# GMS 7.0 TUTORIALS

# SEAM3D – BTEX

## 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.

### 1.1 Contents

## 1.2 Outline

This is what you will do:

1. Import a MODFLOW model.
2. Define conditions.
3. Run MODFLOW.
4. Run SEAM3D.
5. Create a time series plot.

## 1.3 Required Modules/Interfaces

You will need the following components enabled to complete this tutorial:

- Grid
- Map
- MODFLOW
- SEAM3D

You can see if these components are enabled by selecting the *File* | *Register* command.

 

# 2 Description of Problem

The problem we will be solving 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 ground water and are being transported to the right.

We will 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) and a non-conservative tracer.

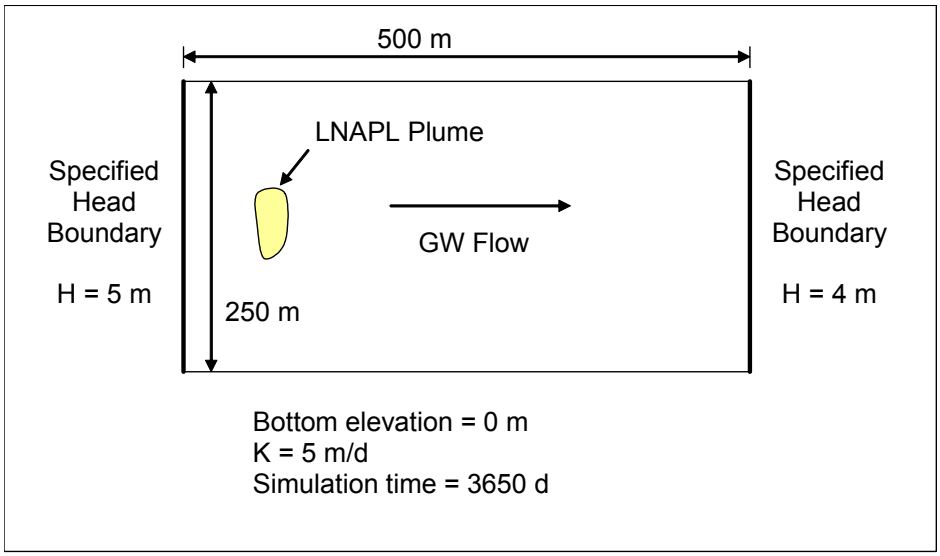


*Figure 1. Problem to be Solved in* SEAM3D *Tutorial.*

# 3 Getting Started

If you have not yet done so, launch GMS. If you have already been using GMS, you may wish to select the *New* command from the *File* menu to ensure the program settings are restored to the default state.

# 4 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 .

 

2. In the *Open* dialog, locate and open the file entitled **tutfiles\SEAM3D\seam3d\flowmod.gpr**

At this point, you should see a grid appear with contours indicating a uniform flow field from the left side to the right side.

# 5 Defining the Units

First of all, we will define the units. The length and time units will already be set by the MODFLOW model. We will specify the mass and concentration units.

1. Select the *Edit* | *Units* command.
2. Select the following units:

| | |
|---|---|
| *Length* | **m** |
| *Time* | **d** |
| *Mass* | **g** |
| *Force* | **N** |
| *Concentration* | **mg/l** |

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

The units we have entered are for convenience only and do not affect the calculations. GMS displays these units next to the input fields to remind us of the proper units for each item. It is still up to the user to enter consistent units.

# 6 Initializing the SEAM3D Simulation

To create a new SEAM3D simulation:

1. Right-click *grid* in the Project Explorer and select the *New MT3D* command.
2. In the *Model* section of the *Basic Transport Package* dialog select the ***SEAM3D*** option.

## 6.1 Setting up the Stress Periods

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

1. Select the *Stress Periods* button.
2. Change the *Length* of the stress period to **3650**.
3. Select the *OK* button to exit the *Stress Periods* dialog.

