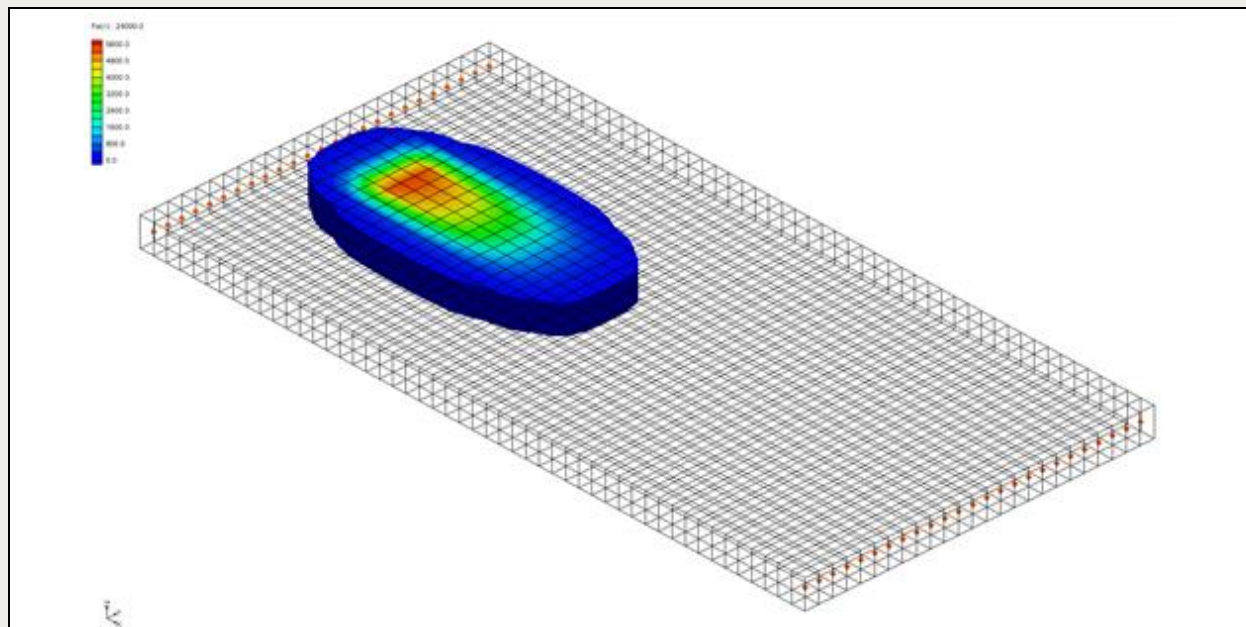




GMS 10.9 Tutorial

SEAM3D – BTEX

Using SEAM3D with BTEX



Objectives

This tutorial shows how to use the SEAM3D Biodegradation and NAPL Dissolution packages.

Prerequisite Tutorials

- MT3DMS – Grid Approach

Required Components

- GMS Core
- MODFLOW Interface
- SEAM3D

Time

- 25–40 minutes

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1 Introduction

SEAM3D is a reactive transport model used to simulate complex biodegradation problems involving multiple substrates and multiple electron acceptors. It is based on the MT3DMS code. In addition to the regular MT3DMS modules, SEAM3D includes a Biodegradation package and NAPL Dissolution package. This tutorial illustrates how to use both of these packages to set up a reactive transport simulation.

The problem in this tutorial is illustrated in Figure 1. The site represents a shallow unconfined aquifer with a uniform flow field from left to right. A NAPL plume is located on the left side of the model. The NAPL plume contains two primary hydrocarbons, benzene and toluene. The benzene and toluene are dissolving into the groundwater and are being transported to the right.

Set up a SEAM3D simulation that models the transport and sequential degradation of the contaminants via aerobic degradation and sulfate reduction over a 2000-day period. The model will include dispersion and retardation due to sorption. The reactions will be modeled using the Biodegradation package. The gradual release of contaminants from the NAPL plume will be modeled as a source term using the NAPL Dissolution package. For comparison purposes, the model will include a conservative (no sorption) tracer and a non-conservative tracer.

