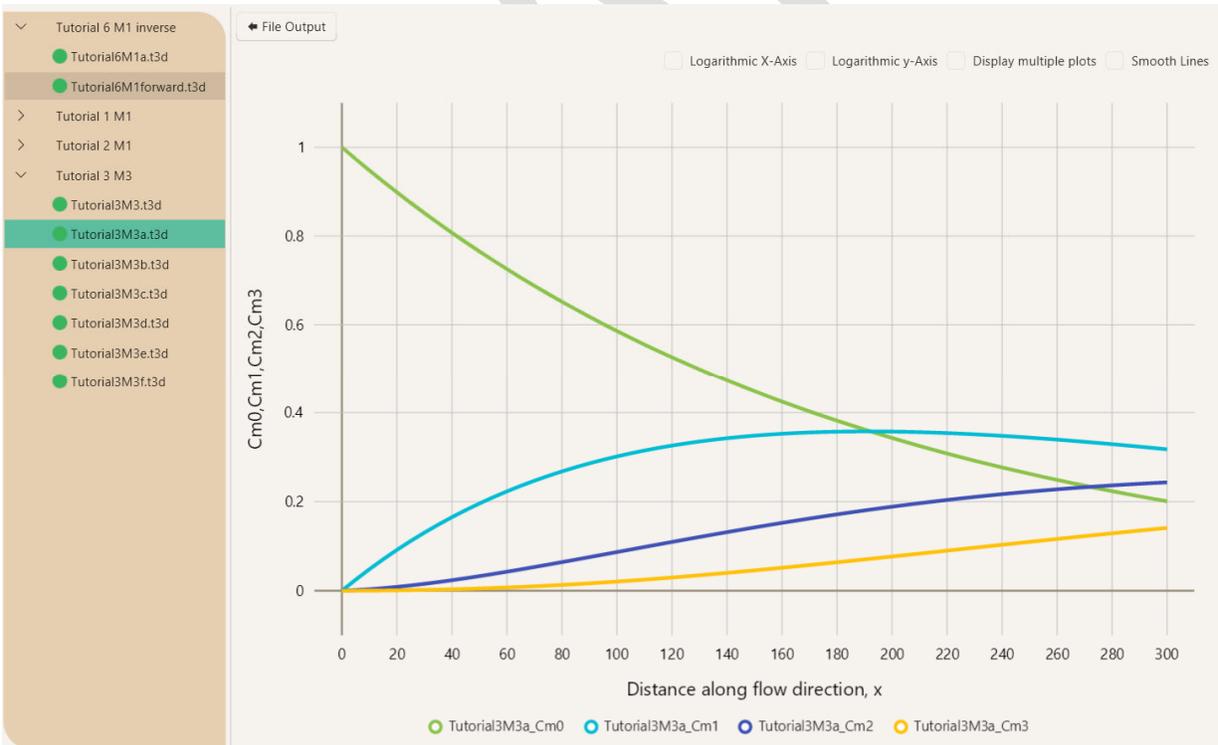


Figure 5: An Example Graphical Display for Model 3 Output – concentration vs distance

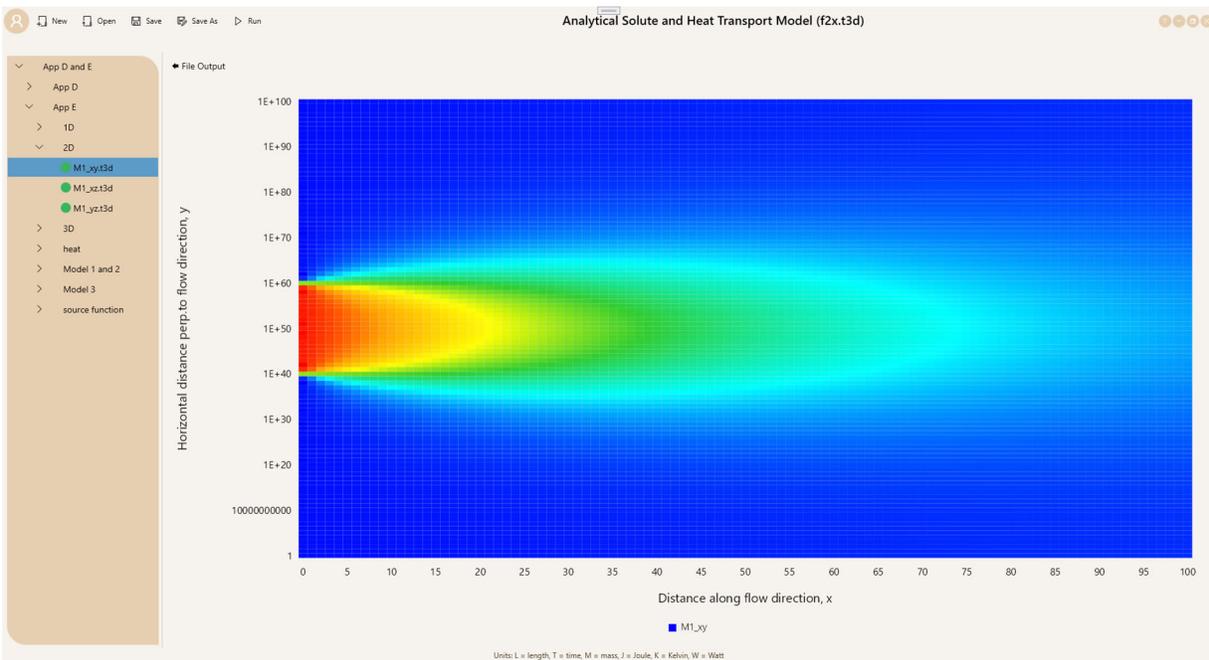


Figure 6: Illustration of a 2-Dimensional Graphical Output

Users can select logarithmic scale for either the horizontal (x) or vertical (y) axis. By default, the line is displayed as piece-wise linear plot (with line segments between computed points); it can be smoothed by selecting the “Smooth Lines” option.

When the 'Display Multiple Plots' checkbox is present in the upper right corner of the Graphical Output page, users gain the capability to perform the comparative analysis of outputs across multiple projects, all within a single consolidated graph. By clicking on various project nodes within the Project Explorer, they can include graphical outputs from different models or projects in a single graph. It's important to note that this function operates under the condition that multiple graphs will be displayed only when the selected project node shares the same x-axis variable as the preceding one (i.e. all simulations compute time-concentration plot, x-concentration plot, etc.). The 'Display Multiple Plots' option is not available for two- or three-dimensional model outputs.

For two-dimensional outputs, the graphical output is presented as a concentration “intensity map”, depicting values over x-y, y-z, or z-x dimensions, as determined by the model output settings configured on the input page. In Figure 6, we show a representative instance of 2D graphical output, where concentration is visualized relative to x and y distances along the flow direction. The intensity map's color spectrum ranges from blue to red, indicating varying concentrations from low to high. Similarly, for three-dimensional models, an intensity map offers insight into concentration variations across all three x, y, and z dimensions. Refer to Figure 7 for an illustrative demonstration of a 3D output display.

[placeholder for 3D output Figure 7]

The 'Graphical Output' page also provides users with a context menu option to capture the 1D and 2D graphical displays as images, which could be used in reports. However, this feature is not

available for the 3D display in the current software version. As an alternative, users can resort to use the Windows screen capture function (or other snapshot software).

Inverse Simulation

Inverse simulation allows estimating unknown model parameters by optimizing model fit to observations recorded during controlled tests or during water quality monitoring. For example, a set of concentrations measured over time in monitoring wells downgradient from a source is available; this data set is referred to as observations. Another example is a set of concentration (or temperature) measurements during a controlled tracer test conducted for the purpose of quantifying the unknown transport parameters by inverse modeling. ASHTM is set up to use transient observation data sets.

Some of the model inputs are known, such as aquifer thickness, locations of monitoring wells, etc. The values for other model inputs are not known, for example the Darcy flux, dispersivity, degradation rate, or fraction of mobile (effective) porosity. Yet other model inputs may not be precisely known but their values may be reasonably estimated based on other information about the site, for example aquifer porosity, source concentration, or source dimensions. The unknown model inputs to be estimated by inverse modeling are referred to as “parameters.” Some parameters may be tied to others (for example, transverse dispersivity may be defined as a fraction of longitudinal dispersivity), these are referred to as “tied parameters.” The set of values for the estimated parameters represents a possible solution to the inverse problem and may be referred to as parameter vector.

Inverse simulation has additional input variable groups (Figure 8). The user must enter values for all model inputs, including the values for the unknown parameters to be estimated. This input is used to calculate an initial fit of the model to the observations; the main purpose of the initial execution is to assure that all inputs to the model are specified, and their values result in plausible output (even if the initial fit to observations is poor). The execution then proceeds to estimate the parameter values.

Any of the model inputs listed in the parameter drop-down menu may be selected as estimated parameter. However, not any model input can be reasonably estimated from a given set of observations. Some parameter combinations can lead to “ill-posed” inverse problem; they are usually recognized by inverse modeling leading to unrealistic values for estimated parameters.

Note: *The performance of the 3D graphics library is governed by your system's graphics card. If the 3D graphical output is not visible for a specific model output, it may indicate an incompatibility between the software's graphics library and your system's graphics card. To address this, you might consider selecting an alternative version of the graphics library through the 'Switch Library' option available in the 'Graphical Output' page's context menu. Should this step not yield the desired results, please reach out to our support team, providing them with your graphics card details for further assistance.*

Figure 8. Parameters Input Page for an Example Inverse Simulation Mode.

Two inverse methods are used in a sequence: genetic algorithm (GA) followed by Markov chain Monte Carlo (MCMC). The GA finds good enough parameter values to start the MCMC, which then converges to the parameter distribution. Either GA or MCMC may be used independently but the sequence is much more efficient in solving the inverse problem.

Like the Forward Simulation, users must choose the Inverse Simulation Mode when initiating a new project for inverse simulation. Once the simulation mode is configured to 'Inverse,' it remains fixed and cannot be changed thereafter.

Inputs

The input page has similar functionality and appearance as the forward simulation page. However, for an inverse run, a distinct set of categorized parameters is defined. When selecting the simulation mode, a new page is displayed, showing the chosen simulation mode for the project at the top of the page, accompanied by a menu bar below it. This menu bar enables users to control the visibility of input variable groups specific to the inverse model, allowing them to toggle these groups on or off as needed for display on the input page (see Figure 9).

Out of those seven input variable groups, users can define multiple sets of variables for 'Test' (one for each tracer test included in the simulation), 'Parameter' (one for each estimated model

Figure 9. Test Parameter Group for the Inverse Model

parameter), and 'Tied Parameter' (one for each dependent parameter) groups. Each Test, Parameter, and Tied Parameter has a set of several variables that must be given values. To define a new parameter, first make the parameter group visible using the menu bar option, and then select the 'Add' option to add a new parameter. Once a new parameter is added, the dropdown box shows the name of the newly added parameter set (e.g., Test 1 in Figure 8) and then user can enter the parameter values in the fields displayed for the current parameter set.

Aquifer Input

In the Aquifer input block, the user inputs values for various transport variables, including aquifer thickness (b), Darcy flux (q), and the first-order decay coefficient for the simulated species. Figure 9 displays only a portion of this input block. For a comprehensive list of variables within this input block, please refer to the Model Input Variables section.

Aquifer	
b (L)	10.67
w (L)	10
q (L/T)	1.0e-6
theta (-)	0.35
phi (-)	0.5
alpha (1/T)	0.05
Dm (L ² /T)	0.00093e-4
ax (L)	1

Figure 7. Partial snapshot of the Aquifer Input Group

Add Source	
source	pulse
PointSource	no
V (L ³)	0.378
r0 (L)	0.072
x0 (L)	0
y0 (L)	5
z1 (L)	2.13

Figure 8. Source input parameters for Test input group

Add Observations	
obswellname	FC1029A
index	
x	0.0
y	5
z	6.4
stdv	0.1
file	Add file

Figure 9. Observation input parameters for Test input group

Test Input

The Test input block encompasses the specification of the chosen transport model type (heat or mass), model number, considerations of time dependency, source magnitude, and observation parameters. To configure source parameters, utilize the 'Add Source' option, which opens the source input window (as shown in Figure 10).

Likewise, for configuring observation inputs, use the 'Add Observations' option within the Test input group (Figure 11). The Observation input requires information such as the location name, coordinates, and standard deviation. The set of observations, whether in the form of time-concentration or time-temperature data pairs, should be copied from an external source (e.g., a spreadsheet) and then pasted into the designated small cell that appears upon clicking "Add file."

Multiple Tests may be included in one inverse simulation. Each test may contain multiple observation data sets.

Users may de-activate a Test or set of observations from the context menu in order to exclude it from the inverse simulation (rather than deleting it).

Parameter Input

For each estimated parameter, the input consists of the following attributes:

- Parameter "name" (selected from a pull-down menu) that identifies the parameter as a model input.
- The "index" is relevant only for parameters representing multiple species in Model 3; otherwise, it is set to 0.
- The probability "distribution" is denoted by "G" for Gaussian, "U" for uniform, and "T" for triangular and is used for generating parameter values.
- The "log" input specifies whether the parameter value is treated internally as a natural log transformation, with options "yes" or "no." When "yes" is selected, the inverse algorithms operate on the natural logarithm of the parameter.
- The "prior" input represents the prior parameter value, estimated using information other than the observation dataset employed in inverse modeling. It can be left blank, and the "ini" value is used as a substitute.
- The "ini" value is the initial value assigned to the parameter, utilized in computing the initial model fit to observations (typically, this corresponds to the best guess value).
- The "stdv" is the standard deviation of the parameter. In cases where the parameter is log-transformed (log=yes), the standard deviation is as a multiplying factor.
- The "min" and "max" indicate the minimum and maximum permissible values for the parameter to limit its values to a reasonable (or physically plausible) range.
- The "cv" denotes the coefficient of variation, expressed as a fractional value, which is employed to generate a perturbed value of the parameter in the MCMC process.

Parameter	
	Parameter1 ▾ ...
name	q ▾
index	0
distribution	G
log	yes ▾
prior	1.0e-6
ini	1.0e-6
stdv	5
min	1.0e-10
max	1.0e-1
cv	0.01

Figure 12. Parameter input group for the Inverse model

Tied Parameter Input

A tied parameter (P_{tied}) value is dynamically updated to preserve its connection with the "master" parameter (P_{master}) value. This relationship is established as $P_{\text{tied}} = P_{\text{master}} * \text{multiplier} + \text{offset}$. Users can select both the tied and master parameters from dropdown lists and must define the multiplier and offset values.

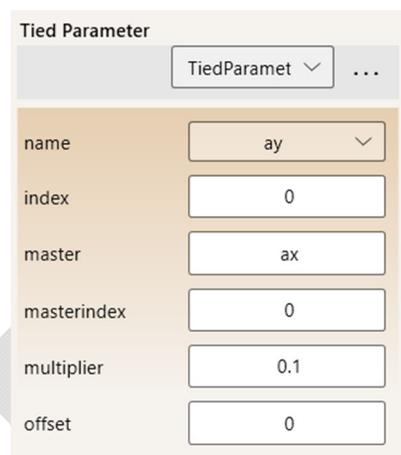


Figure 10. Tied Parameter input group for the Inverse model.

Adding, Deleting, and Deactivating Parameters and Tests

Users can define multiple Tests, Parameters, and 'Tied Parameters' for an Inverse model. To add a new parameter, simply click the '+Add' option. To remove an existing parameter from the group, select the parameter from the dropdown list and use the delete option. Alternatively, the 'Set Inactive' option allows the user to decide whether a selected parameter should be included in the estimation process; when a parameter is marked as inactive, its input value remains unchanged throughout the inversion. The parameter can be re-activated in a later simulation. If these options are not visible, these can be revealed by expanding the overflow options list, which is accessible through the ellipsis dots displayed in the upper right corner of the input parameter window.

Genetic Algorithm Input

The Genetic Algorithm (GA) is conceptually rooted in the principles of evolution of species and its terminology draws from its biological origins. When applied to an inverse problem, the GA represents the response of a population to changed environmental conditions. It comprises three fundamental processes: cross-over (replication with inheritance), competition, and mutation. When these processes are completed, a new generation emerges, with each successive generation featuring parameter vectors that represent improved solutions to the inverse problem. The main advantage of a GA is that it performs a wide search for the best parameter vector. If used alone to find the best solution to the inverse problem, its disadvantage is that it requires long execution. In the GA-MCMC sequence, the GA is used to find a good-enough solution to the inverse problem that is used as the starting parameter vector for MCMC.

The GA's input parameters encompass the population size (the count of parameter vectors), the number of generations, the mutation rate (indicating the probability of mutation occurring), and the size of a tournament group. The tournament group is randomly selected from the population, and the parameter vector that represents the optimal solution within the group is retained, while the others are discarded. These retained parameter vectors, known as "survivors," serve as the "parents" for the following generation; the inclusion of survivors in the new generation is optional. Including survivors assures faster convergence to a solution while excluding them assures a wider search for the best solution. Either option works for the GA-MCMC sequence.

Typically, a population size (Nchromosomes) of 99, a tournament group size (Ntournament) of 3, a mutation rate (mutation) of 0.05, and 10 generations (Ngenerations) result in a close enough fit of the model to observations, offering a robust starting point for the Markov Chain Monte Carlo (MCMC) process. Increasing the population size and the number of generations enhances the thoroughness of the search for the best parameter vector, but this comes at the expense of extended computation time. The option "keepsurvivors" can expedite convergence to a solution when set to "yes," whereas selecting "no" facilitates a more exhaustive search; in either case, the best solution is retained.

In most cases, the variable "alpha" should be left blank. To exclude parameter constraints from the objective function, input 0. For a comprehensive description of this aspect, please refer to the 2023 revised Appendix C User Instructions (APTIM 2022). It's important to note that, despite sharing the same name, this "alpha" is not the rate coefficient for mobile-immobile porosity.

Genetic	
Ngenerations	<input type="text" value="10"/>
Nchromosomes	<input type="text" value="99"/>
Ntournament	<input type="text" value="3"/>
keepsurvivors	<input type="text" value="yes"/>
alpha	<input type="text"/>
mutation	<input type="text" value="0.05"/>

Figure 11. Genetic (Algorithm) input group for the Inverse model

MCMC Input

The Markov Chain Monte Carlo (MCMC) process involves taking random steps from the current parameter vector, and each step is either accepted or rejected based on conditional probability. A step proposing a parameter vector that improves the solution to the inverse problem compared to the current one is accepted. In contrast, a step proposing a worse solution is accepted with a probability contingent on how unfavorable the proposed solution is relative to the current one. MCMC progressively converges towards the probability distribution of the estimated parameters. Multiple successive chains are generated, each offering an enhanced probability distribution and using the parameter probability distribution computed from the previous chain to draw the proposed values in each step.

MCMC	
N	<input type="text" value="1000"/>
Nchain	<input type="text" value="3"/>
Nb	<input type="text" value="100"/>
Gibbs	<input type="text" value="no"/> ▼
restart	<input type="text" value="no"/> ▼
alpha	<input type="text"/>
Nhist	<input type="text" value="50"/>

Figure 12. MCMC input group for the Inverse model

For MCMC configuration, users need to specify the length of the burn-in chain (whose results are discarded and not used to compute the parameter distribution from which steps are drawn in the second chain), the number of sequential chains, and the chain length. When the MCMC follows the Genetic Algorithm (GA), a burn-in length of 100 is generally sufficient. Subsequently, 3-4 chains, each with a length of 1,000, typically achieve robust convergence to the parameter distribution. Beyond 4 chains is typically unnecessary, while 2 chains usually prove insufficient. Extending the chain length over 1,000 may enhance the parameter distribution, whereas considerably shorter chain lengths tend to yield under-sampled parameter distributions.

MCMC can also be utilized without the preceding GA. While it can solve the inverse problem independently, combining the GA and MCMC sequence is a more efficient approach. If MCMC is used without the GA, setting the restart option to "yes" is recommended, and the algorithm will initiate from randomly selected parameters. To ensure effective results, the length of the burn-in (Nb) should be significantly increased, such as to the full length of the chain (N).

Execution

Once all input data is provided and the simulation is saved, simply click the "Run" button, and the model will commence execution. The processing time can vary, with Models 4, 4.1, 4.2, or any steady-state or 1D simulation typically taking seconds to minutes, while 3D transient Models 1, 2, and 3 may require many hours for the inverse execution. The execution time is, of course, dependent on the number of observations because a model value is calculated for each observation.