 

## 6.2 Package Selection

Next, we will select the packages we will be using in the simulation.

1. Select the *Model Setup* button in the *Basic Transport Package* 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.

## 6.3 Defining the Species

Next, we will 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 of the dialog 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 that as we make 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. We will supply more meaningful names to the tracers and hydrocarbons.

5. In the *Names* list, select the *Tracer1* item and change the name to **MTBE**.
6. Select the *Substrate1* item and change the name to **Benzene**.
7. Select the *Substrate2* item and change the name to **TEX**.
8. Select the *Substrate3* item and change the name to **Aliphatics**.
9. Select the *Finish* button.

 

## 6.4 Output Control

We will now edit the *Output Control* data to specify how frequently the solution data should be saved for post-processing. We will save once every 100 days for a total of 20 time steps over the 2000 day simulation.

1. Select the *Output Control* button.
2. Select the *Print or save at specified times* option.
3. Select the *Times* button.
4. Select the *Initialize Values* button.
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.

## 6.5 Entering the Porosity

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

1. Select the *Porosity* button.
2. Select the *Constant* → *Grid* button.
3. Enter a value of **0.25** and select *OK*.
4. Select the *OK* button to exit the *Porosity* dialog.

## 6.6 Starting Concentrations

The mobile species are listed in the lower right corner of the *BTN Package* dialog. We must 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, we must set the starting concentrations of the O2, SO4, and H2S to the correct background values.

1. Select *O2* in the list and select the *Starting Concentration* button.

2. Select the *Constant* → *Grid* button.
3. Enter a value of **3.0** (mg/L) and select the *OK* button.
4. Select the *OK* button to exit the *Starting Concentration* dialog.
5. Repeat this process to enter the following starting concentration:

   Fe(II) = **0.002** mg/L

This concludes the input for the Basic Transport package.

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

# 7 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 and no changes need to be made.

# 8 Dispersion Package

Next, we will 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 *MT3D* | *Dispersion Package* command.
2. Select the *Longitudinal Dispersivity* button.
3. Select the *Constant* → *Grid* button.
4. Enter a value of **5.0** and select *OK*.
5. Select the *OK* button to exit the *Longitudinal Dispersivity* dialog.
6. Enter a value of **0.1** for the *TRPT* value.
7. Select the *OK* button to exit the *Dispersion Package* dialog.

# 9 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 our problem, we have water entering the system on the left side of the model through the specified head boundary. We will enter the correct "background" concentrations for fresh water entering through this boundary.

 

1. Select the *Select j* tool  .
2. Select the leftmost column of cells.
3. Select the *MT3D* | *Point Sources/Sinks* command.
4. Turn on the *Constant head* option for all cells by checking the *All* row for the *Constant head* column.

Once again, the default value is zero. That is the correct value for most of the species. We will change the value for O2 and Fe(II).

5. Select *O2 (mobile)* from the text window containing the species names.
6. Enter a value of **3.0** in the *All* row of the *Constant head* column.
7. Repeat this process to enter a concentration of **0.002** (mg/L) for *Fe(II) (mobile)*.
8. Select the *OK* button to exit the *Point Sources/Sinks* dialog.

## 10 Chemical Reaction Package

Next, we will 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. We will use the *Chemical Reaction* package to simulate retardation due to sorption.

1. Select the *MT3D* | *Chemical Reaction Package* command.
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 O2and CH4. We will enter a non-zero value for Fe(II) and for the two substrates.