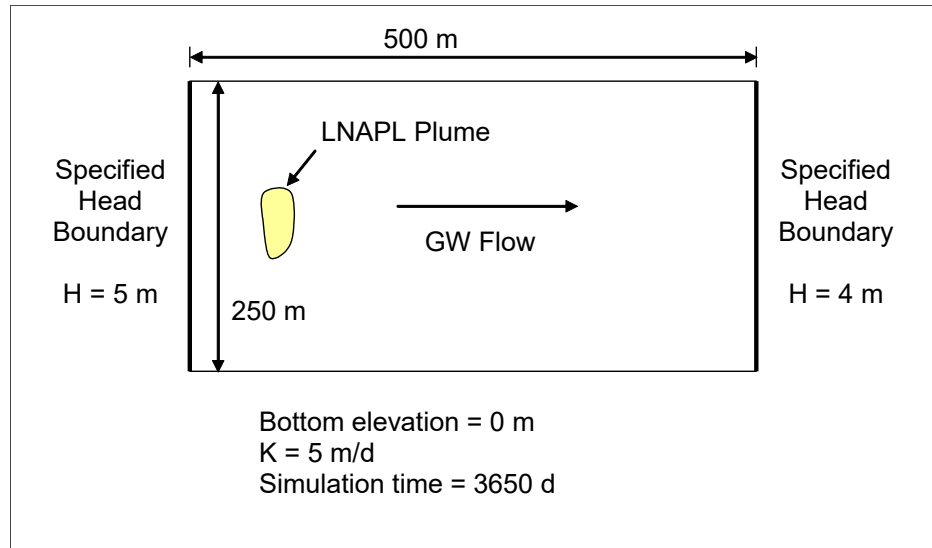


Figure 1 Problem to be solved in SEAM3D tutorial

This tutorial will review importing a MODFLOW model, defining SEAM3D conditions, running MODFLOW and SEAM3D then finally creating a time series plot.


1.1 Getting Started

Do the following to get started:

1. If GMS is not open, launch GMS.
2. If GMS is already open, select the *File* | **New** command to ensure the program settings are restored to the default state.

2 Importing the Flow Model

The first step in setting up the SEAM3D simulation is to import the MODFLOW flow model. A steady state flow model has been previously computed and is supplied with the tutorial files.

1. Select the **Open**  button to bring up the *Open* dialog.
2. Navigate to the *BTEX\BTEX* folder.
3. Select the file entitled “flowmod.gpr” and click **Open** to exit the *Open* dialog.

At this point, a grid should appear with contours indicating a uniform flow field from the left side to the right side (Figure 2).

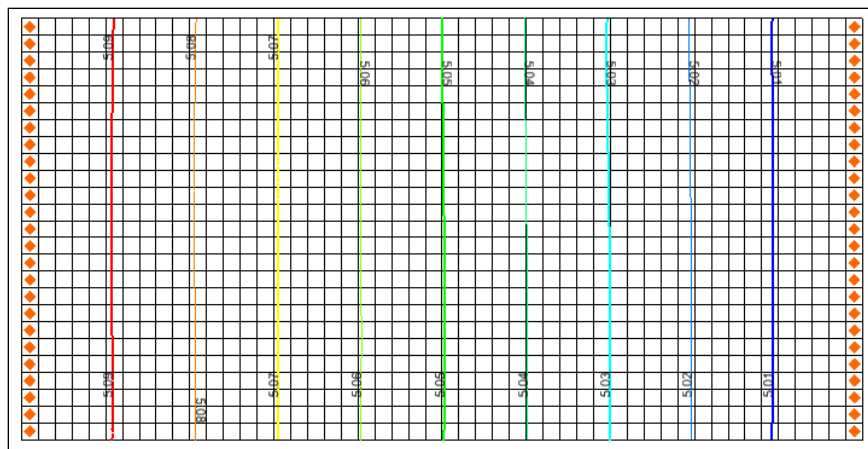


Figure 2 Grid with uniform flow field

3 Defining the Units

First it is necessary to define the units. The length and time units will already be set by the MODFLOW model, so it is only necessary to specify the mass and concentration units.