Users have the option to open and review the output file(s) during the run using software like Notepad or an equivalent program. Following inspection, these files can be closed without saving any changes.

File Output

The inverse simulation generates multiple output files, with comprehensive details provided in the 2023 revised Appendix C User Instructions accompanying the APTIM 2022 report. The estimated transport parameters, along with their mean values, standard deviations, and correlation matrix, are written in the output file named "`*_MHres.txt`," where "`*`" signifies the input file name. The mean parameters derived from the last chain are the solution to the inverse problem, representing the parameter values. The primary output file, "`*_MHres.txt`," also encompasses the parameter correlation matrix, standard deviations, and various additional outcomes. The file "`*_MH mean Prsq.txt`" contains essential fit statistics, including Pearson's R^2 , weighted residuals, and more. The file "`*_pdf.txt`" includes computed distributions for the estimated parameters as histograms and kernel density estimates. For user convenience, a spreadsheet is provided, containing dedicated tabs for each output file, graphical representations, and comprehensive explanations of the file contents; this spreadsheet can be used as template.

Graphical Output

The graphical user interface (GUI) presents both observations (represented as symbols) and model-computed values (displayed as lines) within a single graph. This graph is configured to depict concentration (or temperature) against time, a format commonly used for observation datasets. If your observations, as well as the model fit curves, exhibit significant variations spanning several orders of magnitude, consider utilizing the option to apply a logarithmic transformation to the vertical axis for enhanced clarity.

Additionally, the included spreadsheet offers a range of graphical displays. These encompass visualizations of the model's alignment with the observations, tracking of parameter changes across the Markov Chain Monte Carlo (MCMC) chain, histograms, and more. This facilitates a comprehensive and user-friendly analysis of the results and parameter behavior.

Model Input Variables

Please refer to the following tables for comprehensive information regarding various model input parameters and their corresponding example values:

- Table 1a Forward Simulation Input Variables
- Table 1b Inverse Simulation Input Variables
- Table 2 Source Types
- Table 3 Summary of Source Options
- Table 4 Example Values for Selected Variables

DRAFT

Tutorials

Getting Started

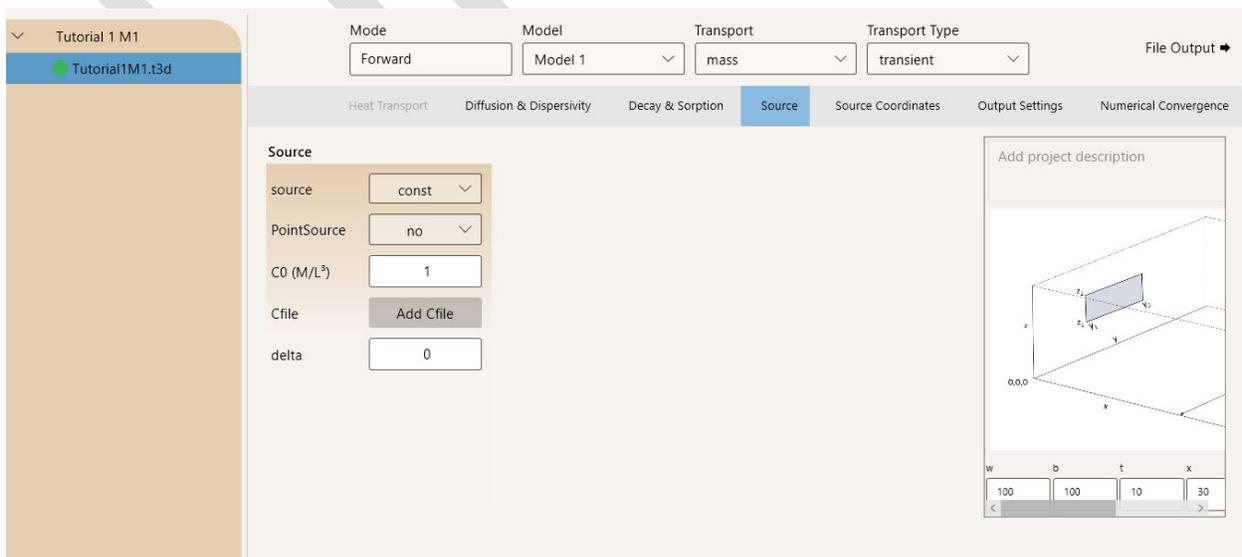
Install ASHTM following the instructions in section *Software Installation and Computer Requirements*.

Tutorial 1 – Model 1 with Constant Source:

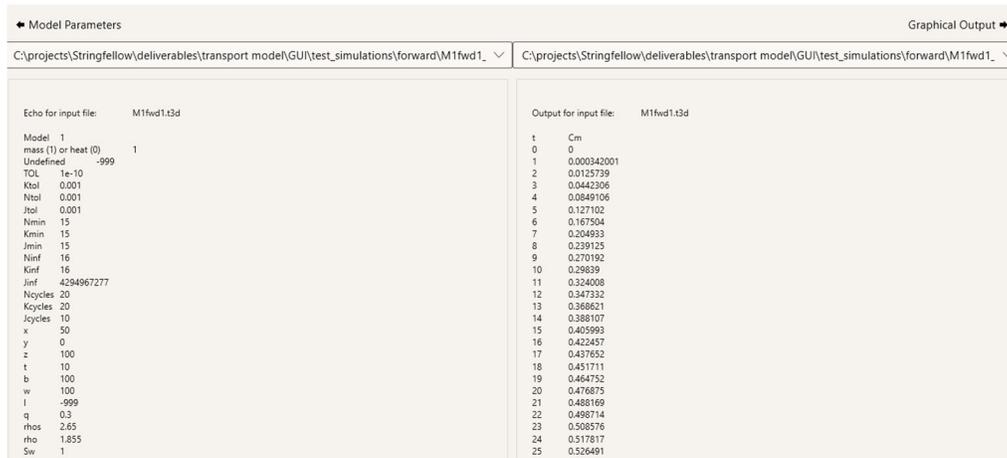
1. In the upper left menu, click Open and select the folder where tutorial input files are stored; this location depends on user's selections during installation. For the examples provided, navigate to folder "Tutorials" and click "select folder." This folder has subfolders with files for each tutorial.



2. Open the "Tutorial 1" folder, select simulation Tutorial1M1.t3d. This uses transient Model 1 (vertical patch source with specified concentration). The units are feet and days (or could be meters and days) except for sorption coefficient – sorption coefficient and soil density may be in different units from the rest of input because they cancel out. Click on Source to verify a constant source is specified. Variable delta is set to zero so the source represents the first type (Dirichlet) condition.
3. Click on Run. The hourglass next to the file name turns green, indicating the execution completed. The execution is fast.



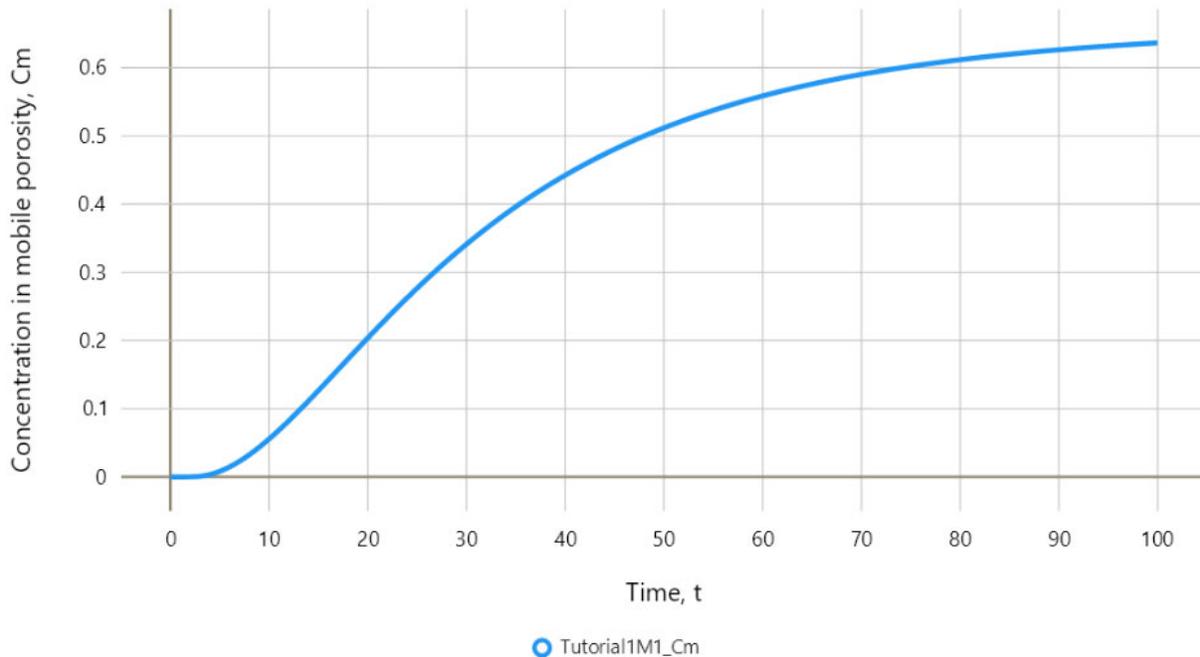
- Click File output in the upper right. Select the “echo” file and “out” file. The echo file lists the input values, the out file has the computed output.



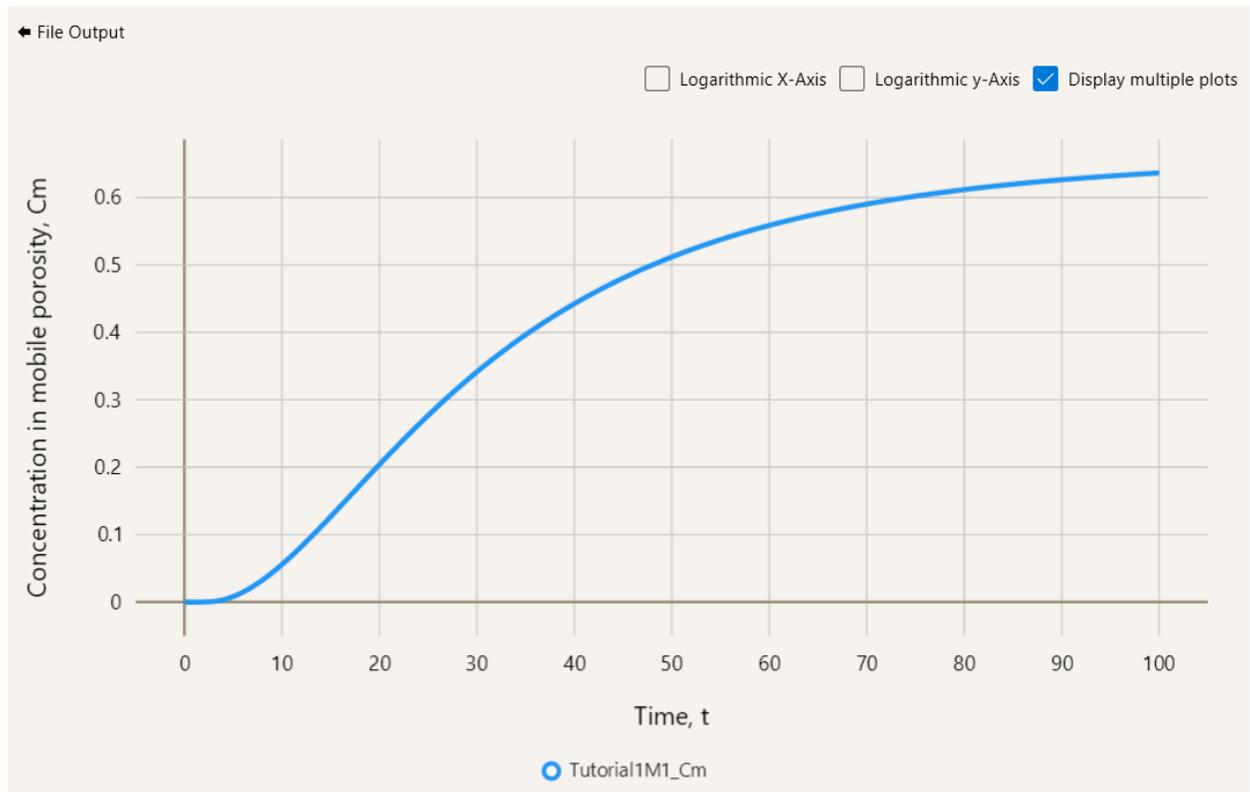
The screenshot shows two windows from a software application. The left window, titled "Model Parameters", displays a list of input parameters for a simulation. The right window, titled "Graphical Output", displays the corresponding output values for these parameters.

Echo for input file: M1fwd1.t3d		Output for input file: M1fwd1.t3d	
Model	1	t	Cm
mass (1) or heat (0)	1	0	0
Undefined	-999	1	0.000342001
TOL	1e-10	2	0.0125739
Ktol	0.001	3	0.0442306
Ntol	0.001	4	0.0849106
Jtol	0.001	5	0.127102
Nmin	15	6	0.167504
Kmin	15	7	0.204933
Jmin	15	8	0.239125
Ninf	16	9	0.270192
Kinf	16	10	0.29839
Jinf	4294967277	11	0.324008
Ncycles	20	12	0.347332
Kcycles	20	13	0.368621
Jcycles	10	14	0.388107
x	50	15	0.405993
y	0	16	0.422457
z	100	17	0.437652
t	10	18	0.451711
b	100	19	0.464752
w	100	20	0.476875
l	-999	21	0.488169
q	0.3	22	0.498714
rhos	2.65	23	0.508576
rho	1.855	24	0.517817
Sw	1	25	0.526491

- One can scroll down to view the rest of the files.
- Click Graphical Output and a graph of concentration versus time is displayed. The graphic below was produced by right-clicking the displayed graph to copy image and pasting it into this manual.



- There are options in the upper right corner to change either axis to logarithmic, or to display multiple plots, i.e., plots from multiple simulations (for the same type of output, e.g., concentration versus time). Select the box for Display Multiple Plots.

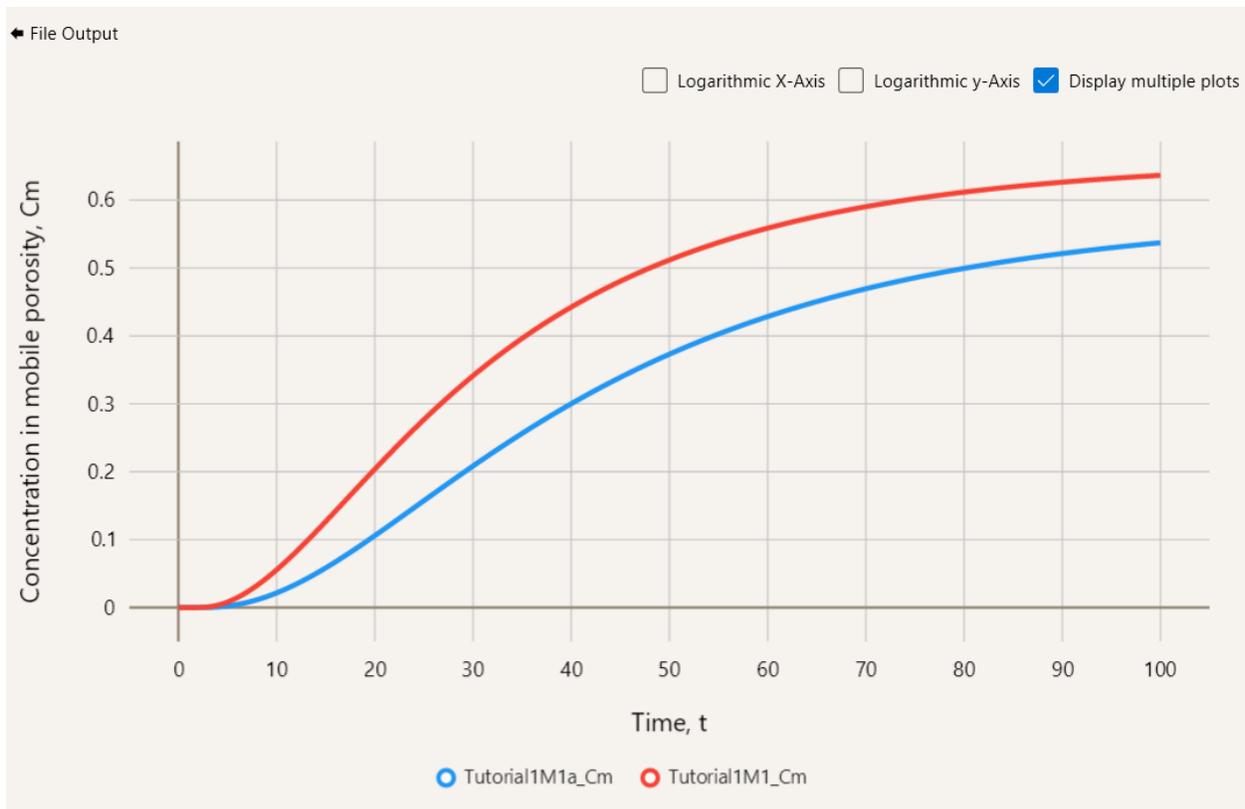


8. Click File Output in the upper left and then Model Parameters (upper left again) to navigate back to the main input menu.
9. Click Source and enter 1 in the cell for delta.

Source

source	const
PointSource	no
C0 (M/L ³)	1
Cfile	Add Cfile
delta	1

10. In the upper left, click Save As and enter a new file name M1fwd1a (the file extension t3d will be added automatically).
11. The new simulation uses type 3 (Cauchy) boundary condition for the source. All other input is the same. Click Save As at the top and save as Tutorial1M1a. Click Run, then File Output. When finished (dot turns green), click File Output and Graphical Output. Now there are two graphs. This example illustrates the difference between the two boundary conditions that may be chosen to represent the source.



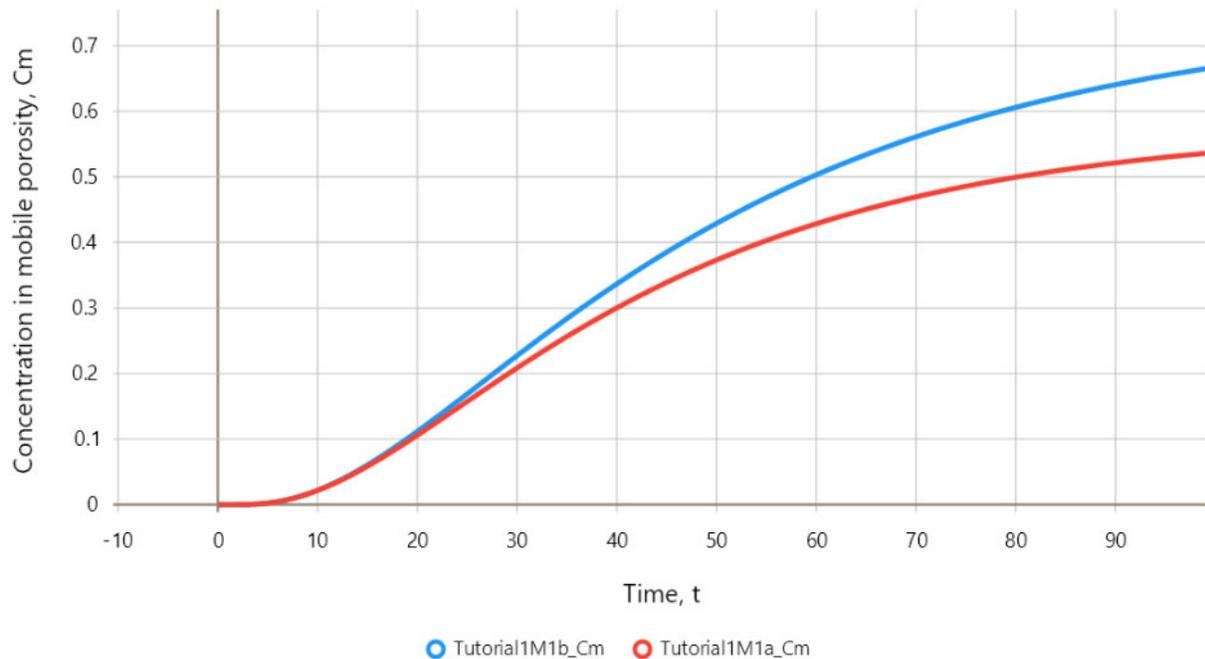
12. In the file menu on the left, select M1fwd1.t3d again. Click Decay & Sorption and enter zeros for λ_{dai} , λ_{dais} , and λ_{dams} . Leave λ_{dam} at 0.01. This will result in only the dissolved mass within the mobile domain undergoing first order decay. Sorbed mass and mass in immobile porosity will not decay.