3. Enter the values shown in for *Bulk Density* and *1st sorption const*.

 

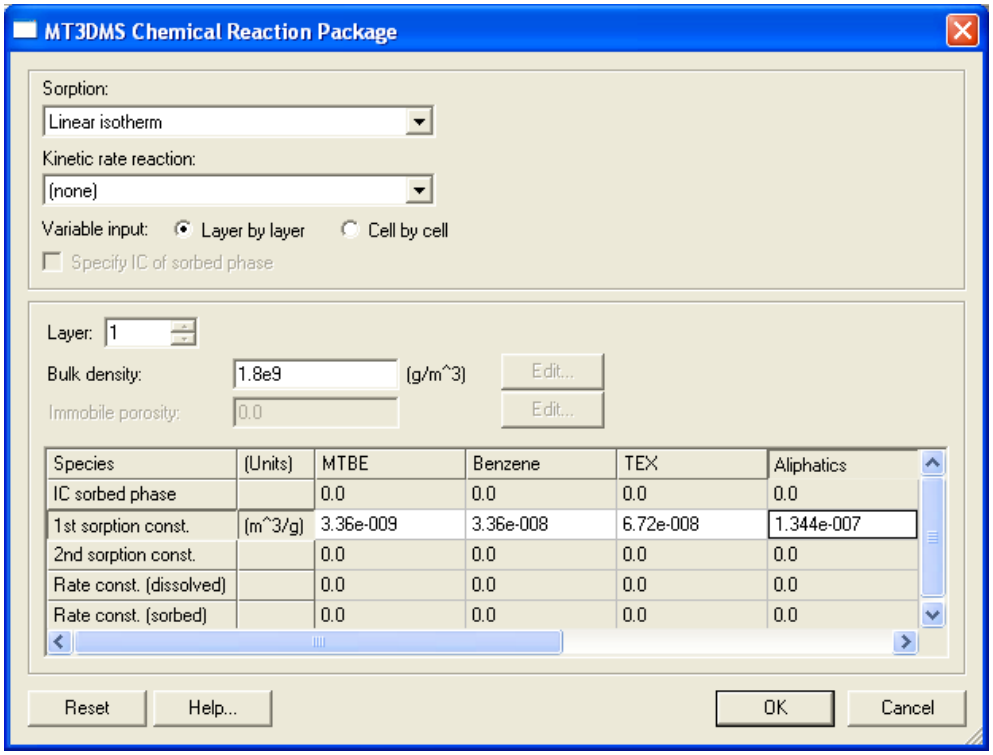


*Figure 2. MT3DMS Chemical Reaction Package dialog.*

4. Select *OK* to exit the *MT3DMS Chemical Reaction Package* dialog.

# 11 NAPL Dissolution Package

We are now ready to enter the data for the *NAPL Dissolution* package. For our problem we must 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, we identify the cells containing the plume and enter the initial concentration and dissolution rate for the contaminants. We also 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 duration of the simulation.

## 11.1 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.
3. Enter **11**, **6**, and **1** for the I, J, K value respectively and select *OK*.

 

4. 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.