1. Select the *Edit | Units...* command to open the *Units* dialog.
2. Ensure the following units agree:



<i>Length</i>	ft
<i>Time</i>	d
<i>Mass</i>	g
<i>Force</i>	N
<i>Concentration</i>	mg/l

3. Select the **OK** button to exit the *Units* dialog.

The units entered here are for convenience only and do not affect the calculations. GMS displays these units next to the input fields as a reminder of the proper units for each item. It is still necessary to enter consistent units.

4 Initializing the SEAM3D Simulation

To create a new SEAM3D simulation:

1. In the Project Explorer, expand the “ 3D Grid Data” folder.
2. Right-click on “ grid”.
3. Select the **New MT3DMS...** command to open the *Basic Transport Package* dialog.
4. In the *Model* section, select the *SEAM3D* option.

4.1 Setting up the Stress Periods

The next step is to set up the stress periods. Since none of the sources change over the simulation, it is possible to use a single stress period with a single time step of 2000 days. For the transport step size, use the default value of zero. This forces SEAM3D to compute the appropriate transport step size automatically.

1. Select the **Stress Periods...** button to open the *Stress Periods* dialog.
2. Change *Length* to “3650”.
3. Select the **OK** button to exit the *Stress Periods* dialog.

4.2 Package Selection

Next, to select the packages for the simulation:

1. Select the **Model Setup...** button to open the *MT3DMS/RT3D Packages* dialog.
2. Make sure the following packages are selected:
 - *Advection package*
 - *Dispersion package*
 - *Source/sink mixing package*
 - *Chemical reaction package*
 - *Biodegradation package*
 - *NAPL dissolution package*
3. Select the **Next>** button to open the *Define Species* dialog.

4.3 Defining the Species

Next, to define the species used in the simulation:

1. Change *Number of nondegradable tracers* to “1”.
2. Change *Number of hydrocarbon substrates* to “3”.
3. In the *Microbial Processes* section, turn on *Fe(III) reduction* and *Methanogenesis*.
4. In the *Products to track* section, turn on *Fe(II)*.

Notice while making changes in the left side of the dialog, the species names are listed on the right side of the dialog. Some of these names are fixed, but some are user-defined. Supply more meaningful names to the tracers and hydrocarbons:

5. In the *Names* list, double-click “tracers1”, and change the name to “MTBE”.
6. Double-click “Substrate1”, and change the name to “Benzene”.
7. Double-click “Substrates2”, and change the name to “TEX”.
8. Double-click “Substrates3”, and change the name to “Aliphatics”.
9. Select the **Finish** button to close the *Define Species* dialog.

4.4 Output Control

Now to edit the *Output Control* data to specify how frequently the solution data should be saved for post-processing:

1. Select the **Output Control...** button to open the *Output Control* dialog.
2. Select the *Print or save at specified times* option.
3. Select the **Times...** button to open the *Variable Time Steps* dialog.
4. Select the **Initialize Values...** button to open the *Initialize Time Steps* dialog.
5. For *Initial time step size*, enter “182.5”.
6. For *Maximum time step size*, enter “182.5”.
7. For *Maximum simulation time*, enter “3650”.
8. Select the **OK** button to exit the *Initialize Time Steps* dialog.
9. Select the **OK** button to exit the *Variable Time Steps* dialog.
10. Select the **OK** button to exit the *Output Control* dialog.

4.5 Entering the Porosity

SEAM3D requires a porosity value for each cell in order to compute a correct seepage velocity for transport. This tutorial will use a constant porosity for the entire grid. To enter the porosity:

1. Select the **Porosity...** button to open the *Porosity* dialog.
2. Select the **Constant** → **Grid** button to open the *Grid Value* dialog.
3. Enter “0.25”.
4. Select **OK** to close the *Grid Value* dialog.
5. Select the **OK** button to exit the *Porosity* dialog.