Decay & Sorption

λ_{dai} (1/T)	<input type="text" value="0.0"/>
λ_{dais} (1/T)	<input type="text" value="0.0"/>
λ_{dam} (1/T)	<input type="text" value="0.01"/>
λ_{dams} (1/T)	<input type="text" value="0.0"/>
K_i (L ³ /M)	<input type="text" value="0.01"/>
K_m (L ³ /M)	<input type="text" value="0.01"/>
gamma	<input type="text"/>
f (-)	<input type="text" value="0.5"/>

13. Click Save As and specify filename Tutorial1M1b.

14. Click Run and navigate to Graphical Output. Limiting decay to just the dissolved mass in the mobile porosity result in higher concentrations.

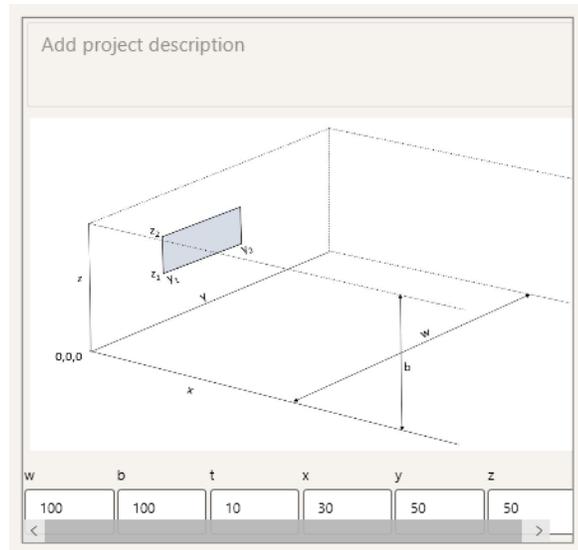


15. Navigate to Model Parameters. Click Source Coordinates. Now you see that $y_1 = 0$, $y_2 = 100$, $z_1 = 0$, and $z_2 = 100$. This means that the source extends over the entire model domain in the yz plane and consequently, the model simulates one-dimensional (1D) transport. The 1D execution is fast because the model calculations are greatly simplified. Now click Source Coordinates and change the source coordinates to $y_1 = 40$, $y_2 = 60$, $z_1 = 40$, and $z_2 = 60$. This will result in a three-dimensional (3D) transport problem.

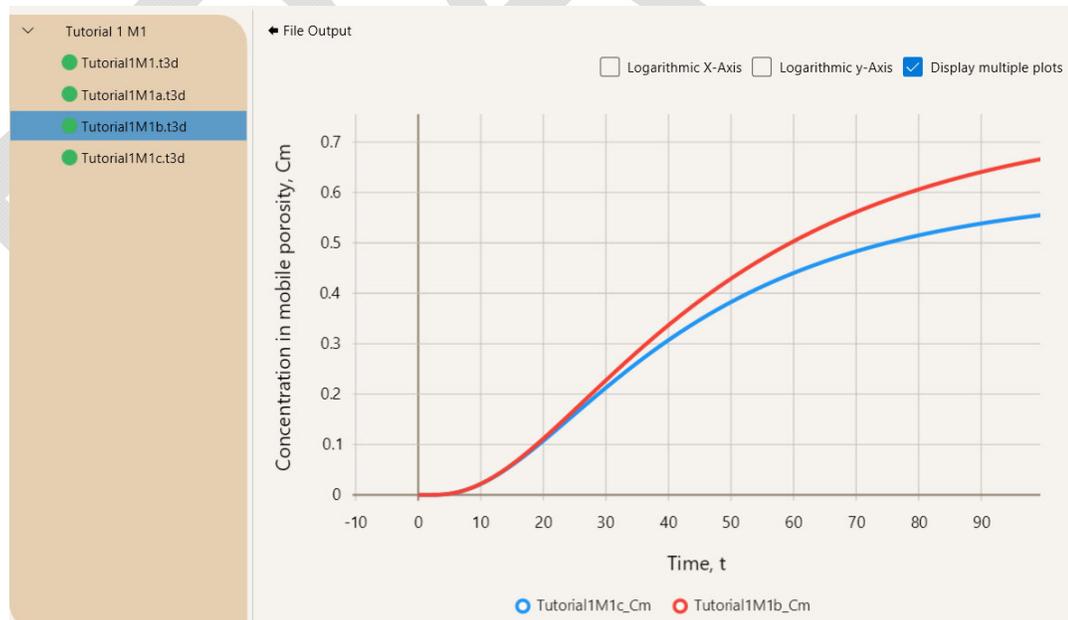
Source Coordinates	
x1 (L)	<input type="text"/>
x2 (L)	<input type="text"/>
y1 (L)	<input type="text" value="40"/>
y2 (L)	<input type="text" value="60"/>
z1 (L)	<input type="text" value="40"/>
z2 (L)	<input type="text" value="60"/>
x0 (L)	<input type="text"/>
y0 (L)	<input type="text"/>
z0 (L)	<input type="text"/>

16. Check the model geometry shown in the box on the right. The x , y and z coordinates specify the observation point for which concentration-time curve will be computed. The specified x , y and z

mean the point is in the center of the source in the yz plane at a distance of 40 m along the flow direction (x).

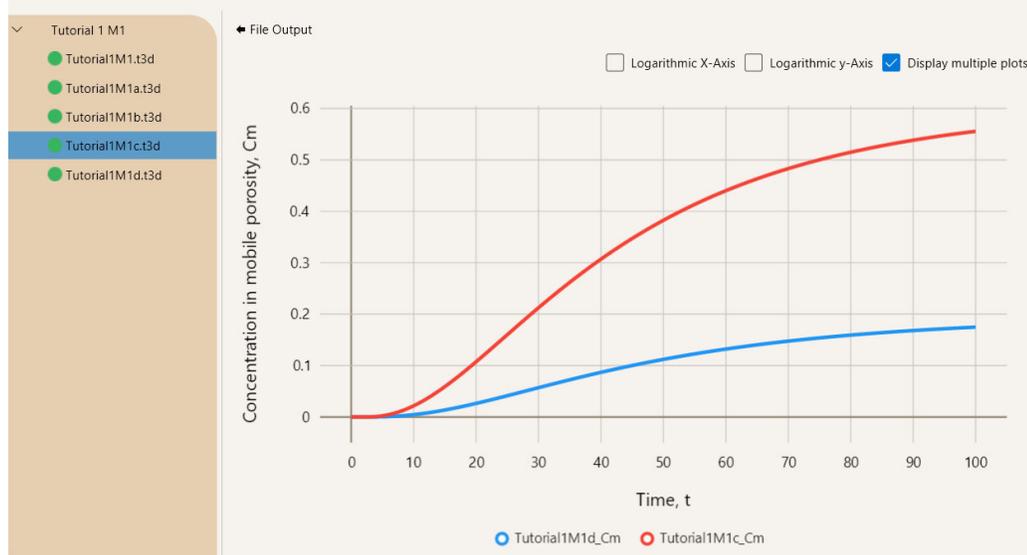


17. Click Save As and specify file name: Tutorial1M1c. Click Run. The execution is much slower than for the previous (1D) simulations.
18. Navigate to Graphical Output. Select Display Multiple Plots and click on simulation Tutorial1M1b in the list on the left. Now the results for both “b” and “c” simulations are shown. This comparison illustrates how a 1D simulation (“b”) overestimates concentrations in the aquifer.



19. If you specify the observation point coordinates such that the point is not directly along a flow path from the source, the calculated concentrations will be much lower for the new location. For example, change the point elevation to $z = 61$ in the box on the right under Model Parameters and

save the simulation as Tutorial1M1d. Click Run and when the dot turns green navigate to Graphical Output. Click Display Multiple Plots, then click Tutorial1M1c in the list on the left.

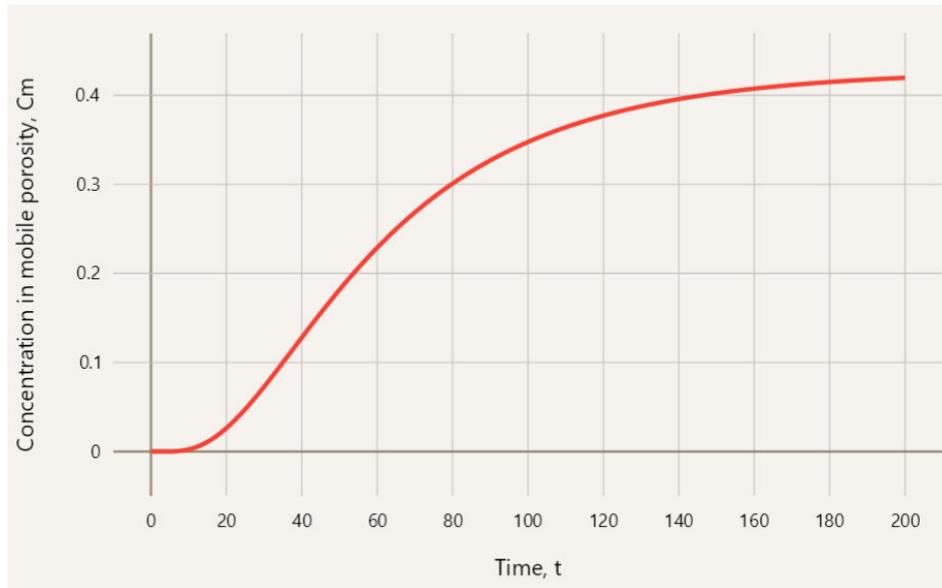


20. The concentrations are much lower for the new point (“d” simulation) because vertical transverse dispersivity is very low. Users can alternatively change the y-coordinate of the observation point to, for example, $y = 35$ and leave $z = 50$. The calculated concentration will be higher now because horizontal transverse dispersivity is 10-times higher than vertical in this example (see Diffusion & Dispersivity under Model Parameters); the concentration will still be lower than in simulation “c” where the observation point is in the direction of groundwater flow along the plume centerline.

Tutorial 2 – Model 1 with Time Dependent Source:

Model 1 source time dependency

1. In this tutorial, we are modifying the source and saving over the existing file, rather than saving a separate input file for each simulation. Users can elect to use the “Save As” option instead and save each simulation in a separate input file so that multiple graphs can be displayed or users can go back to a simulation with a different source definition.
2. Click “Open” at the top menu and navigate to the folder “Tutorial 2.” Click “Run” and then “File Output” and “Graphical Output.” A graph of concentration versus time is shown for a source defined by constant concentration in time.

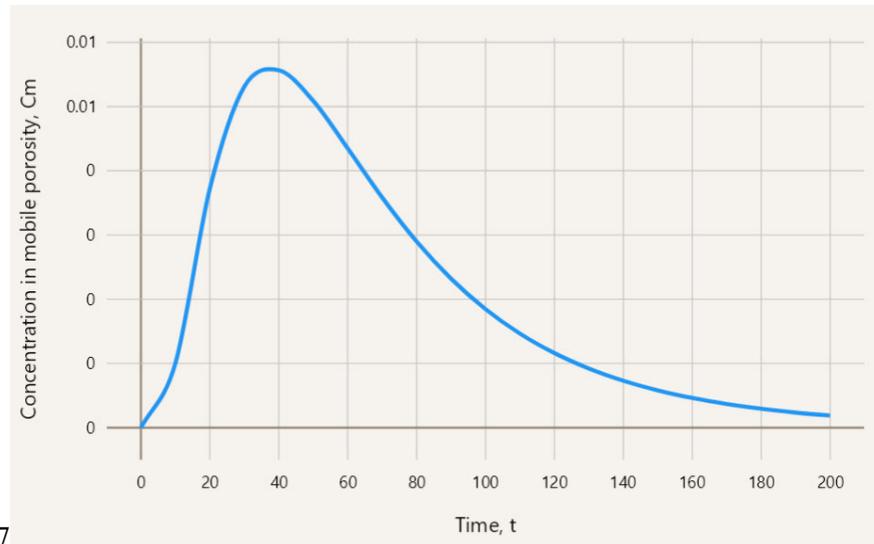


3. Navigate back to “Model Parameters.”
4. Click “Source” and select “pulse” from the pull-down menu for source. This is an instantaneous pulse source.

The dialog box titled "Source" contains the following parameters:

Parameter	Value
source	pulse
PointSource	no
C0 (M/L ³)	1
Cfile	Add Cfile
delta	0

5. Click “Save” and then “Run.” Navigate to “Graphical Output.” The graph below is displayed.

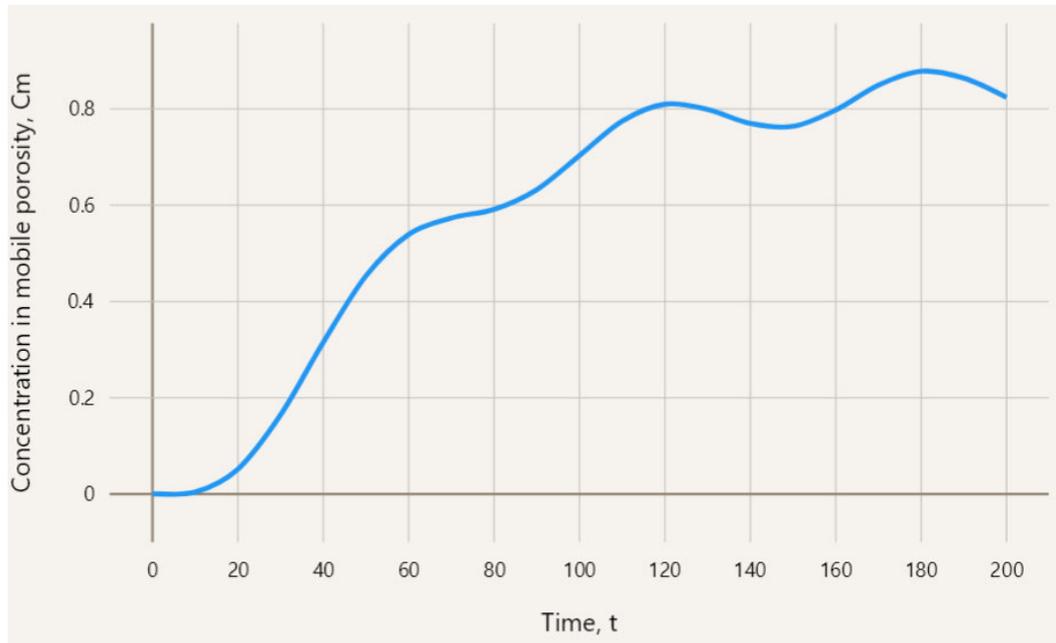


7

6. Navigate back to “Model Parameters” and click “Source.” From the pull down menu, select “sine” source, specify C0 2.0, C1 1.0, phis 0.5 and omegas 0.1.

Source	
source	sine <input type="button" value="v"/>
PointSource	no <input type="button" value="v"/>
C0 (M/L ³)	<input type="text" value="2"/>
C1 (M/L ³)	<input type="text" value="1"/>
Cfile	<input type="button" value="Add Cfile"/>
phis (rad)	<input type="text" value=".5"/>
omegas (rad/T)	<input type="text" value=".1"/>
delta	<input type="text" value="0"/>

7. Click “Save” and “Run.” Navigate to “Graphical Output.” The graph displayed is shown below.



8. Note that this is not a periodic response, because the source is activated at time zero. The computed concentration approaches a periodic response with increasing time.
9. Navigate to “Model Parameters”, select “Source”, specify “exp” source, and lambdas -0.01. This simulation has an exponentially decreasing source concentration.

Source

source

PointSource

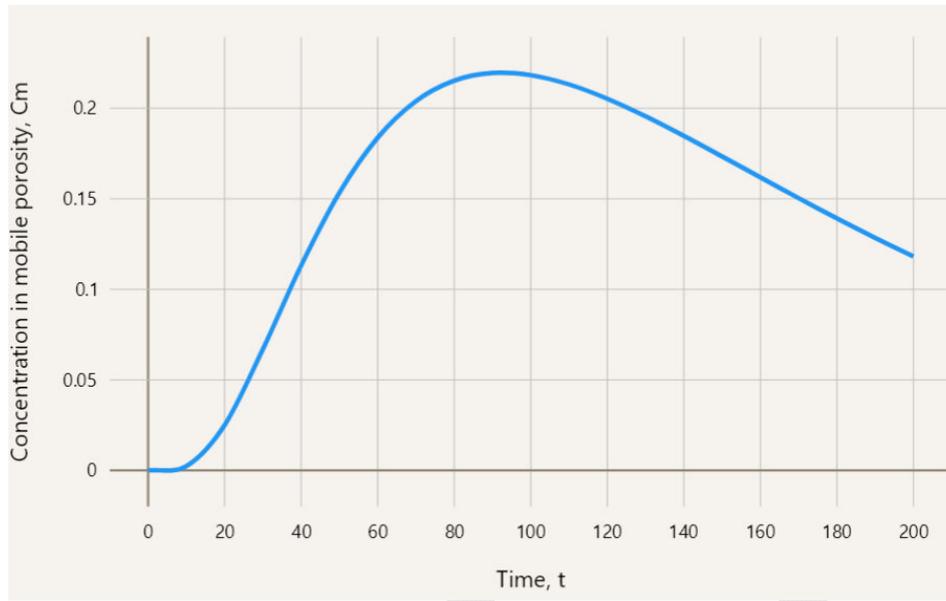
C0 (M/L³)

Cfile

lambdas (1/T)

delta

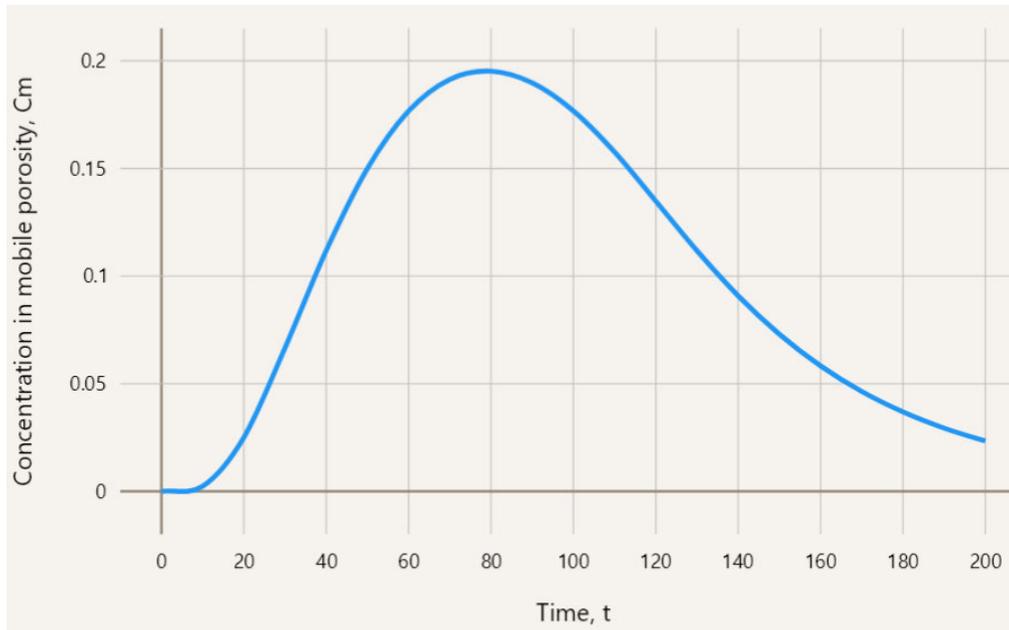
10. Click “Save” and “Run”, then navigate to Graphical Output.” The displayed graph is:



11. Navigate to “Model Parameters”, click “Source” and select “line” source.

Source	
source	line
PointSource	no
C0 (M/L ³)	1
C1 (M/L ³)	-0.01
Cfile	Add Cfile
delta	0

12. This is a linearly decreasing source concentration (at late time, it will be automatically truncated at zero to avoid negative source concentration). Click “Save” and “Run”, then navigate to “Graphical Output.” The graph is



13. Navigate back to “Model Parameters”, click “Source” and select “linear” source.

Source

source

PointSource

C0 (M/L³)

Cfile

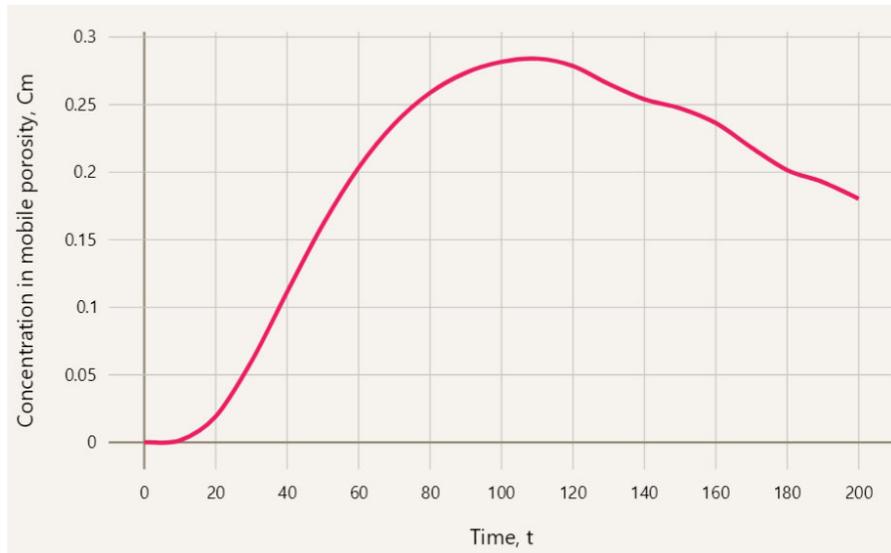
delta

14. The value for C0 will be ignored.

15. In Windows Explorer, open the file “source.txt” located in folder “Tutorial 2” using Notepad or other text editing software. Select all file content and copy to clipboard. This file contains time-concentration data pairs, such as groundwater sample results from a source area monitoring well. The “linear” source means the data points will be linearly interpolated over time to define the source concentration.

