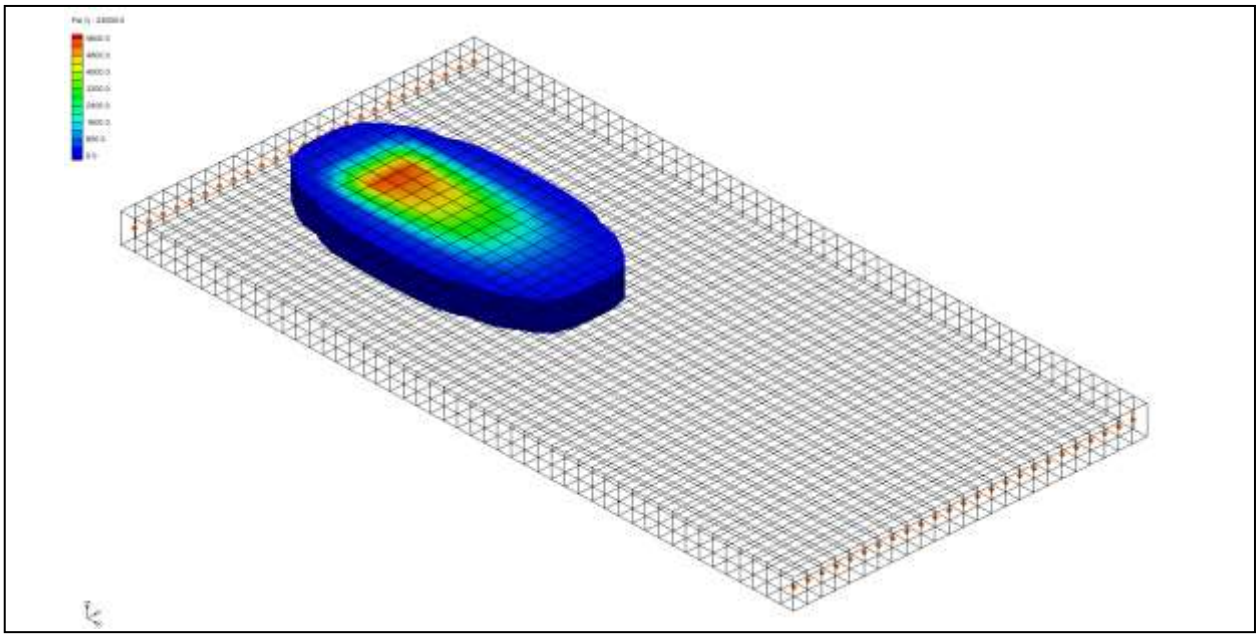
GMS v. 10.5

GMS 10.5 Tutorial

SEAM3D – BTEX



Objectives

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

Prerequisite Tutorials

- MT3DMS – Grid Approach

Required Components

- Grid Module
- Map Module
- MODFLOW
- 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 Biodegration 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.

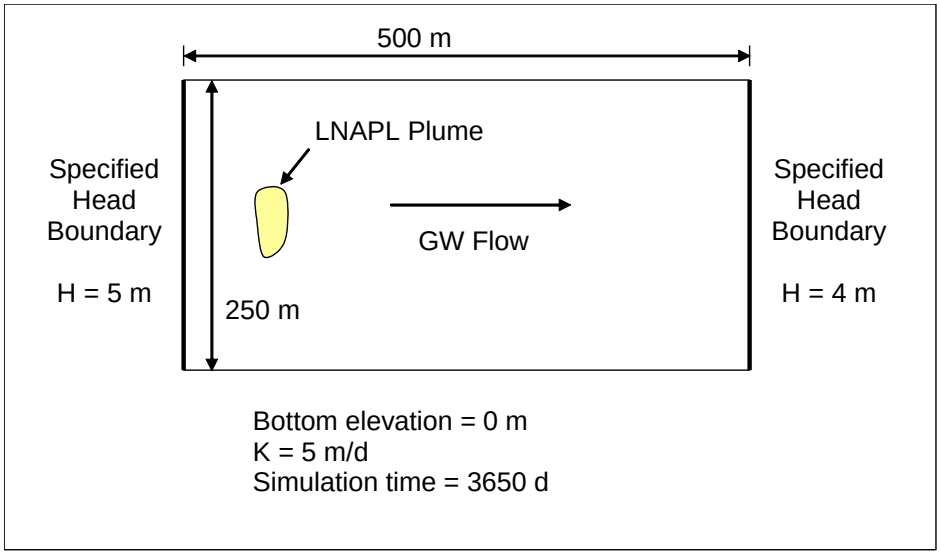

Figure 1 Problem to be solved in SEAM3D tutorial

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).