4.6 Starting Concentrations

The mobile species are listed in the lower right corner of the *Basic Transport Package* dialog. It is necessary to define a set of starting concentrations for each of the species. The default concentration is zero. This will be the correct starting concentration for the hydrocarbon substrates and the tracers. However, it's necessary to set the starting concentrations of the O₂, SO₄, and H₂S to the correct background values.

1. In the spreadsheet, for O₂, under *Starting Conc.(mg/l)*, enter “3.0”.
2. For Fe(II), under *Starting Conc.(mg/l)*, enter “0.002”.

This concludes the input for the Basic Transport package.

3. Select the **OK** button to exit the *Basic Transport Package* dialog.

5 Advection Package

Typically, the next step at this point would be to enter the data for the Advection package. However, the default solution scheme (*Third Order TVD – ULTIMATE*) is adequate for this problem, so no changes need to be made.


6 Dispersion Package

The next step is to enter the data for the *Dispersion* package. The aquifer has a longitudinal dispersivity of 3 m and a transverse (horizontal) dispersivity of 0.15 m. The vertical dispersivity is assumed equal to the longitudinal dispersivity.

1. Select the **SEAM3D | Dispersion Package...** command to open the *Dispersion Package* dialog.
2. For *TRPT*, enter “0.1”.
3. Select the **Longitudinal Dispersivity...** button to open the *Longitudinal Dispersivity* dialog.
4. Select the **Constant** → **Grid** button to open the *Grid Value* dialog.
5. Enter “5.0”.
6. Select **OK** to close the *Grid Value* dialog.
7. Select the **OK** button to exit the *Longitudinal Dispersivity* dialog.
8. Select the **OK** button to exit the *Dispersion Package* dialog.

7 Source/Sink Mixing Package

The next step is to enter the data for the Source/Sink Mixing package. This package is used to establish the concentration of water entering the system. For this problem, water is entering the system on the left side of the model through the specified head boundary. It is needful to enter the correct “background” concentrations for fresh water entering through this boundary.

1. Use the **Select j**  tool to click on any cell in the leftmost column to select the entire column.
2. Select the **SEAM3D | Point Sources/Sinks...** command to open the *MODFLOW/SEAM3D Sources/Sinks* dialog.
3. Click the **Add BC** button near the bottom of the dialog.
4. In the *All* row, change *Type (ITYPE)* to “constant head (CHD)” to apply the type to all the selected cells.

Once again, the default value is zero. That is the correct value for most of the species.

5. In the *All* row, for *O2* column, enter “3.0”.
6. In the *All* row, for *Fe(II)*, enter “0.002”.
7. Select the **OK** button to exit the *MODFLOW/SEAM3D Sources/Sinks* dialog.

8 Chemical Reaction Package

The next step is to enter the data for the Chemical Reaction package. This package is the standard MT3DMS package that is used to simulate sorption and first order decay. The biodegradation reactions are simulated in the Biodegradation package that is unique to SEAM3D. This tutorial uses the Chemical Reaction package to simulate retardation due to sorption.

1. Select the *SEAM3D* | **Chemical Reaction Package...** command to open the *Chemical Reaction Package* dialog.
2. In the *Sorption* combo box, select the “Linear isotherm” option.

The default sorption constant is zero. This is the correct value for the Aliphatics and for O₂ and CH₄. However, it is necessary to enter a non-zero value for Fe(II) and for the two substrates.