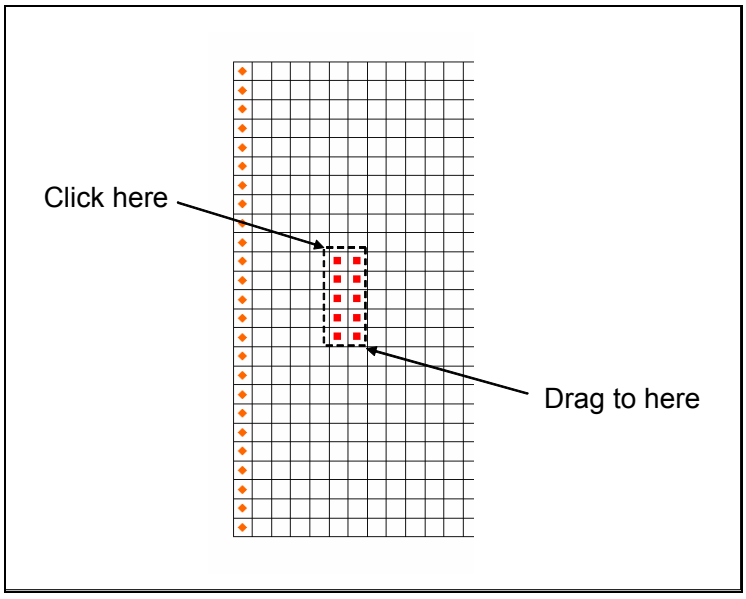


*Figure 3. Selecting the Cells Defining the Plume.*

## 11.2 Assigning the Concentration

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

1. Select the *MT3D* | *Point Sources/Sinks* command.
2. Check the All row in the NAPL column of the lower spreadsheet.
3. Enter a value of **0.001** for the *Initial con.* for all cells
4. Enter a value of **0.5** for the *Dissolution rate* for all cells.
5. Select the *OK* button to exit the *Point Sources/Sinks* dialog.
6. Click anywhere outside the grid to unselect the cells.

## 11.3 Entering the NAPL Data

Finally, we will enter the remaining NAPL plume data using the *NAPL Dissolution Package* dialog.

1. Select the *MT3D* | *NAPL Dissolution Package* command.
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 Figure 4 for all four species.

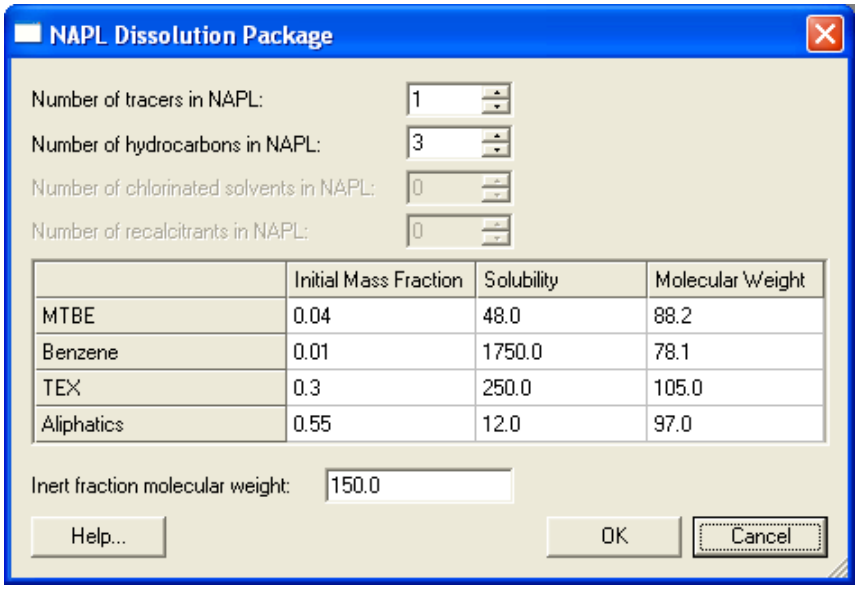


*Figure 4. NAPL Dissolution Package dialog.*

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

# 12 Biodegradation Package

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

1. Select the *MT3D* | *Biodegradation Package* command.

## 12.1 Minimum Concentrations

Notice that the input for the dialog is broken up into a series of property sheets. First, we will enter the data for the minimum concentrations section.

1. Verify that the *Min. Conc.* tab is selected.
2. Enter the values shown in Figure 5 for *Number of bio steps per transport step*, *Microcolony minimum concentration*, and *Minimum Concentration values for the species*.