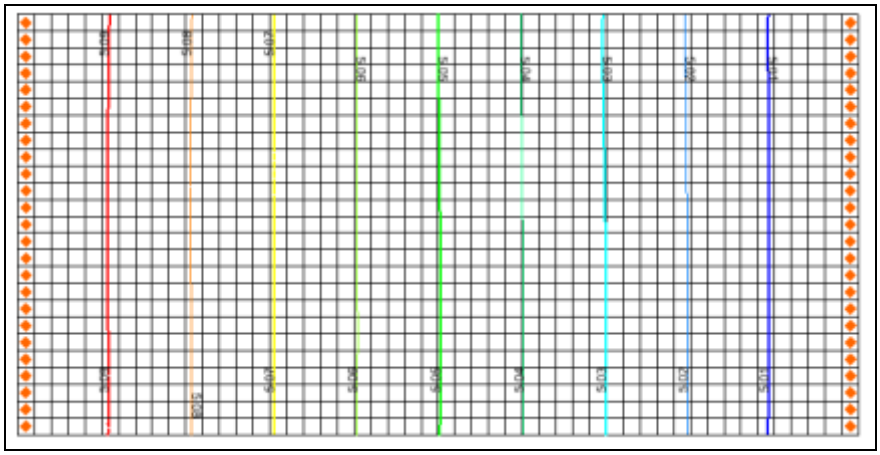

Figure 2 Grid with uniform flow field

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. Make sure the following units are selected:

Length	**m**
Time	**d**
Mass	**g**
Force	**N**
Concentration	**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. Expand the "3D Grid Data" folder.

2. Right-click on the "  grid" item in the Project Explorer.
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 the *Length* of the stress period 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 the *Number of nondegradable tracers* to "1".

2. Change the *Number of hydrocarbon substrates* to "3".
3. In the *Microbial Processes* section, turn on the *Fe(III) reduction* and *Methanogenesis* options.
4. In the *Products to track* section of the dialog, turn on the *Fe(II)* option.

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 the "tracers1" item, and change the name to "MTBE".
6. Double-click the "substrates1" item, and change the name to "Benzene".
7. Double-click the "substrates2" item, and change the name to "TEX".
8. Double-click the "substrates3" item, 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. Enter "182.5" for the *Initial time step size*.
6. Enter "182.5" for the *Maximum time step size*.
7. Enter "3650" for the *Maximum simulation time*.
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 a value of "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. Select *O2* in the spreadsheet then enter a value of "3.0" (mg/L) for the *Starting Conc.(mg/l)*.
2. Select *Fe(II)* in the spreadsheet then enter a value of "0.002" (mg/L) for the *Starting Conc.(mg/l)*.

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. Select the **Longitudinal Dispersivity…** button to open the *Longitudinal Dispersivity* dialog.
3. Select the **Constant → Grid** button to open the *Grid Value* dialog.
4. Enter a value of "5.0".
5. Select **OK** to close the *Grid Value* dialog.
6. Select the **OK** button to exit the *Longitudinal Dispersivity* dialog.
7. Enter a value of "0.1" for the *TRPT* value.
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 select the leftmost column of cells.
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. Change the *Type (ITYPE)* to "constant head (CHD)" in the *All* row; this will 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 *O2* column, enter a concentration of "3.0" (mg/L) in the *All* row.
6. In the *Fe(II)* column, enter a concentration of "0.002" (mg/L) in the *All* row.
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. Select the "Linear isotherm" option in the *Sorption* combo box.

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. Enter "1800000000.0" for *Bulk density*.

4. Enter the following values for *1st sorption const*.

MTBE	3.36e-009
Benzene	3.36e-008
TEX	6.72e-008
Aliphatics	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 the 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. Enter "11" for *I*, "6" for *J*, and "1" for *K* values.

4. Select **OK** to close the *Find Grid Cell* dialog.

5. Drag a rectangle to select a 5x2 rectangular region of cells as shown in Figure 3. The currently selected cell represents the cell in the upper left corner of the grid of cells.