3. For *Bulk density*, enter “1800000000.0”.
4. For *1st sorption const*, enter the following values.

<i>MTBE</i>	3.36e-009
<i>Benzene</i>	3.36e-008
<i>TEX</i>	6.72e-008
<i>Aliphatics</i>	1.34e-007


5. Select **OK** to exit the *Chemical Reaction Package* dialog.

9 NAPL Dissolution Package

It is now possible to enter the data for the NAPL Dissolution package. This tutorial will simulate the gradual dissolution of contaminants from a plume into the groundwater. In MT3DMS, such a situation could be simulated using constant concentration cells, injection wells, or recharge. None of these options results in a realistic simulation of dissolution from a plume. The SEAM3D NAPL Dissolution package provides a more realistic representation of a contaminant plume. With this package, it is possible to identify the cells containing the plume and enter the initial concentration and dissolution rate for the contaminants. It is also possible to enter the initial mass fraction and solubility of each species in the plume. SEAM3D then simulates the release of each of the species over the duration of the simulation.

9.1 Selecting the Cells

The first step is to select the cells where the plume is located.

1. Select the **Select Cells**  tool.
2. Select the *Grid* | **Find Cell...** command to open the *Find Grid Cell* dialog.
3. For *I*, *J*, and *K*, enter “11”, “6”, and “1” respectively.
4. Select **OK** to close the *Find Grid Cell* dialog.
5. Using the selected cell as the upper left corner, drag a rectangle to select a 5x2 rectangular region of cells as shown in Figure 3.

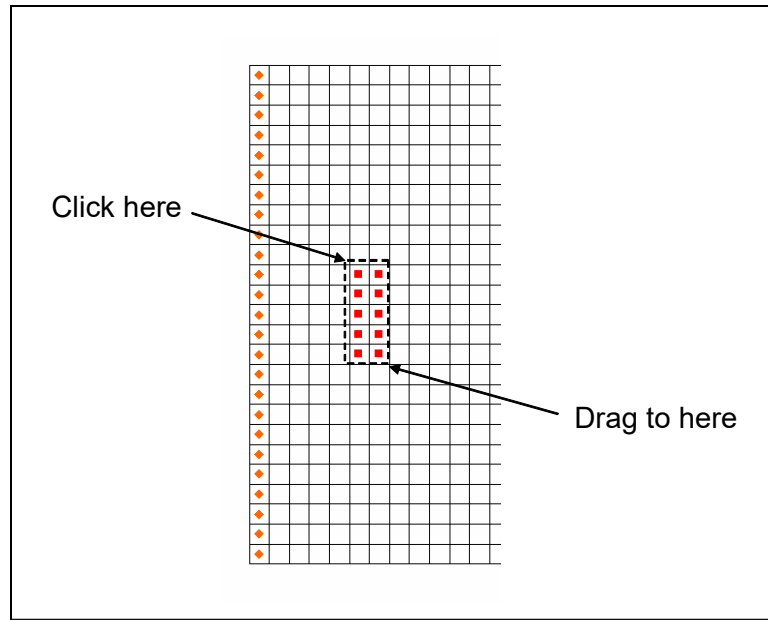


Figure 3 Selecting the cells defining the plume

9.2 Assigning the Concentration

Now that the plume cells are selected, the next step is to assign the concentrations to the cells.

1. Select the **SEAM3D | Point Sources/Sinks...** command to open the *MODFLOW/SEAM3D Sources/Sinks* dialog.
2. In the left window, select *SEAM3D: NAPL*.
3. In the *All* row, in the *NAPL* column, check the box.
4. In the *All* row, for *Initial conc. (mg/l)*, enter "0.001".
5. In the *All* row, for *Rate dissolved (1/d)*, enter "0.5".
6. Select **OK** to exit the *MODFLOW/SEAM3D Sources/Sinks* dialog.
7. Click anywhere outside the grid to unselect the cells.

9.3 Entering the NAPL Data

The next step is to enter the remaining NAPL plume data using the *NAPL Dissolution Package* dialog.

1. Select the **SEAM3D | NAPL Dissolution Package...** command to open the *NAPL Dissolution Package* dialog.
2. Change *Number of tracers in NAPL* to "1".
3. Change *Number of hydrocarbons in NAPL* to "3".
4. At the bottom of the dialog, for *Inert fraction molecular weight*, enter "150".