16. Click “Add Cfile” in the “Source” menu. An open box appears. Place cursor inside and paste the clipboard content.

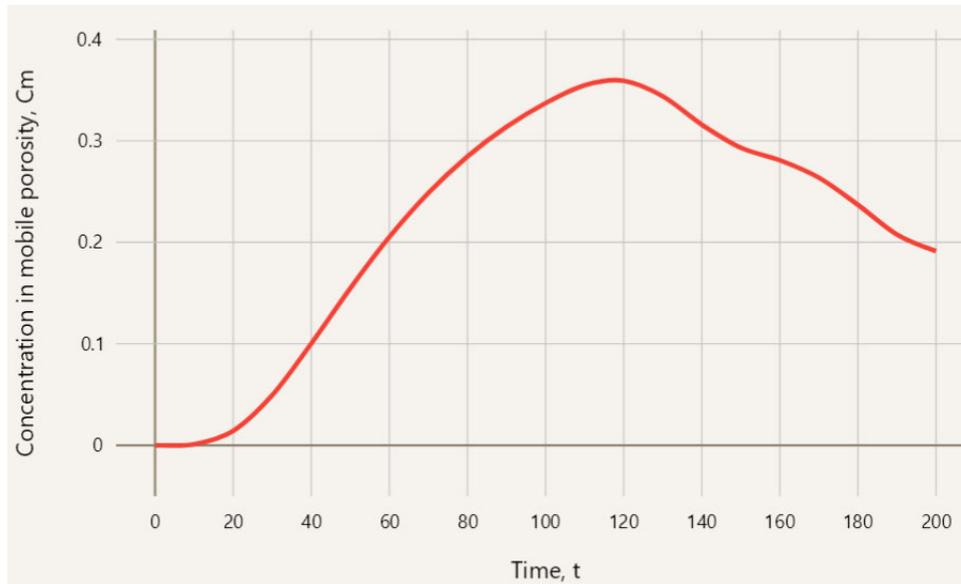
17. Click “Save” and “Run”, navigate to “Graphical Output.” The graph shown is:



18. Navigate back to “Model Parameters, click “Source”, and select “step” source.

Source	
source	step
PointSource	no
C0 (M/L ³)	1
Cfile	Add Cfile
delta	0

19. The step source means the data pairs will be treated as constant steps in time to define the source concentration. Click “Save” and “Run”, the navigate to “Graphical Output.” The graph displayed is:

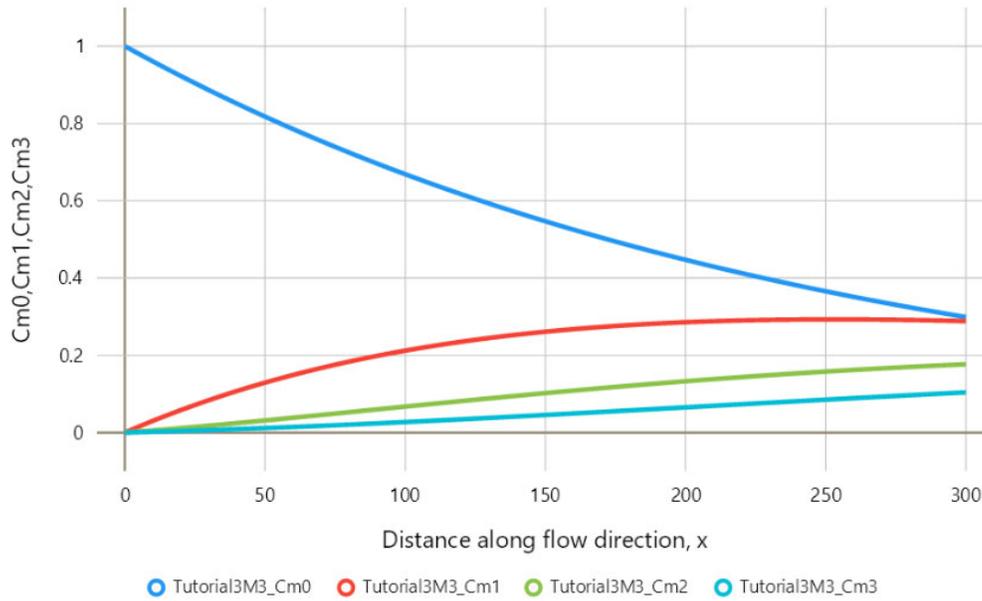


20. Note that the two different representations of the source concentrations given by the same set of time-concentration points result in quite different computed concentrations in the aquifer. The difference would increase for an observation point located closer to the source.

Tutorial 3 – Model 3 with Chain Decay:

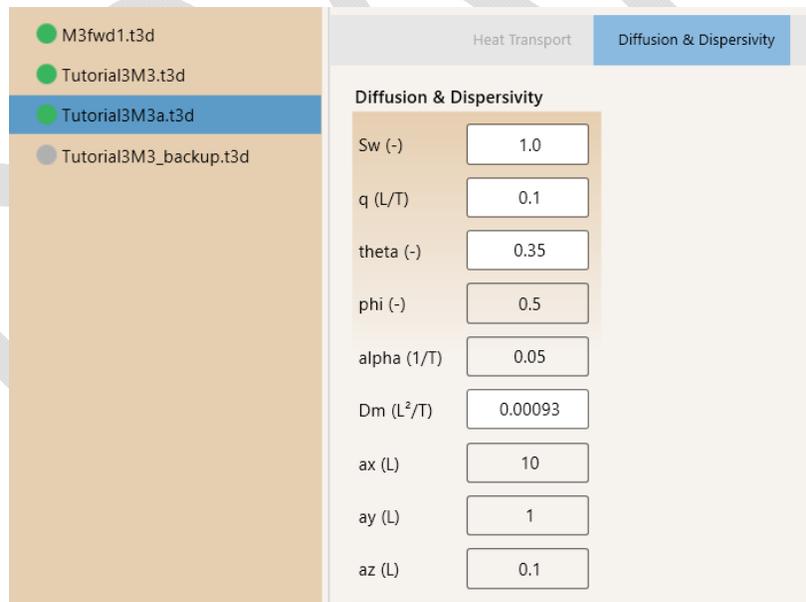
This tutorial is for the solute transport of chain decaying species.

Navigate to folder Tutorial 3 and open project “Tutorial3M3.” The parent species is given a constant source concentration of 1.0 and the daughter species have zero source concentration. The source extends over the entire width and thickness of the aquifer; this makes the transport problem one-dimensional along the x-axis and the execution is faster than for a 3D problem. Also, the transport is steady state. Click “Run” and navigate to Graphical Output to see the plot:

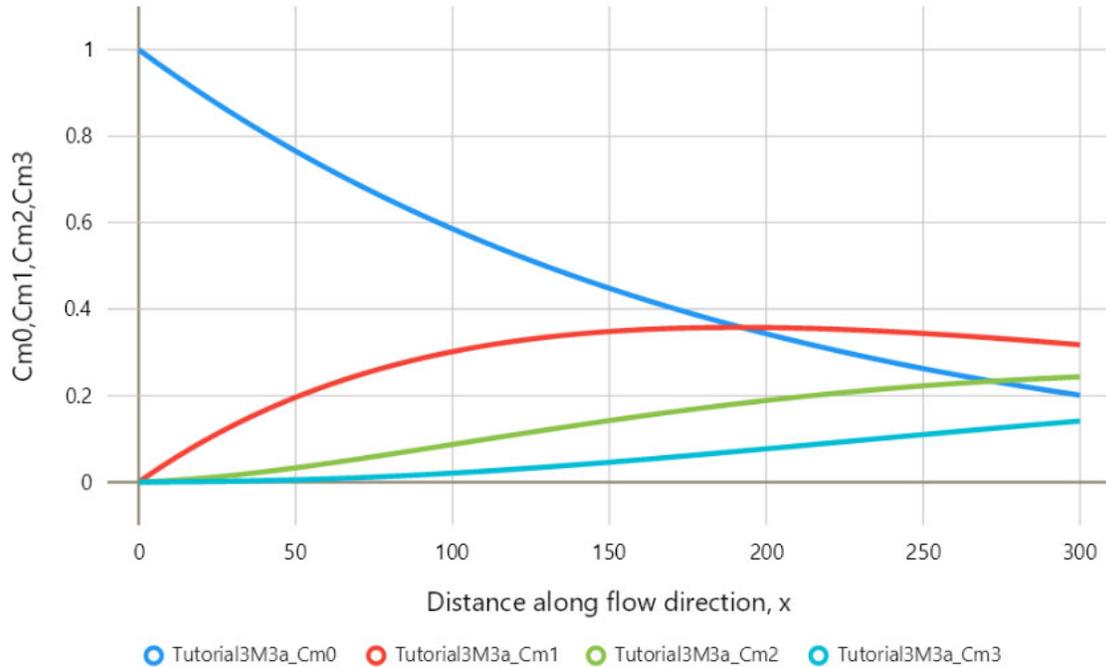


The species are numbered from 0 (parent) to the last daughter species; there are three daughter species in this problem.

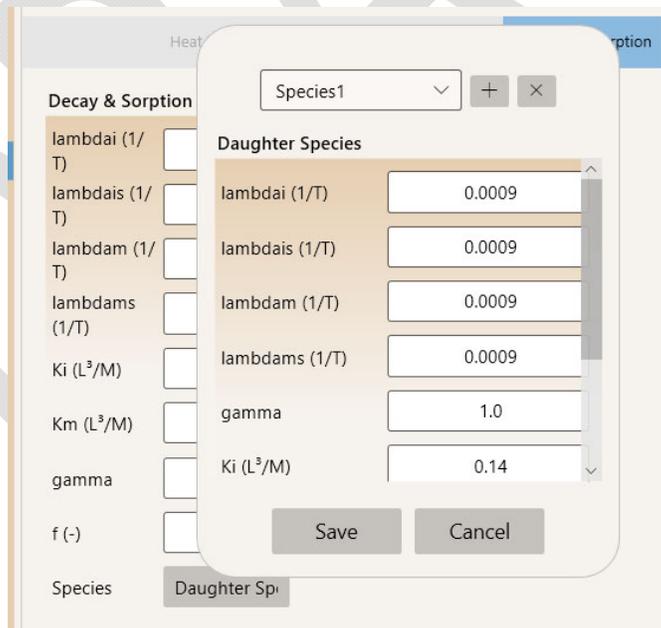
1. Navigate back to Model Parameters, click Save As and specify name “Tutorial3M3a.”
2. Click Diffusion & Dispersivity and change alpha, ax, ay, and az to 0.05, 10, 1, and 0.1, respectively:



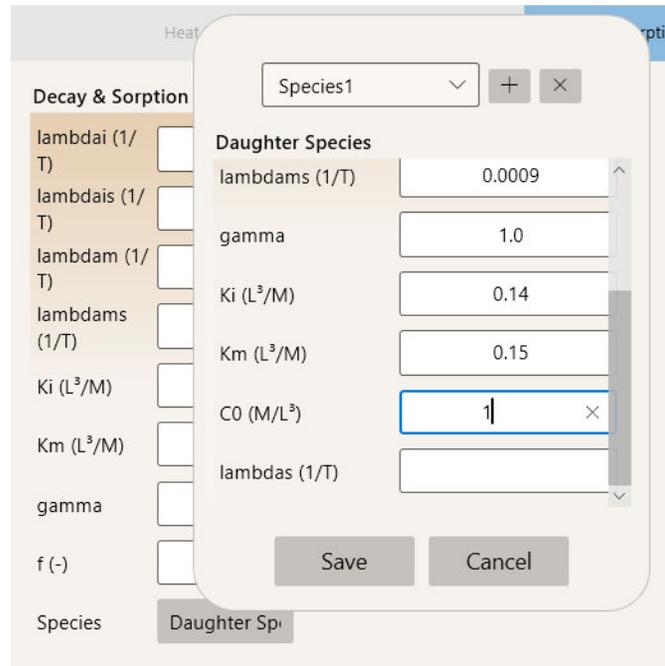
3. Click “Save” and “Run”, then navigate to Graphical Output:



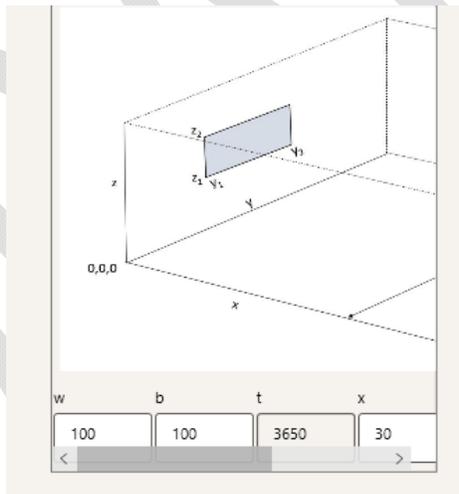
4. Navigate back to Model Parameters, click Save As and specify name "Tutorial3M3b."
5. From the pull-down menu for Transport Type at the top, select "transient."
6. Click Decay & Sorption, then Daughter Sp., and in the top pull-down menu select "Species 1."



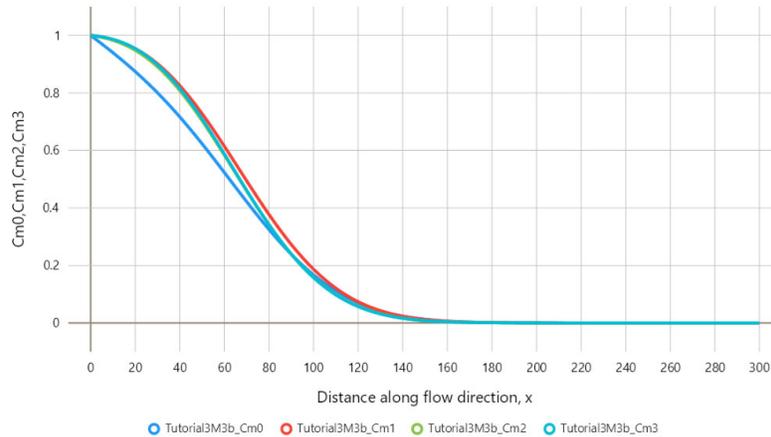
7. Drag the vertical scroll bar down to reveal C0 and enter 1 (it was 0):



8. Click "Save" and repeat this for Species 2 and 3.
9. In the model geometry box, change t to 3650 (10 years in days):



10. Click "Save" and "Run", navigate to Graphical Output to see concentration profile after 10 years for constant source concentrations for all species:



11. Navigate back to Model Parameters, click “Save As” and specify name “Tutorial3M3c.”
12. Click “Source” and select “exp” from the “source” pull-down menu. Change “lambdas (1/T)” to -0.001. The first order coefficient for an exponential source term may be positive or negative to allow for increasing or decreasing source.

Source

source

PointSource

C0 (M/L³)

Cfile

lambdas (1/T)

delta

13. Click Decay & Sorption, then Daughter Sp. And selected Species 1 from the pull-down menu on top. Change “lambdas (1/T)” to the negative of the value of lambdams.

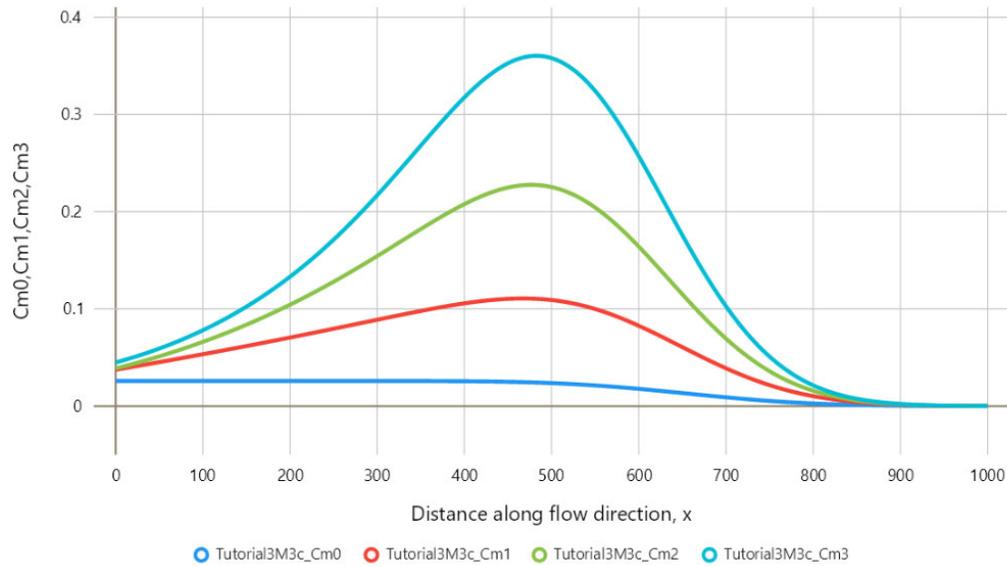
Decay & Sorption	
lambdai (1/T)	0.001
lambdais (1/T)	0.001
lambdam (1/T)	0.001
lambdams (1/T)	0.001
Ki (L ³ /M)	0.12
Km (L ³ /M)	0.13
gamma	1.0
f (-)	0.5
Species	Daughter Spe

Daughter Species	
lambda_dams (1/T)	0.0009
gamma	1.0
Ki (L ³ /M)	0.14
Km (L ³ /M)	0.15
CO (M/L ³)	1
lambda_das (1/T)	-0.0009

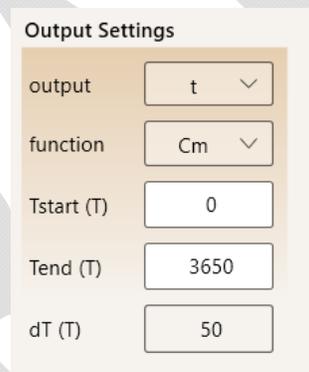
14. Do the same for Species 2 and Species 3. Note that all decay coefficients for dissolved and sorbed mass in the mobile and immobile porosity are the same and also the source decay constant is the same; this would represent a transport problem for radionuclides. For chain decay of chlorinated compounds, the decay coefficients would differ.
15. In Output Settings, change Xend to 1000:

Output Settings	
output	x
function	Cm
Xstart (L)	0
Xend (L)	1000
dX (L)	5

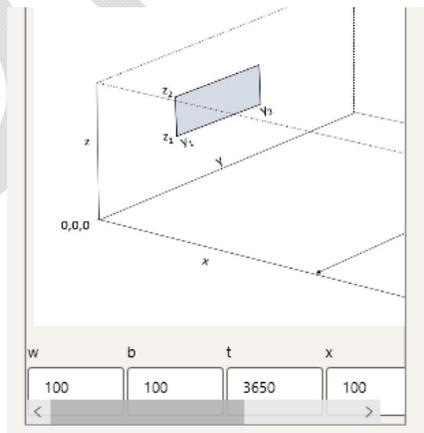
16. Click “Save” and Run” and navigate to Graphical Output:



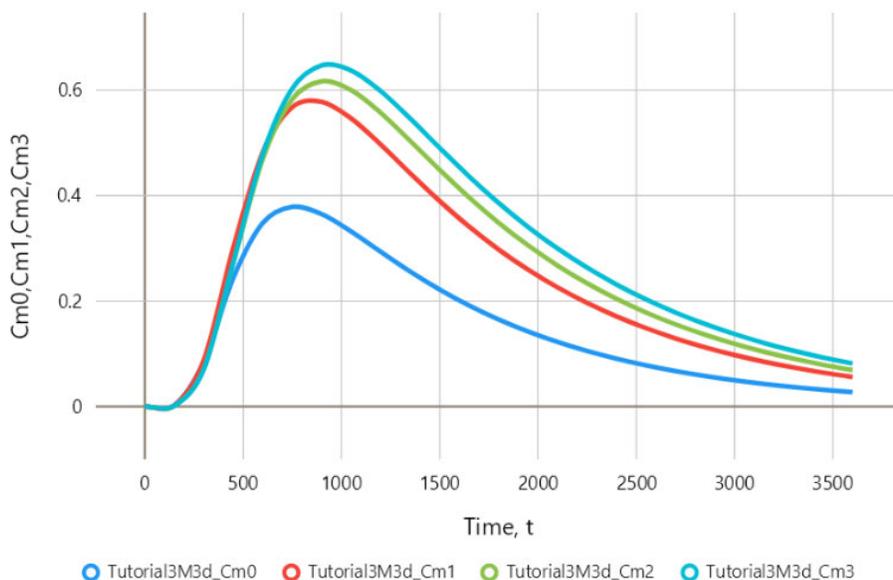
17. Navigate to Model Parameters, click Save As and specify name “Tutorial3M3d.”
18. In Output Settings, change the output to concentration versus time as follows:



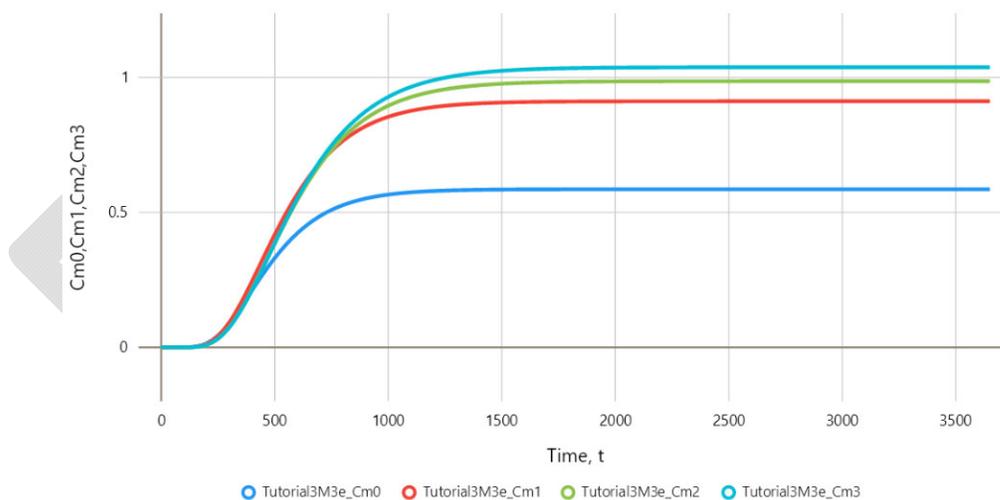
19. In the model geometry box, change x to 100:



20. Now the output will be concentration vs. time at a distance of 100 from the source. Click “Save” and “Run”, navigate to Graphical Output:



21. Navigate to Model Parameters, click Save As and specify name “Tutorial3M3e.”
22. Click Source and select “const” from the pull-down menu.
23. Click “Save” and “Run”, navigate to Graphical Output. As might be expected, constant source concentrations result in quite different time-concentration curves:

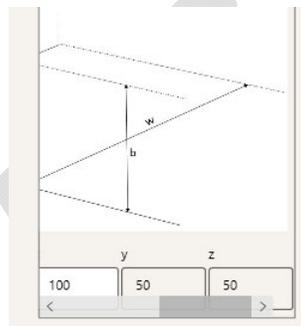


24. Users can change the source type to any choice from the pull-down menu for the parent species (see Tutorial 2). Daughter species may have a non-zero source only if the source type selected is const, pulse, or exp; when any other source type is selected for the parent species, daughter species have no source.
25. Note that at least one of the decay and sorption coefficients must differ (at least slightly) for any two species.
26. Now try changing the source dimensions. Navigate back to Model Parameters, select “Tutorial3M3e” and save as “Tutorial3M3f.”

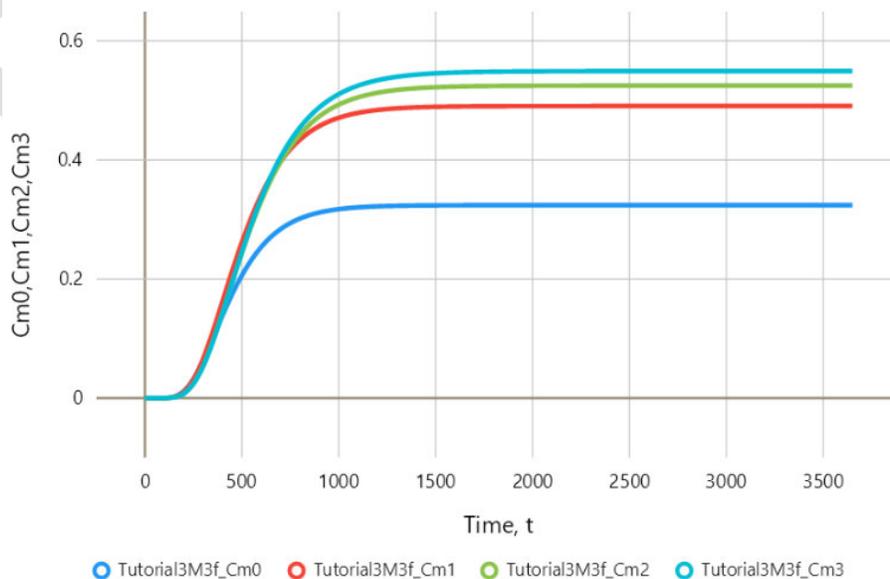
27. Click Source Coordinates and change y_1 , y_2 , z_1 , z_2 as follows:

Source Coordinates	
x1 (L)	-10
x2 (L)	0
y1 (L)	40
y2 (L)	60
z1 (L)	40
z2 (L)	60

28. In the model geometry box, change both y and z to 50:



29. Click “Save” and “Run.” Now it takes considerably longer to execute the model (the smaller the source dimensions relative to aquifer width and thickness, the longer the execution time). Navigate to Graphical Output to see that computed concentrations are lower (compared to Tutorial3M3e results) for a smaller source rectangle:

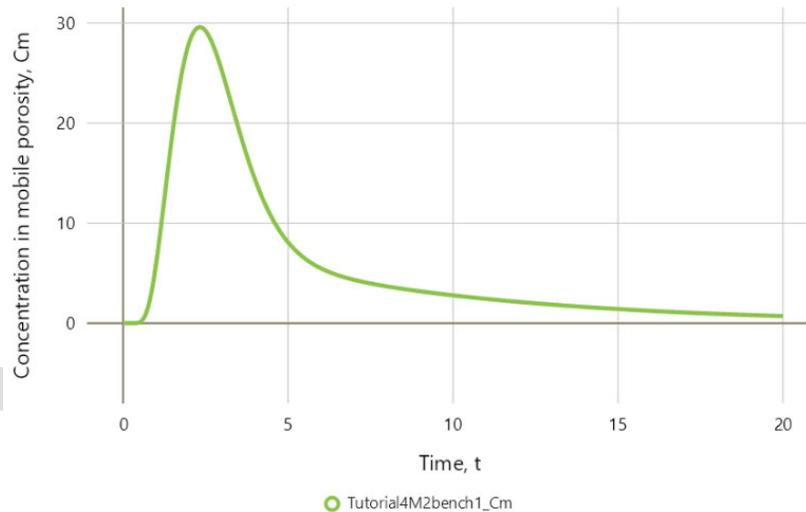


Tutorial 4 – Model 2

Model 2 is for volumetric mass (or heat) generation term or can be used for initial concentration distribution. The source term may be given the same time dependency as the source term for Model 1 (see Tutorial 2). The mass generation is in units of mass per unit volume of the aquifer per unit time. The source has the shape of a rectangular prism and the mass generation is uniform within this volume.

The first tutorial uses a benchmark simulation that was used to test the model against MT3D. The units used are feet and days.

1. Click “Open” and navigate to folder “Tutorial 4 M2.” Select simulation “Tutorial4M2bench1.” Click “Run” and navigate to Graphical Output. The graph displays concentration versus time for a point in the aquifer downgradient of an initial distribution of concentrations.



2. Navigate back to Model Parameters and click “Source.”

Source	
source	<input type="text" value="pulse"/>
PointSource	<input type="text" value="no"/>
injection	<input type="text" value="no"/>
C0 (M/L ³)	<input type="text" value="26.1125"/>
Cfile	<input type="button" value="Add Cfile"/>

- The source is an instantaneous pulse of mass distributed over the source volume (defined in input block "Source Coordinates") and represents mass per unit volume of the aquifer with a value of 26.1125.
- Click "Save As" and specify name "Tutorial4M2bench2."
- Click "Source" and select "none" from the "source" pull-down menu. The input field for C_0 disappears and is replaced by input for C_{m0} and C_{i0} , initial concentrations in mobile and immobile porosity, respectively. Enter 100 for C_{m0} and 0 for C_{i0} .

Source

source

PointSource

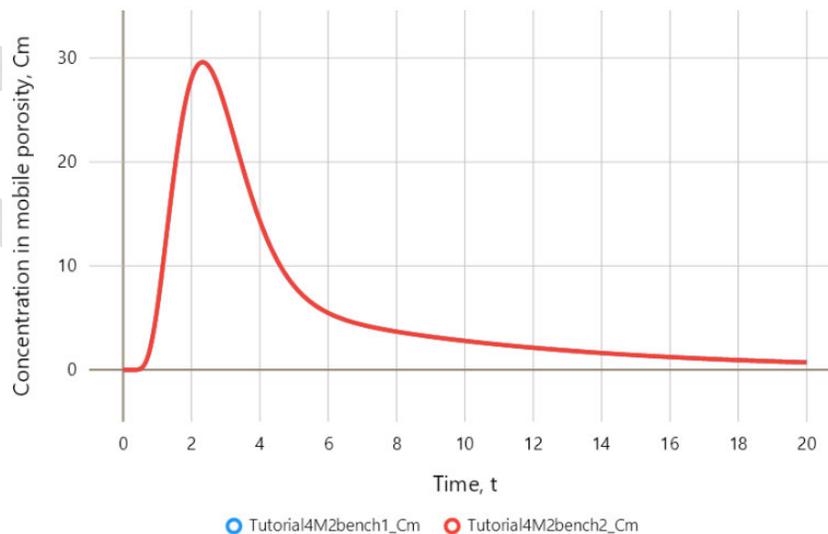
injection

C_{m0} (M/L³)

C_{i0} (M/L³)

Cfile

- Click "Save" and "Run" and navigate to Graphical Output. Check "Display multiple plots" and click "Tutorial4M2bench1" in the list of simulations on the left. The two graphs are identical as shown below. This is because the initial concentration C_{m0} of 100 within the mobile porosity corresponds to the released mass C_0 of 26.1125 per unit aquifer volume.



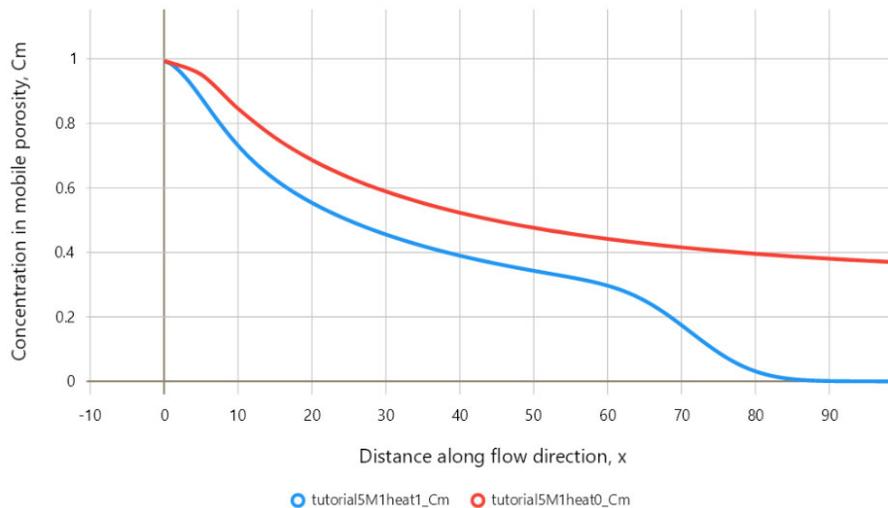
Tutorial 5 – Heat Transport

This tutorial illustrates simulating heat transport using several models. All input is in SI units (m, s, K, W, J, kg). Note that transient execution of Model 1 and Model 2 takes some time, while steady state execution of the two models and transient execution of Model 4 (or 4.1, 4.2) is much faster.

Model 1

This tutorial is a theoretical example of heat transport with a source defined by a specified temperature boundary condition.

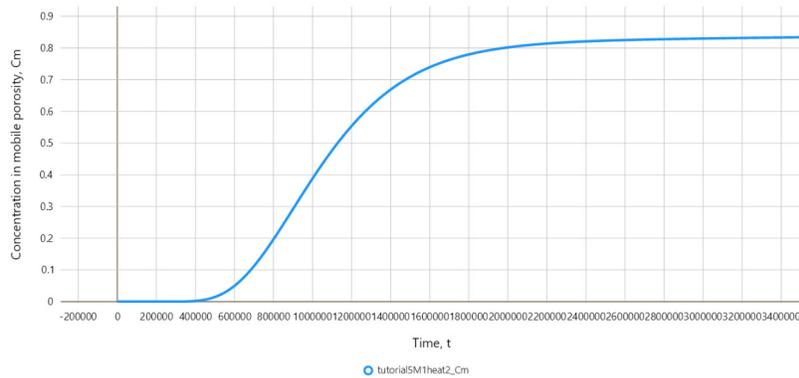
1. Navigate to folder Tutorial 5 and open project “tutoria5M1heat0.” Click Run, File Output, and Click Graphical Output to navigate to the graph. The calculated result is temperature increase over a transect along the flow direction through the center of the specified temperature zone. The boundary condition is set at 1.
2. Navigate back to the main input menu. Click “Save As” and specify filename “tutorial5M1heat1.”
3. From the pull-down menu for “transport Type” select “transient.”
4. At the bottom of the diagram of the model geometry, change t to 1.5768e+7 (half a year in seconds).
5. Click “Save” and “Run.” Navigate to Graphical Output, click Select multiple plots” and click on “tutoria5M1heat0” in the simulation list on the left. The steady and transient temperature profiles are shown.



6. Click “Save As” and specify name “tutorial5M1heat2.”
7. Below the diagram of model geometry, change “x” from 0 to 5.
8. Click Output Settings and change the output to “t”, then specify Tstart, Tend, and dT to 0, 3600000, and 36000 as shown below:

Output Settings	
output	t
function	Cm
Tstart (T)	0
Tend (T)	3600000
dT (T)	36000

- Click “Save” and “Run”, then navigate to Graphical Output to show a graph of temperature versus time.

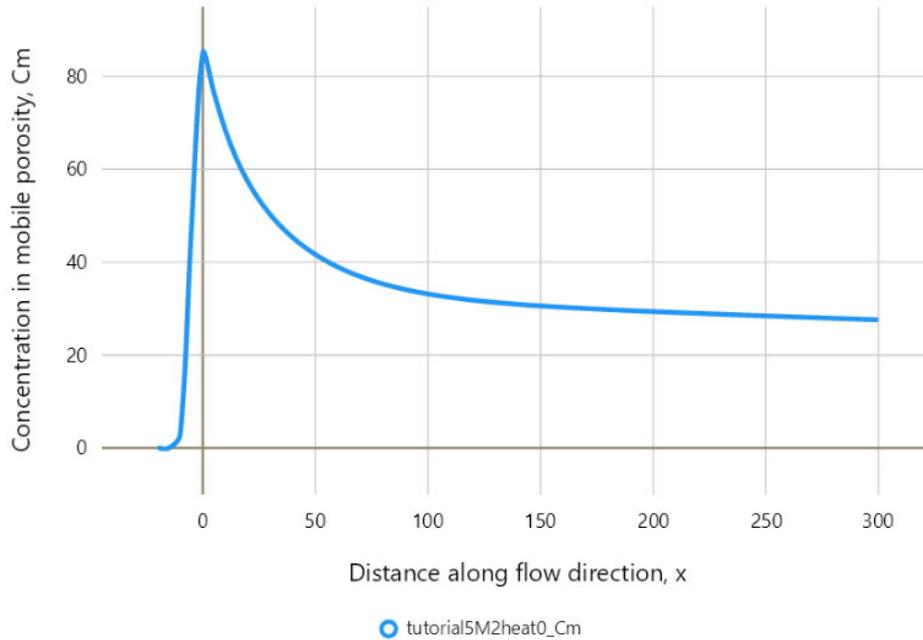


- Any time dependence of the source term can be selected from the pull-down menu “source” as shown in Tutorial 2.

Model 2

This example is a model for simplified heat transport through a thermal treatment zone with constant heat source at a New York site. The length of the treatment zone along groundwater flow direction is 10 m (x_2-x_1), its width is 40 m (y_2-y_1), and thickness (z_2-z_1) is 6 m. The energy input (as heat) within the treatment zone volume is 131.6 W/m^3 (uniformly distributed). The treatment zone is in the middle of the aquifer vertically. This is a steady state simulation. For a transient simulation, any time dependence of the source term can be selected from the pull-down menu “source” as shown in Tutorial 2.

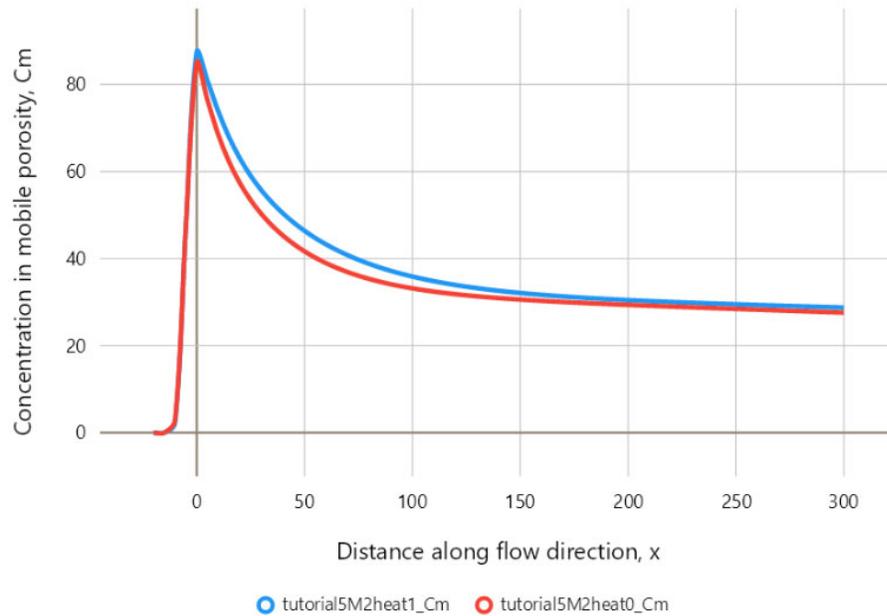
- Navigate to folder Tutorial 5 and open project “tutoria5M2heat0.” Click Run, File Output, and Click Graphical Output to navigate to the graph. The calculated result is temperature increase over a transect along the flow direction through the center of the zone. The temperature increase profile is computed from $x = -20 \text{ m}$ to $x = 300 \text{ m}$. The temperature increase is linear through the treatment zone (from $x = -10$ to $x = 0$), then the temperature decreases with distance due to dispersion and heat conduction perpendicular to groundwater flow.