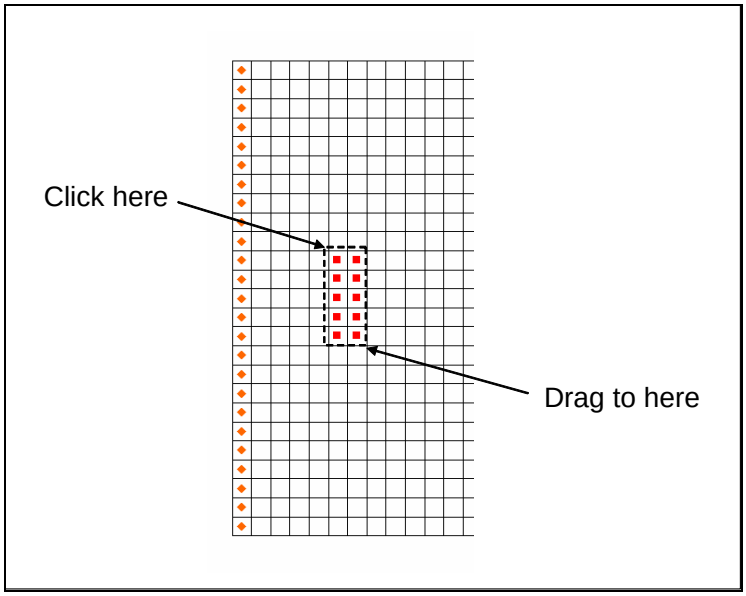

Figure 3 Selecting the cells defining the plume

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. Select the *SEAM3D: NAPL* in the left window.
3. Check the box in the *NAPL* column in the *All* row.
4. Enter a value of "0.001" for the *Initial conc.(mg/l)* for all cells.
5. Enter a value of "0.5" for the *Rate dissolved (1/d*) for all cells.
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 the *Number of tracers in NAPL* value to "1".

3. Change the *Number of hydrocarbons in NAPL* value to "3".

4. At the bottom of the dialog, enter "150" for the *Inert fraction molecular weight*.

5. Enter the values shown in the table for all four species.

	Initial Mass Fraction	*Solubility*	*Molecular Weight*
MTBE	0.04	48.0	88.2
Benzene	0.01	1750.0	78.1
TEX	0.3	250.0	105.0
Aliphatics	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. Enter "2" for *Number of bio steps per transport step*.

3. Enter "0.001" for *Microcolony minimum concentration*.

4. For the *Minimum Concentration* enter the values in the following table for each of the species.

Benzene	0.002
TEX	0.005
Aliphatics	0.1
O2	0.0
Fe(III)	5.0

10.2 Electron Acceptor Coefficients

Next, to enter the electron acceptor data:

1. Select the *Elec. Acc.* tab in the dialog.
2. Enter the following values for *Inhibition coefficient*.

Fe(III)-O2	0.5
Methane-O2	0.2
Methane-Fe	25

3. Enter the following values for *Yield coefficient*.

O2-Benzene	0.4
O2-TEX	0.5
O2-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. Enter "0.10" in the *Product coefficient* value for *Fe(II)*.
3. Enter the following values for the *Methane coefficient*:
   - *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 in the dialog.
2. Enter the following values for the *Electron acceptor use coefficient*:

O2-Benzene	3.1

O2-TEX	3.0
O2-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. Enter a value of "50" for the *Hydro. half saturation constant* for all species except the following:
   - *O2-Benzene*: "15"
   - *O2-TEX*: "10"
   - *Fe(III)-TEX*: "30"
3. Under *Electron acceptor half saturation Constant*, enter "1" for O2.

10.6 Rates

Do as follows to enter the rate data:

1. Select the *Rates* tab.
2. Make sure that, in the *Death rate* portion of the dialog, the *Calculated by model* option is selected.
3. Enter the following values for the *Max. specific rate of substrate utilization*:

O2-Benzene	0.4
O2-TEX	0.5
O2-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. For the *Fe(III)* entry on the list, select the **Edit**... button to open the *Starting Concentration Array* dialog.
3. Select the **Constant → Grid** button to open the *Grid Value* dialog.
4. Enter a value of "50" (mg/kg).
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. Locate and open the directory entitled *BTEX\BTEX*.
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. The solution is imported 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 the **Contour Options** button to open the *Dataset Contour Options – 3D Grid – MTBE* dialog.
2. Change the *Contour method* to "Color fill".
3. Make sure 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. Select the "MTBE" dataset in the Project Explorer.
2. Select the last time step listed in the Project Explorer.

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. Select the *Active Dataset Time Series* option for the plot type.
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 this tutorial. Continue to explore the SEAM3D options or exit the program.