5. For all four species, enter the values shown in the table.

	<i>Initial Mass Fraction</i>	<i>Solubility</i>	<i>Molecular Weight</i>
<i>MTBE</i>	0.04	48.0	88.2
<i>Benzene</i>	0.01	1750.0	78.1
<i>TEX</i>	0.3	250.0	105.0
<i>Aliphatics</i>	0.55	12.0	97.0

6. Select **OK** to exit the *NAPL Dissolution Package* dialog.

10 Biodegradation Package

The last package to set up is the Biodegradation package. It is possible to enter the yield coefficients, inhibition coefficients, and other reaction parameters controlling the degradation of benzene and toluene.

1. Select the *SEAM3D* | **Biodegradation Package...** command to open the *Biodegradation Package* dialog.

10.1 Minimum Concentrations

Notice that the input for the dialog is broken up into a series of property sheets.

1. Verify that the *Min. Conc.* tab is selected.
2. For *Number of bio steps per transport step*, enter “2”.
3. For *Microcolony minimum concentration*, enter “0.001”.
4. For *Minimum Concentration*, enter the following values:

<i>Benzene</i>	0.002
<i>TEX</i>	0.005
<i>Aliphatics</i>	0.1
<i>O2</i>	0.0
<i>Fe(III)</i>	5.0

10.2 Electron Acceptor Coefficients

Next, to enter the electron acceptor data:

1. Select the *Elec. Acc.* tab.
2. For *Inhibition coefficient*, enter the following values:

<i>Fe(III)-O2</i>	0.5
<i>Methane-O2</i>	0.2
<i>Methane-Fe</i>	25

3. For *Yield coefficient*, enter the following values:

O ₂ -Benzene	0.4
O ₂ -TEX	0.5
O ₂ -Aliphatics	0.2
Fe(III)-Benzene	0.15
Fe(III)-TEX	0.20
Fe(III)-Aliphatics	0
Methane-Benzene	0.01
Methane-TEX	0.02
Methane-Aliphatics	0

10.3 Generation Coefficients

Do the following to enter the generation coefficient for H₂S:

1. Select the *Gen. Coeff.* tab.
2. Under *Product coefficient*, for *Fe(II)*, enter “0.10”.
3. Under *Methane coefficient*, enter the following values:

Benzene	0.77
TEX	0.8
Aliphatics	0.7

10.4 Use Coefficients

Do the following to enter the electron acceptor use coefficients:

1. Select the *Use Coeff.* tab.
2. For *Electron acceptor use coefficient*, enter the following values:

O ₂ -Benzene	3.1
O ₂ -TEX	3.0
O ₂ -Aliphatics	3.0
Fe(III)-Benzene	41
Fe(III)-TEX	42
Fe(III)-Aliphatics	0

10.5 Saturation Constants

Do the following to enter the saturation constants:

1. Select the *Sat. Const.* tab.
2. Under *Electron acceptor half saturation Constant*, for O₂, enter “1”.

3. For *Hydro. half saturation constant*, enter the following values:

O ₂ -Benzene	15
O ₂ -TEX	10
O ₂ -Aliphatics	50
Fe(III)-Benzene	50
Fe(III)-TEX	30
Fe(III)-Aliphatics	50
Methane-Benzene	50
Methane-TEX	50
Methane-Aliphatics	50

10.6 Rates

Do as follows to enter the rate data:

1. Select the *Rates* tab.
2. Under *Death rate*, ensure *Calculated by model* is selected.
3. For *Max. specific rate of substrate utilization*, enter the following values:

O ₂ -Benzene	0.4
O ₂ -TEX	0.5
O ₂ -Aliphatics	0.2
Fe(III)-Benzene	0.001
Fe(III)-TEX	0.02
Fe(III)-Aliphatics	0
Methane-Benzene	0.002
Methane-TEX	0.01
Methane-Aliphatics	0.002

10.7 Starting Concentrations

At this point, the only remaining data for the Biodegradation package are the starting concentrations for the microcolonies and Fe(III). To enter the starting concentration data, do the following:

1. Select the *Start. Conc.* tab.
2. Next to *Fe(III)*, click **Edit...** to open the *Starting Concentration Array* dialog.
3. Select **Constant** → **Grid** to open the *Grid Value* dialog.
4. Enter "50".
5. Select **OK** to close the *Grid Value* dialog.
6. Select **OK** to close the *Starting Concentration Array* dialog.
7. Repeat steps 2–6 for the remaining species with the following grid values:

Aerobes: "0.25" *Fe(III) Reducers*: "0.025" *Methanogens*: "0.025"

8. Select the **OK** button to exit the *Biodegradation Package* dialog.

11 Saving the Simulation

At this point, it is possible to save the model and run SEAM3D.

1. Select the *File* | **Save As...** command to open the *Save As* dialog.
2. Navigate to the *BTEX\BTEX* directory.
3. Enter “run1.gpr” for the *File name*.
4. Select the **Save** button to save the files and exit the *Save As* dialog.

12 Running MODFLOW

SEAM3D requires the HFF file generated by MODFLOW. Since the project is saved in a different folder than the one where the MODFLOW simulation was opened, the HFF file does not exist in the new location. It's necessary to rerun MODFLOW so that it will recreate the HFF file in the current folder.

Do the following to run MODFLOW:

1. Select the *MODFLOW* | **Run MODFLOW** command to bring up the *MODFLOW* dialog.
2. Select **OK** at the prompt if it appears.
3. When the simulation is finished, click the **Close** button to exit the *MODFLOW* dialog to import the solution automatically.


13 Running SEAM3D

To run SEAM3D:


1. Select the *SEAM3D* | **Run SEAM3D...** command to open the *SEAM3D* dialog.
2. Select **Yes** at the prompt to save changes.
3. When the simulation is finished, hit the **Close** button to exit the *SEAM3D* dialog.

14 Setting the Contouring Options

Now to turn on color shaded contours and set up a color legend:

1. Select **Contour Options**  to open the *Dataset Contour Options – 3D Grid – MTBE* dialog.
2. Change the *Contour method* to “Color fill”.
3. Ensure the *Legend* option is turned on.
4. Select **OK** to close the *Dataset Contour Options – 3D Grid – MTBE* dialog.

15 Viewing the Concentration Contours

1. In the Project Explorer, select “ MTBE”.
2. In the *Time Steps* window, select the last time step.

This plot illustrates the concentration contours corresponding to no sorption and no reactions. This is a useful benchmark to consider when viewing the other datasets.

To quickly switch between datasets, do as follows:

3. Click on the  "MTBE" dataset.

This plot (non-conservative tracer) represents sorption but no reactions.




4. Use the down arrow key to view the other datasets.

While viewing the datasets, note the relationship between the substrates and the electron acceptors. If desired, use the *Time Steps* list to view the solution at different time steps.

16 Generating a Time History Plot

A useful way to compare two transient solutions is to create an observation point and generate a time history plot. The fastest way to do this is to create an "Active Dataset Time Series" plot.

16.1 Creating a Time Series Plot

1. Click on the  "O2" dataset.
2. Select the **Plot Wizard**  button to open the *Plot Wizard* dialog.
3. For *Plot Type*, select "Active Dataset Time Series".
4. Select the **Finish** button to close the *Plot Wizard* dialog and generate the plot.
5. Use the **Select Cells**  tool to select a cell in the grid near the contaminant source.

Notice that the plot shows the concentration v. time.

6. Select a different cell and notice that the plot updates.

If desiring to take the plot data and put it into Excel, right-click on the plot and select the **View Values...** option. This brings up a spreadsheet that can be copied into Excel.

17 Other Viewing Options

At this point, experiment with other viewing options if desired. For example, try setting up an animation using the **Animate** command in the *Display* menu.

18 Conclusion

This concludes the "SEAM3D – BTEX" tutorial. Continue to explore the SEAM3D options or exit the program.