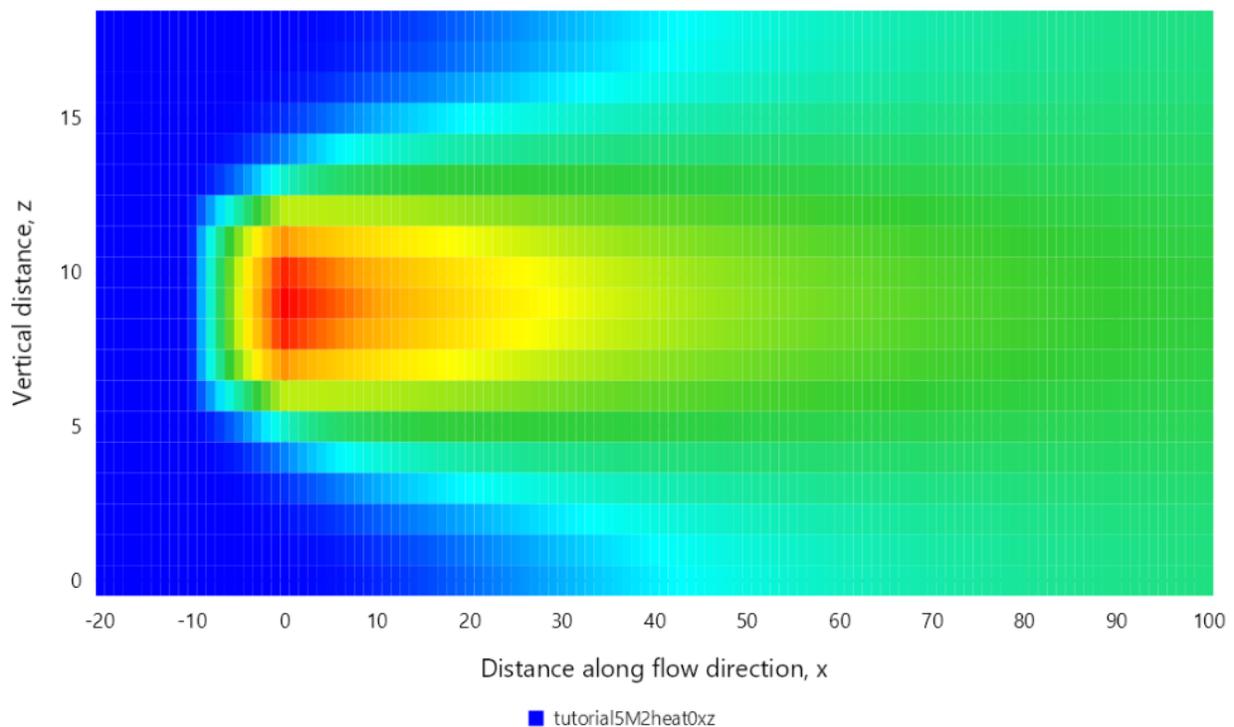
2. Click File Output in the upper left and then Model Parameters (upper left again) to navigate back to the main input menu.
3. Click “Diffusion & Dispersivity” and change the total porosity theta from 0.35 to 0.45.



4. Click “Save As” and save the file as “tutorial5M2heat1”, click Run, then navigate to Graphical Output. Click “Display multiple plots” and select “tutorial5M2heat0” in the simulation list. Now both graphs appear and one can see the effect of increased porosity on the calculated temperature.



5. Select file “tutorial5M2heat0xz”, click “Run”, and when it finishes, navigate to Graphical Output. The result is temperature increase over a vertical cross-section of the aquifer through the center of the heated zone. The source extends from $x_1 = -10$ to $x_2 = 0$ along the x-axis.



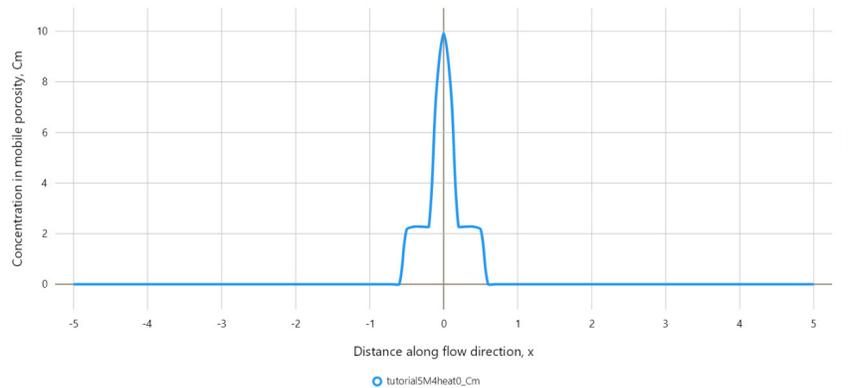
6. Try increasing the dispersivity – navigate to Parameter Input, select Diffusion & Dispersivity, and change a_x to 1, a_y to 0.1, and a_z to 0.01. Click Save and Run, navigate to Graphical Output. The plot

is only slightly different because dispersivity has smaller effect on heat transport than on solute transport.

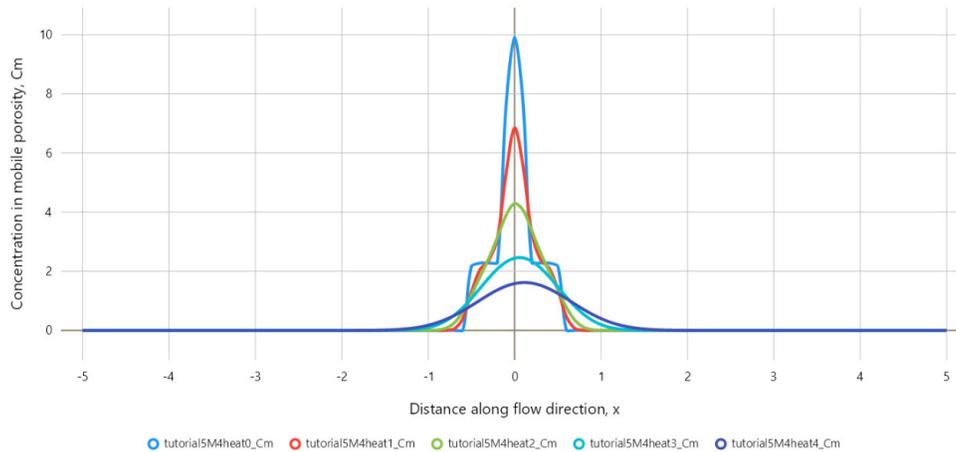
Model 4.1

This tutorial is a model of instantaneous injection of 378 l (100 gal) of water into a well. The injected water is at a temperature 10 °C warmer than the aquifer. The actual injected zone has cylindrical shape and is represented by a rectangular prism in the model.

1. In the simulation list, select “tutorial5M4heat0.” Click “Run” and navigate to Graphical Output. The displayed graph is a temperature profile along the direction of groundwater flow at an elevation of the mid-point of the screen interval (between z_1 and z_2) after 60 seconds following injection. The wellbore is represented by a superposition of an additional small prism. The horizontal resolution of the graph can be increased by specifying a smaller value of dx in output settings.

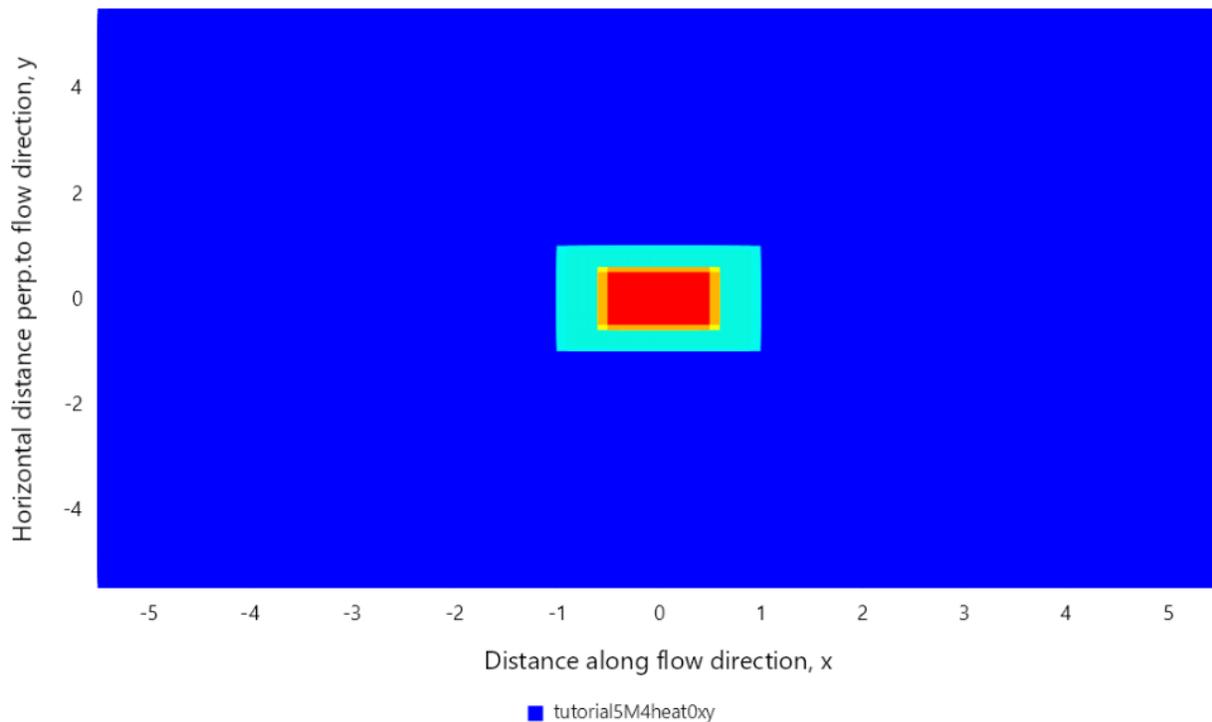


2. Now navigate to the Parameter Input, click “Save As” and specify name “tutorial5M4heat1”. Change the value of “t” below the model geometry diagram to 3600. Click “Save” and “Run.”
3. Repeat step 2 three more times and save and run input files for t of 10800, 43200, and 86400 (time in seconds corresponding to 3 hours, half a day, and one day).
4. Navigate to Graphical Output, click “Display multiple plots” and click on all 5 simulations with Model 4.1. The graph shown below appears. The peak temperature decreases with time and also moves with groundwater flow in the positive x-direction.

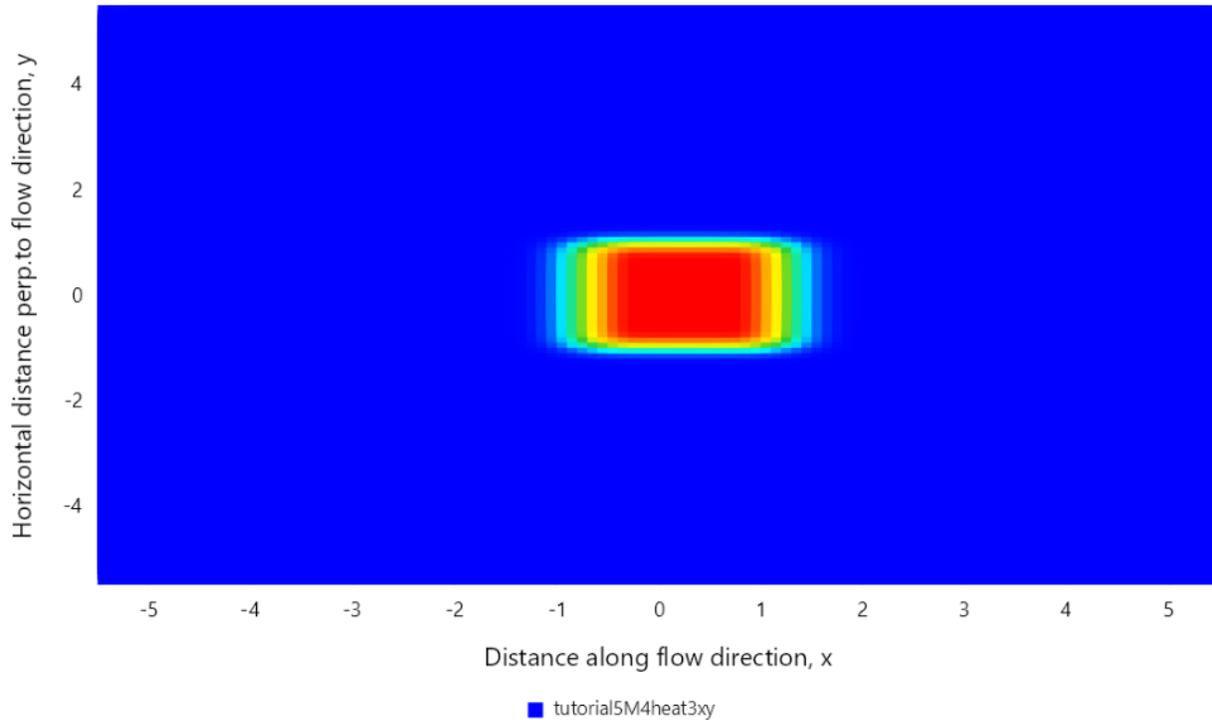


Model 4.1, 4.2

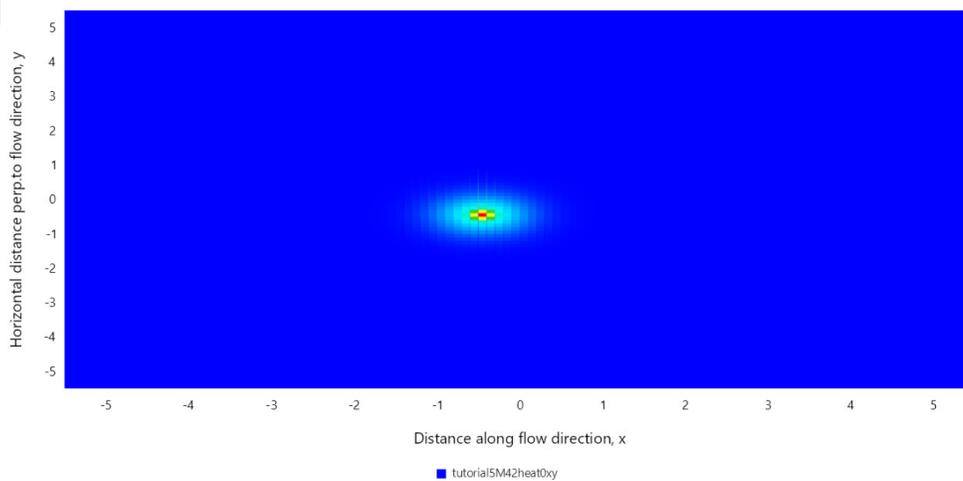
1. In the simulation list, select “tutorial5M4heat0.” Click “Save As” and specify name “tutorial5M4heat0xy.”
2. Click “Output Settings”, select “xy” and set Ystart, Yend, and dY to 5, 5, and 0.1 (same as for Xstart, Xend, and dX). Click “Save” and “Run”, then navigate to Graphical Output. The displayed temperature distribution is still rectangular after 60 seconds. Note that the heat plume is a square in plane view; the shape is distorted by different x and y scale on the image displayed.



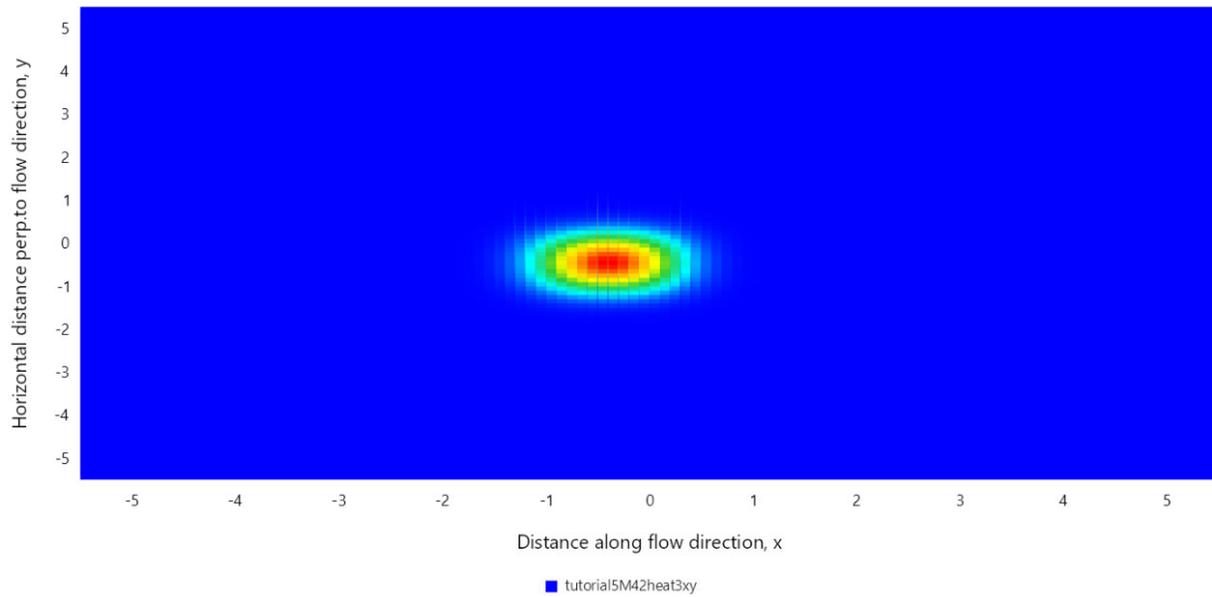
3. Navigate to main input, click “Save As” and specify name “tutorial5M4heat3xy”, change t to 43200, click “Save” and “Run”, navigate to Graphical Output to see that the heat plume has spread out after half a day.



4. Select simulation “tutorial5M4heat0xy” in the list, click “Save As” and specify name “tutorial5M42heat0xy”.
5. Select “Model 4.2” from the “Model” pull-down menu. Click “Save” and “Run”, navigate to Graphical Output. The initial temperature distribution is a Gaussian in the xy plane (with constant temperature between z_1 and z_2). The different x and y scales cause a display distortion.
6. [need to replace figures]



7. Navigate to main input, click “Save As” and specify name “tutorial5M42heat3xy”. Set t to 43200 below the model geometry diagram. Click “save” and “Run”, navigate to Graphical Output.



Tutorial 6 – Inverse Modeling of Concentration History:

Inverse analysis with synthetic example using Model 1

[explain how to deactivate/activate Parameter]

This modeling exercise illustrates how to set up an inverse simulation. Furthermore, this example uses synthetic “observations” generated using known model variables and then attempts to estimate some of them as unknown parameters; this type of exercise is useful for planning tracer tests or inverse analysis of historical water quality data.

A forward simulation was used to generate observations with white noise added in Excel. The forward simulation is saved as “Tutorial2M1forward.” All input is in units of feet and days. The source is defined using the following series of time, concentration data pairs:

0	0.5
10	1
100	0.6
110	0.25
130	0.7

150 0.1
180 0.65

All decay coefficients are set to 0.001, both sorption coefficients to 0.01, and fraction of mobile sorption sites to 0.5. The source coordinates are set to span the entire width and thickness of the aquifer so that the model is executed as 1D (at significantly shorter time than a 3D simulation).

Source	Decay & Sorption	Source Coordinates
source: linear	lambdai (1/T): 0.001	x1 (L):
PointSource: no	lambdais (1/T): .001	x2 (L):
C0 (M/L ³): 1	lambdam (1/T): 0.001	y1 (L): 0
Cfile: Add Cfile	lambdams (1/T): 0.001	y2 (L): 100
delta: 0	Ki (L ³ /M): 0.01	z1 (L): 0
	Km (L ³ /M): 0.01	z2 (L): 100
	f (-): 0.5	x0 (L):

The remaining input is:

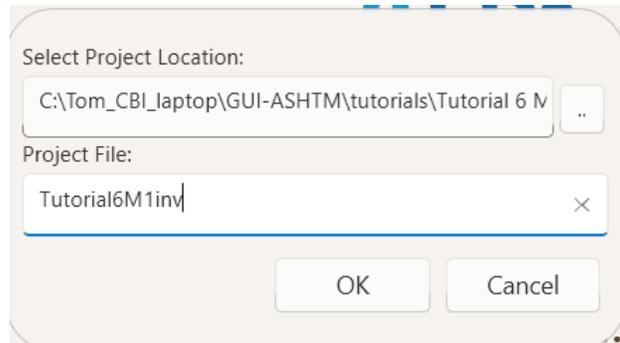
Diffusion & Dispersivity	
Sw (-)	1.0
q (L/T)	0.1
theta (-)	0.35
phi (-)	0.5
alpha (1/T)	0.07
Dm (L ² /T)	0.00093
ax (L)	10
ay (L)	1
az (L)	0.1

Output is computed for a point at $x=15$, $y=50$, $z=100$.

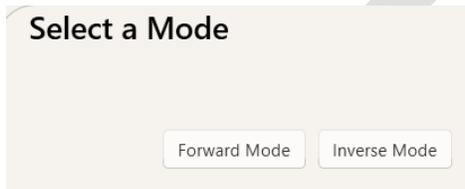
The computed concentration time series was reduced to 11 observation data pairs and white noise added. These synthetic observations are saved in "obsFile_Tutorial6M1a1.txt."

Tutorial2M1a – inverse analysis assuming steps

1. Start a new simulation, select Tutorial 6 folder and type simulation name "Tutorial6M1inv"



2. Click OK and select Inverse Mode



3. Click “Aquifer” input block and enter the same values for corresponding variables as were used in the forward simulation listed above.
4. Click “Test” and enter a test name (any), select Model 1, transient mass transport:



5. Click “Source” and select “linear” from the pull-down menu for “source.”
6. Copy the source defining time-concentrations data pairs listed above, click “AddCfile” and past the copied content into the open box

lambdas (1/T)	
0	0.5
10	1
100	0.6
110	0.25
130	0.7
150	0.1
180	0.65

- Click Save, then click Observations and enter the coordinates of the observation point, the standard deviation of observed concentrations (here assumed to be 0.01)

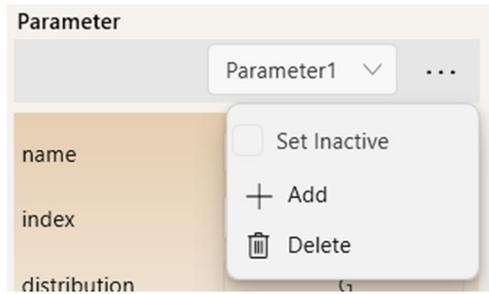
- Open the file with observations “obsFile_Tutorial6M1a1.txt” from Windows Explorer (or similar application), copy its entire content (if using Notepad, press Ctrl-a and then Ctrl-c), then in ASHTM click “Add file” and past the clipboard into the pop-up box

40	0.496555143
60	0.600775938
80	0.625246617
100	0.630346125
120	0.501548547
140	0.497589119
160	0.394570925
180	0.38130251
200	0.297710831

9. Click Save.
10. Click “Genetic” and “MCMC.” For this simulation, keep the default settings.
11. Click “Parameter”, select “q” from the pull-down menu and enter the values shown below:

name	q
index	1
distribution	G
log	yes
prior	0.05
ini	0.05
stdv	4
min	.0001
max	10
cv	.01

12. Click the three dots and select “+Add”



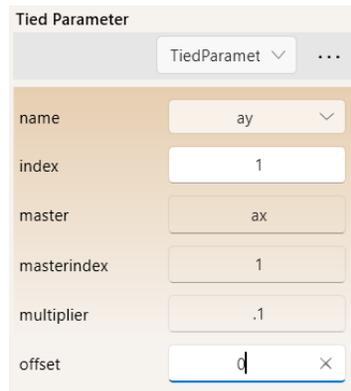
13. Select “ax” from the pull-down menu and enter the following values:



14. Click the three dots and “+Add” again, select “phi” and enter the following values:



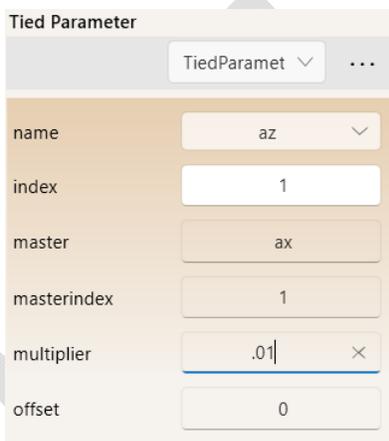
15. Click “Tied Parameter” in the top menu, select “ay” from the pull-down menu and enter these values:



The screenshot shows a dialog box titled "Tied Parameter". At the top, there is a dropdown menu with "TiedParamet" selected and three dots to its right. Below this, the following fields are visible:

name	ay
index	1
master	ax
masterindex	1
multiplier	.1
offset	d

16. Click the three dots and “+Add”, then select “az” from the pull-down menu and enter these values:



The screenshot shows a dialog box titled "Tied Parameter". At the top, there is a dropdown menu with "TiedParamet" selected and three dots to its right. Below this, the following fields are visible:

name	az
index	1
master	ax
masterindex	1
multiplier	.01
offset	0

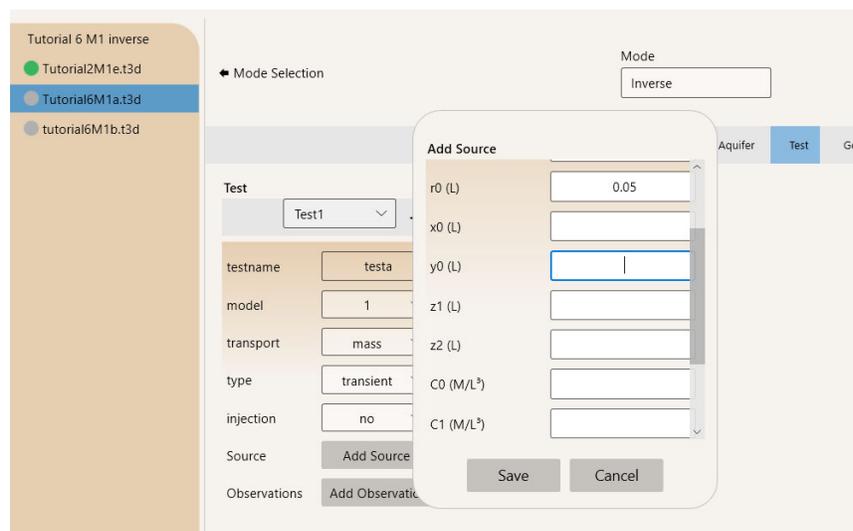
17. Click “Save” and “Run”

18. Problem in assigning source coordinates

19. T3D needs to read Cfile or steps

Tutorial2M1b – inverse analysis using linear

Tutorial2M1c – inverse analysis assuming decay of dissolved phase only



Tutorial 7 – Tracer Test Interpretation:

This tutorial covers inverse analysis of Stringfellow and Barstow tracer tests with models 2 and 4.1. The tests were conducted on single wells, i.e. the tracer was added to the well and tracer migration under natural groundwater flow was recorded in the same well.

Navigate to folder “Tutorial 7 M4 Inverse. Simulations “MW6A-a”, “MW6A-b”, and “MW6A-d” are for a tracer test conducted in 2024 on a well in the Mojave River Basin, in Barstow, CA. A tank with 946 l (250 gal) of water was quickly drained into the well. The injected water contained dissolved sodium chloride and was at a temperature several degrees lower than the aquifer temperature. Temperature and electrical conductivity were recorded every minute with a multi-parameter probe placed in the middle of the well screen. As groundwater flow carried the injected “plume”, the conductivity and temperature signals decreased over time. The test response dissipated in 5 days. The electrical conductivity is a proxy for concentration of a non-reactive tracer. The recordings were converted to the difference from pre-test aquifer temperature and groundwater electrical conductivity. Then each set of observations was normalized by the initial difference in temperature and conductivity, respectively. The normalization is required to obtain observations that are of comparable magnitude (otherwise one observation data set may dominate the other in the parameter estimation process unless one uses weighting). The observations were interpolated at 50 points each to reduce the computational effort.

The estimated unknown aquifer properties, or model parameters, selected for this inverse problem include q (Darcy flux), ϕ (fraction of mobile porosity), and a_x (longitudinal dispersivity). Tied parameters are a_y and a_z (transverse horizontal and vertical dispersivities); they are tied to a_x . The key parameter of interest is the Darcy flux q .

Other model inputs are assumed to be known. This includes the total porosity (θ). Experience shows that the total porosity cannot be reliably estimated from this type of tracer test (single well). The good news is that porosity can be measured in soil samples, or its range of values can be constrained by the soil

type. (Users are encouraged to try to include porosity as an unknown parameter and assess whether the estimated value is realistic.)

1. Select simulation “MW6A-a”. Click on Aquifer, Test, Genetic, and MCMH to see input values. Note that all initial model input must be specified, including values for inputs that will be estimated as unknown parameters; this is because the model is executed once to test all inputs prior to starting the inverse simulation. Note that Model 4.1 is selected for each test (single-porosity transport with initial concentration/temperature distribution).

Aquifer	Test	Genetic	MCMH
b (L) [50]	Test1	Ngenerations [20]	N [1000]
w (L) [10]	testname [MW6A-T]	Nchromosomes [99]	Nchain [3]
q (L/T) [1e-06]	model [4.1]	Ntournament [3]	Nb [100]
theta (-) [0.35]	transport [heat]	keepsurvivors [yes]	Gibbs [no]
phi (-) [0.5]	type [transient]	alpha []	restart [no]
alpha (1/T) [5e-06]	injection [yes]	mutation [0.05]	alpha []
Dm (L ² /T) [9.3e-08]	Source [Add Source]		Nhist [50]
ax (L) [1]	Observations [Add Observation]		
ay (L) [0.1]			
az (L) [0.01]			

2. Click on “Add Source” and scroll down to see that the value for C0, the initial temperature, is 1. This is because the observations were normalized. Click “Cancel” and if you select Test2 from the scroll-down menu, you can similarly verify that initial concentration is also 1.

Test	Coefficients
Test1	r0 (L) [0.0508]
testname [MW6A-T]	x0 (L) [0]
model [4.1]	y0 (L) [0]
transport [heat]	z1 (L) [45.19]
type [transient]	z2 (L) [50]
injection [yes]	C0 (M/L ³) [1.0]
Source [Add Source]	C1 (M/L ³) []
Observations [Add Observation]	
	Save Cancel

3. Click on Aquifer, Test, Genetic, and MCMH again to hide them and then click Parameter and Tied Parameter. You can scroll between the three parameters and two tied parameters. All Parameters are specified as log (“yes”) which means that the inverse algorithm will operate on the natural logarithm

of the parameter value; this is important for parameters whose values may span several orders of magnitude.

Parameter		Tied Parameter	
	Parameter1 ▾ ...		TiedParamet ▾ ...
name	q ▾	name	ay ▾
index	0	index	0
distribution	G	master	ax
log	yes ▾	masterindex	0
prior	1e-06	multiplier	0.1
ini	1e-06	offset	0
stdv	5		
min	1e-10		
max	0.1		
cv	0.01		

- Click “Run.” It will take several minutes to finish the execution because the model will be executed over 5,000 times for every observation (see settings for GA and MCMH), this is over 500,000 model executions for the combined 100 observations.
- Navigate to File Output, select file “MW6A-a_MHres.txt” and scroll to the bottom to see the results for the last Markov chain. The mean parameters are the representative result for this inverse problem. Inspect the correlation matrix for any off-diagonal coefficients with absolute values greater than 0.9, these indicate the corresponding two parameters are not independent (re-running the inverse simulation is recommended before concluding this is indeed the case). The diagonal entries are always 1 and the matrix is symmetric. The text file is tab-separated for copying and pasting into a spreadsheet and the results are not always clearly displayed in the File View.

Mean parameters:

	Name	Location	Mean	Stdv	Log	95% conf limit	
1	q	aquifer	9.43505e-07		1.00852	yes	9.27634e-07 9.59647e-07
2	phi	aquifer	0.1443031.01394		yes		0.1403610.148355
3	ax	aquifer	0.5333831.0175		yes		0.5151890.55222

Covariance matrix:

	q	phi	ax
q	7.19469e-05	7.92355e-05	-6.68001e-05
phi	7.92355e-05	0.000191724	-0.000138055
ax	-6.68001e-05	-0.000138055	0.000301142

Correlation matrix:

	q	phi	ax
q	1	0.674646	-0.453822
phi	0.674646	1	-0.574549
ax	-0.453822	-0.574549	1

Tied parameters:

number	name	index	value	master	masterindex	multiplier	offset
1	ay	0	0.0533383	ax	0	0.1	0
2	az	0	0.00533383	ax	0	0.01	0

- Open file "MW6A-a_MH mean Prsq.txt" in the second window. This has fit statistics including the square of Pearson's correlation coefficient R2. The file is again tab-delimited for copying and posting its content to a spreadsheet.

GWFi results for input file: MW6A-a

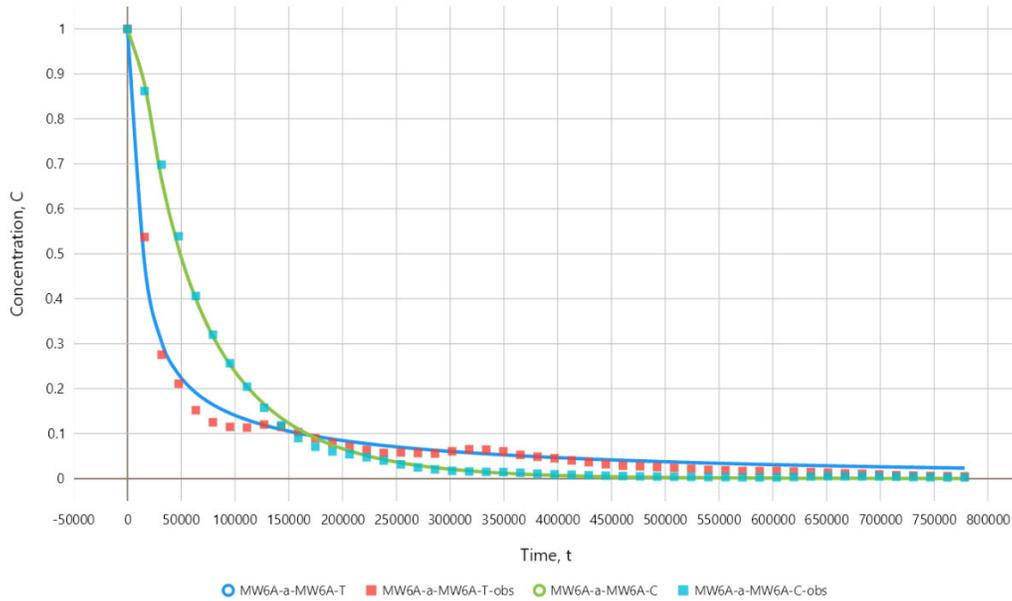
Inverse Method: MH mean P

N = number of observations
R = Pearson product moment correlation coefficient
R2 = R-squared
RMS = root of mean squared error
ME = mean error
AME = mean absolute error
ResW = sum of weighted residuals
Objective function used: RSS

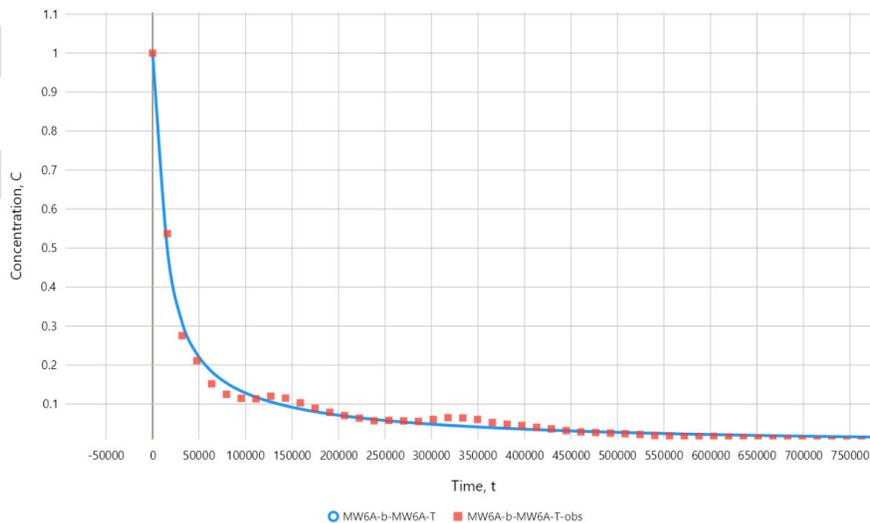
Observations:

Well	Test	Wellfunction	N	R2	RMS	ME	AME	ResW	
MW6A	MW6A-T	undefined	50	0.9922610.0175107			0.0101964	0.0140157	153.313
MW6A	MW6A-C	undefined	50	0.9984460.00880104			-0.000472357	0.0053947	38.7291
all data			100	0.9955510.0138579		0.00486205	0.00970518	192.042	

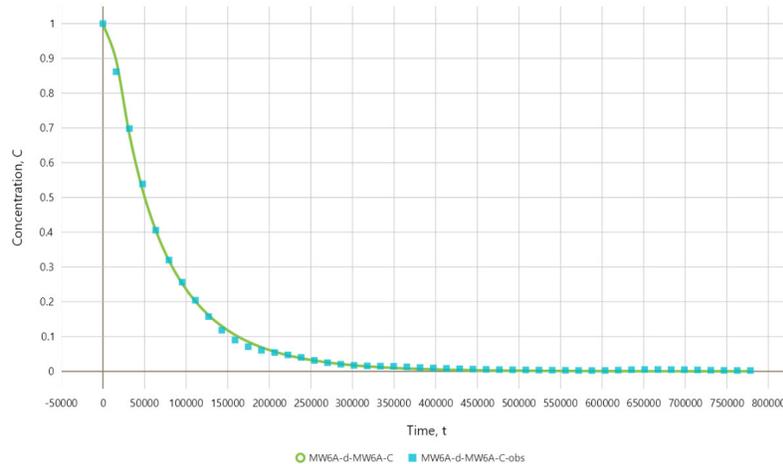
- Navigate to Graphical Output. Observations are shown as symbols, model fit is shown as continuous line for each observation data set. Note that there is more "noise" in the temperature observations ("T") than in the conductivity observations ("C").



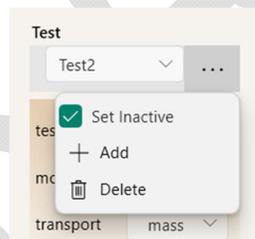
8. Simulation “MW6A-a” was simultaneous fitting of heat transport and solute transport models to the respective observations which provides a more robust approach to parameter estimation. Now we can test what results would be obtained if only heat tracer test or only solute tracer test were performed.
9. Navigate back to main input and select simulation “MW6A-b.” If you click “Test” you will see that only one test is included in this simulation, the temperature observations; this simulation is heat transport only. Click “Run” and when it finishes, inspect files “MW6A-b_MH mean Prsq.txt” and “MW6A-b_MHres.txt” to see the fit statistics and results. Navigate to Graphical Output to see the plot.



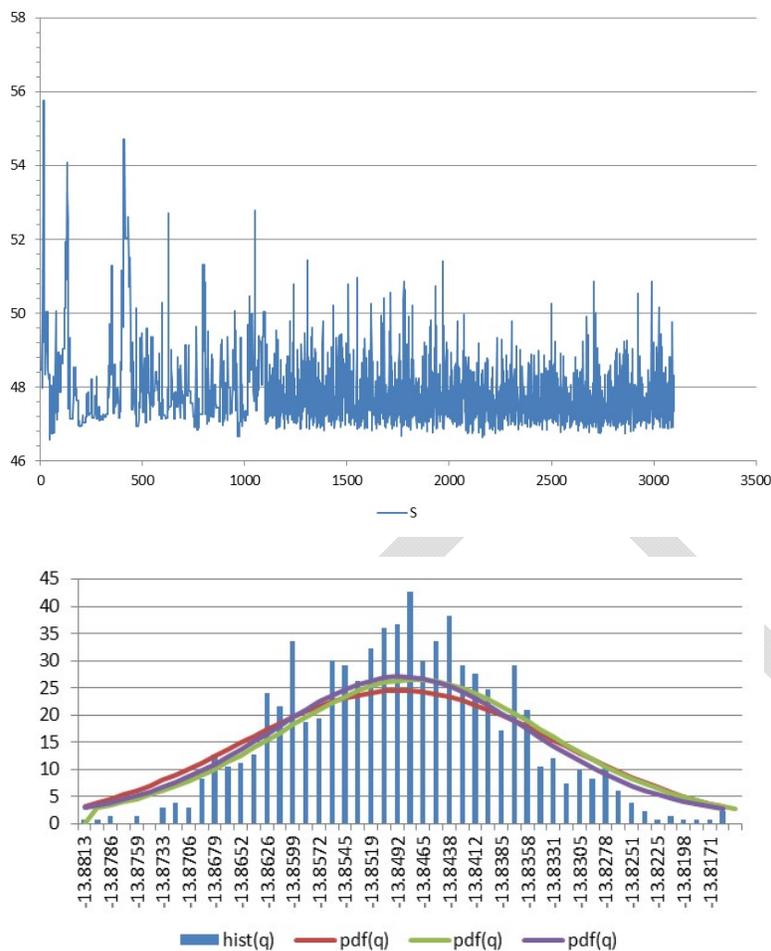
10. Repeat the procedures in step 8 for simulation “MW6A-d” which is solute transport only.



11. How do the results compare for the three simulations? Please note that precision beyond two significant digits is rarely meaningful for the estimated values.
12. Simulations “MW6A-b” and “MW6A-d” were saved as separate input files each containing one test only. Users can prepare simulation “MW6A-a” with both tests and then deactivate one of the tests to run heat or mass transport tracer test simulation only. To deactivate a test, click the three dots to the right of the test pull-down menu and check the “Set Inactive” box, then click Save. The test with all input variables and observations stays in the input file but is not used in the inverse simulation (the test is marked by the symbol * in the input file). To re-activate the test, unselect the check box and click Save.

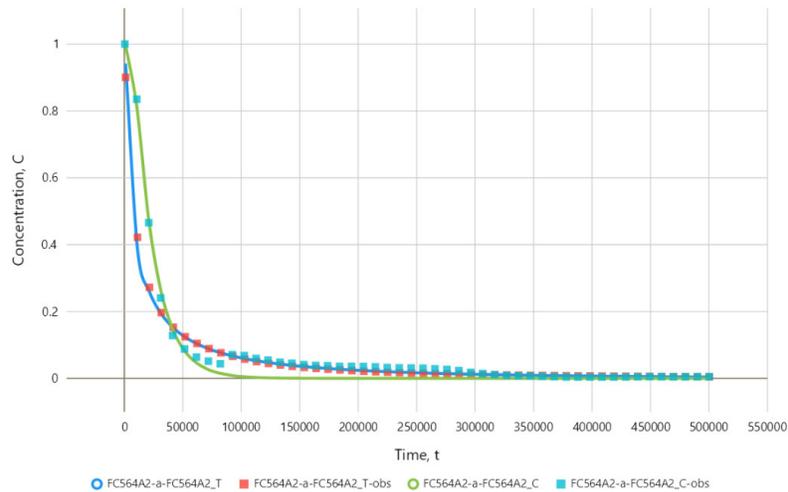


13. ASHTM only displays a graph of the model fit to observations. Users who want to see plots of the Markov chain or probability distributions of the estimated parameters may use the included spreadsheet as template to copy and paste respective output files. The spreadsheet contains plots for various output. For example, Markov chain (value of objective function S versus step number) and probability distribution (histogram with successive adaptive kernel density curves) graphs are shown below.



14. The simulations shown above are for single-porosity model (Model 4.1). This choice was made because Model 4.1 execution is very fast compared to the execution of Model 2 for double porosity. Single porosity model is suitable for heat transport (the model accounts for advective transport via mobile porosity while using the total porosity and soil matrix for heat conduction and storage) but double porosity model is more accurate for solute transport. Simulation “MW6A-f1” uses Model 4.1 for heat transport and Model 2 for solute transport. The number of observations was reduced to 10 for both temperature and conductivity data sets to shorten execution time and maintain balance between the effect of both data sets on the parameter estimation process. There are 4 estimated parameters; the coefficient alpha for mass transfer between mobile and immobile porosity was added. Also note that because Model 2 is for a finite-width aquifer, the coordinates of the injection location (x_0 , y_0) were modified accordingly for solute transport. Users who chose to execute simulation “MW6A-f1” should be prepared for a run time in excess of 24 hours (depending on processor speed).
15. Stringfellow test - The Stringfellow test was conducted in 2021 by gravity draining a 100 gallon tank of distilled water at temperature higher than the aquifer temperature into well FC564A2. Simulations FC564A2-a, FC564A2-b, and FC564A2-d use Model 4.1 and simulation FC564A2-f uses Models 4.1 for heat and Model 2 for solute transport.

16. Click on simulation FC564A2-a. In the Model Parameters menu, check Test, Parameter, etc. The same settings are used for the estimated parameters, Genetic, and MCMC as for the Barstow test on MW6A. Navigate to Graphical Output to see the model fit to observations.



17. Click on simulations FC564A2-b, FC564A2-d, and FC564A2-f to see model fit for temperature observations only, conductivity observations only, and both temperature and conductivity observations with Model 2 used for mass transport, respectively.
18. Select simulation FC564A2-b, navigate to Model Parameters, and save under a new name. Click Parameter. Click the three dots to the right of “Parameter1” and select “+Add” from the menu. Select theta (total porosity) from the pull-down menu for “name.” Enter the values shown below for the remaining variables. Click the three dots again and unselect “Set Inactive.” Click Save.

Parameter4	
name	theta
index	1
distribution	G
log	yes
prior	.35
ini	0.3
stdv	5
min	0.1
max	0.5
cv	0.01

19. Click run, wait for the execution to finish (this may take a few minutes). Navigate to File Output and select the file with MCMC results (with name “..._MHres.txt”), then scroll to the end to see chain 3 results. The mean parameters (q, phi, ax) are similar to the results of simulation FC564A2-b and the value of theta is plausible. However, this is not guaranteed for this type of tracer test; estimation of both phi and theta often fails in the sense that the estimated values are implausible and/or correlated.

The goodness of fit (navigate to Graphical Output) is not by itself a reliable indicator of successful inverse simulation.

20. Final Notes:

- a. Pre-processing and reduction of observations is done outside of ASHTM to allow users maximum flexibility and using methodologies suitable to their data recording and test procedures.
- b. Because inverse execution takes substantial time for dual-porosity solute transport, it may be worthwhile to use a single-porosity, time-domain model first before running a dual-porosity simulation and inspect the results and check for input errors.
- c. The executable called by ASHTM writes two echo files: first after reading input and before executing the model to calculate initial fit (“..._ech.txt” file), the second after calculating the initial fit (“..._ech1.txt” file). The echo file would list input errors at the end. Inspection of the echo of input is recommended to ensure that all the instructions are what the user intended.
- d. The initial fit is written in file “..._ini.txt.” The initial fit file may be inspected to see if the calculated values meet expectations.
- e. Try to execute the same inverse simulation again (perhaps save it with a new file name). The results will not be exactly the same but should be very close. If they are not, the MCMC did not converge to the target distribution and the number of chains (Nchain) should be increased or a difficult to estimate parameter should be excluded.
- f. Running inverse simulations with Model 1, Model 2, and especially Model 3 takes considerable execution time even with a reduced number of observations. Users may find it convenient to run several of these simulations concurrently by invoking the T3D executable from the command prompt (see User Instructions) after having prepared the input files in ASHTM.

Tutorial 8 – Plume Assessment Using Forward Modeling:

This tutorial covers forward analysis of an existing plume. An apparently isolated PCE plume, detected by only a single monitoring well, has existed for years at the Fresno Sanitary Landfill Superfund Site in California. No source of PCE associated with this plume is known and it is interpreted as being limited in extent. This conceptual model represents a solute transport scenario with no source and only initial distribution of PCE. Forward transport modeling is used to test this conceptual model. The model inputs are based on measured and estimated plume concentrations and aquifer properties. For example, the input value for the Darcy flux q was calculated using hydraulic conductivity from a pumping test and hydraulic gradient from measured water levels. A range of transport scenarios can be used to confirm or disprove assumptions and/or previous estimates of aquifer properties, existence of sources, or plume size.

1. Navigate to folder Tutorial 8 and click simulation “b0”. The units used are feet and days. The initial concentration distribution is based on interpreted plume extent and the output is specified to be a concentration profile through the plume center along the flow direction after one year.

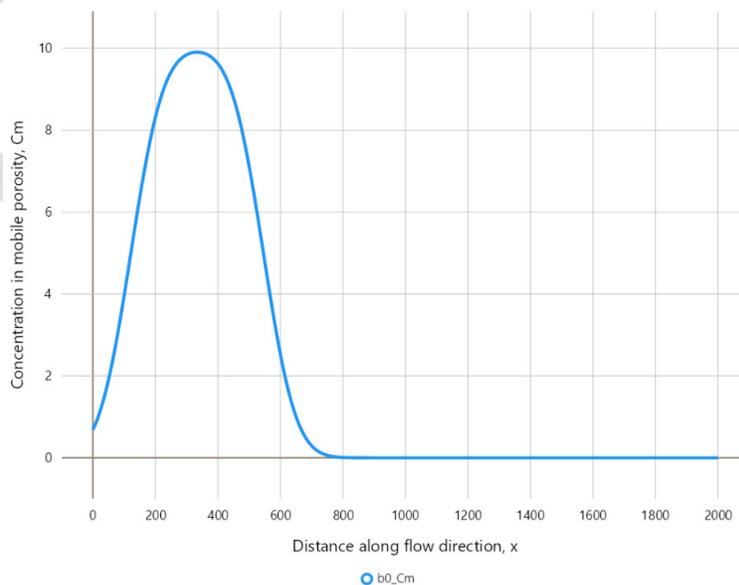
Diffusion & Dispersion		Decay & Sorption		Source	
Sw (-)	1.0	lambdai (1/T)	0	source	none
q (L/T)	.219	lambdais (1/T)	0	PointSource	no
theta (-)	.45	lambdam (1/T)	0	injection	no
phi (-)	.5	lambdams (1/T)	0	C0 (M/L ³)	10
alpha (1/T)	.86	Ki (L ³ /M)	.02	Cfile	Add Cfile
Dm (L ² /T)	9.3e-4	Km (L ³ /M)	.02		
ax (L)	10	gamma			
ay (L)	1	f (-)	.5		
az (L)	.1				

Source Coordinates		Output Settings	
x1 (L)	-212	output	x
x2 (L)	212	function	Cm
y1 (L)	787.87	Xstart (L)	0
y2 (L)	1212.13	Xend (L)	2000
z1 (L)	0	dX (L)	10
z2 (L)	24		

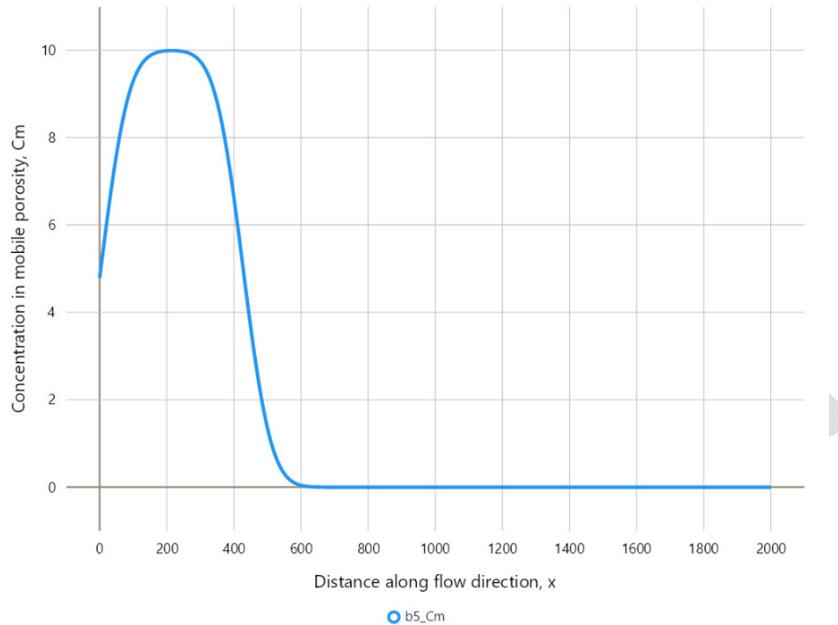
Add project description

w: 2000, b: 24, t: 365, x: 100

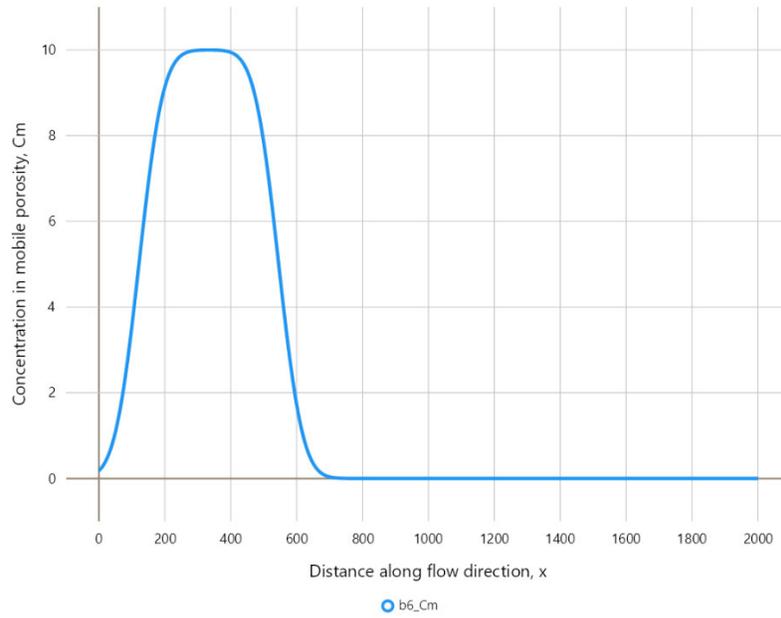
2. Click “Run” and navigate to Graphical Output.



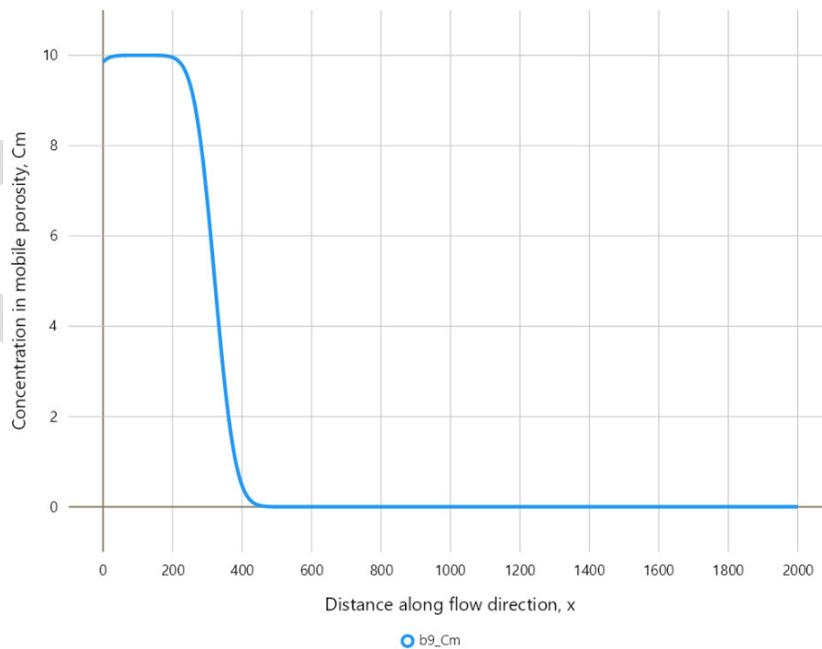
3. The center of plume has moved away within a year for this scenario. This does not agree with observations.
4. Now navigate to Model Parameters, click Decay & Sorption, and change K_i and K_m from 0.02 to 0.2 (note only K_m is used with Model 4). Click Save and Run, navigate to Graphical Output. Note that this tutorial keeps saving over the original simulation file but some of the graphical output shown is for simulations saved under different names.



5. The plume migration is delayed compared to the base case but still moves away in one year.
6. Go back to Model Parameters, change sorption back to 0.02, click Diffusion & Dispersivity and decrease dispersivity by changing a_x , a_y , and a_z from 10, 1, and 0.1 to 5, 0.5, and 0.05.
7. Click Save and Run, navigate to Graphical Output.



8. The result is similar to increased sorption.
9. Navigate back to Model Parameters, click Diffusion & Dispersivity, and change the Darcy flux q from 0.219 to 0.072.
10. Click Save and Run, then navigate to Graphical Output.



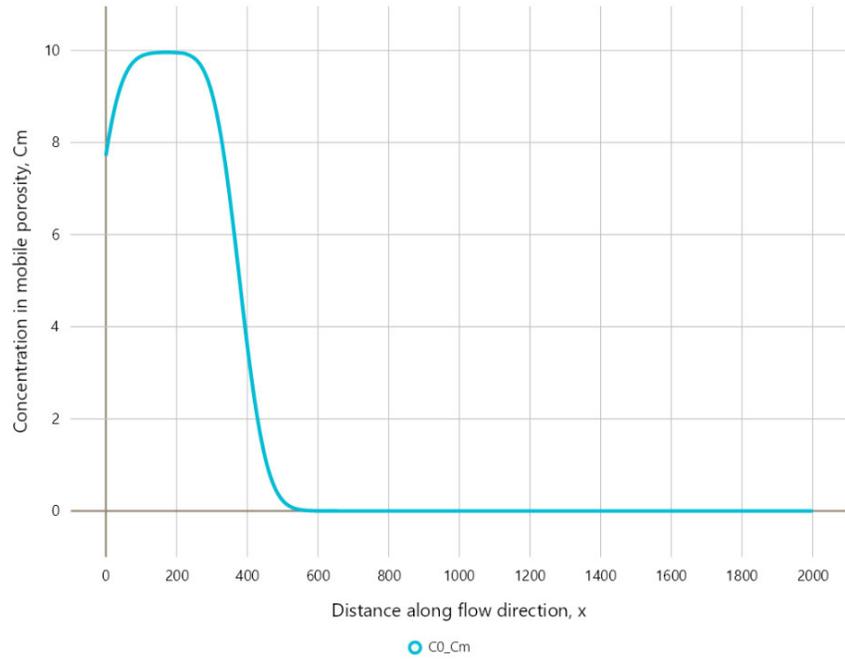
11. As expected, changing q has the most effect on the plume movement.
12. Now go back to Model Parameters and select Model 2 from the Model scroll-down menu. Model 2 accounts for dual porosity.

13. Click Diffusion & Dispersivity, change q back to 0.219 and change value of α to 0.09 (now α is being used because Model 2 was selected).
14. Click Source and change values of both C_{m0} and C_{i0} to 10 (variable C_0 is not used with Model 2 when “no source” is selected).
15. Click Source Coordinates and change z_1 from 0 to 0.1 (this last change is for improved numerical convergence).

Mode	Model	Transport	Transport Type
Forward	Model 2	mass	transient

Heat Transport	Diffusion & Dispersivity	Decay & Sorption	Source	Source Coordinates	
Diffusion & Dispersivity					
Sw (-)	1.0	Decay & Sorption		x1 (L)	-212
q (L/T)	.219	lambdai (1/T)	0	x2 (L)	212
theta (-)	.45	lambdais (1/T)	0	y1 (L)	787.87
phi (-)	.5	lambdam (1/T)	0	y2 (L)	1212.13
alpha (1/T)	.09	lambdams (1/T)	0	z1 (L)	0.1
Dm (L ² /T)	9.3e-4	Ki (L ³ /M)	.02	z2 (L)	24
ax (L)	10	Km (L ³ /M)	.02		
ay (L)	1	gamma			
az (L)	.1	f (-)	.5		

16. Click Save and Run (the execution takes substantially longer), navigate to Graphical Output.



17. One can decrease the q value again, save, and run to get a result representative of a persistent small plume.

DRAFT

References

APTIM. 2023. Tracer Test Report Stringfellow Acid Pits Superfund Site Jurupa Valley, California. February.

APTIM. 2022. Analytical Solute Transport Model Development Report Stringfellow Acid Pits Superfund Site Jurupa Valley, California. May.

Perina, T. 2021. Semi-analytical three-dimensional solute transport of sequentially decaying species with mobile-immobile regions, sorption, decay, and arbitrary transient source. *Mathematical Geosciences*, <https://doi.org/10.1007/s11004-021-09975-5>

Perina, T. 2022. Semi-analytical model for solute transport in a three-dimensional aquifer with dual porosity and a volumetric source term. *Journal of Hydrology* 607, 127520. <https://doi.org/10.1016/j.jhydrol.2022.127520>

DRAFT