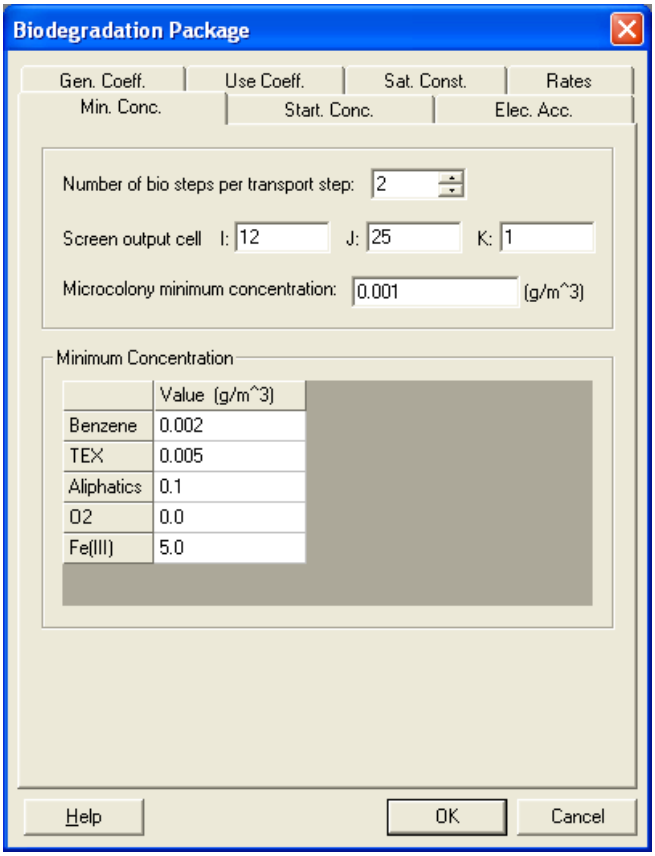


*Figure 5. Biodegradation Package (Min. Conc.) dialog.*

## 12.2 Electron Acceptor Coefficients

Next, we will 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** |

## 12.3 Generation Coefficients

To enter the generation coefficient for H2S:

1. Select the *Gen. Coeff.* tab.
2. Enter **0.10** in the *Production Coefficient* value for *Fe(II)*.
3. Enter the following values for the *Methane Generation Coefficient*:
   - *Benzene*: **0.77**
   - *TEX*: **0.8**
   - Aliphatics: **0.7**

## 12.4 Use Coefficients

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** |

## 12.5 Saturation Constants

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.

## 12.6 Rates

To enter the rate data:

1. Select the *Rates* tab.
2. Make sure that in the *Death Rate* portion of the dialog that 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** |

## 12.7 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:

1. Select the *Start. Conc*. tab.
2. Select *Fe(III)* in the list and select the *Edit…* button.
3. Select the *Constant* → *Grid* button.
4. Enter a value of **50** (mg/kg) and select the *OK* button.
5. Select *OK* to return to the *Biodegradation Package*.
6. Repeat steps 2-5 for the remaining species with the following grid values:

 

| | |
|---|---|
| *Aerobes* | **0.25** |
| *Fe(III) Reducers* | **0.025** |
| *Methanogens* | **0.025** |

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

## 13 Saving the Simulation

At this point, we are ready to save the model and run SEAM3D.

1. Select the *File* | *Save As* command.
2. Select the *Save File* dialog, locate and open the directory entitled **tutfiles\seam3d**.
3. Enter **run1** for the filename.
4. Select the *Save* button to save the files.

## 14 Running MODFLOW

SEAM3D requires the .hff file generated by MODFLOW. Since we saved the project in a different folder than the one where we opened the MODFLOW simulation from, the .hff file does not exist in the new location. We need to rerun MODFLOW so that it will recreate the .hff file in the current folder.

To run MODFLOW:

1. Select the *MODFLOW* | *Run MODFLOW* command.
2. Select *OK* at the prompt if it appears.
3. When the simulation is finished, close the window and return to GMS. The solution is imported automatically.

## 15 Running SEAM3D

To run SEAM3D:

1. Select the *MT3D* | *Run* SEAM3D command.
2. Select *Yes* at the prompt.
3. When the simulation is finished, hit the *Close* button.

 

# 16 Setting the Contouring Options

We will now turn on color shaded contours and set up a color legend.

1. Select the *Contour Options* button .
2. Change the *Contour method* to *Color fill*.
3. Turn on the *Legend* option.
4. Select the *OK* button.

# 17 Viewing the Concentration Contours

First, we will view the conservative tracer solution at 2000 days.

1. Select the *MTBE* data set  in the *Project Explorer*.
2. Select the *Time Steps* list in the *Project Explorer*, select the time step at t=**3650** days

This plot illustrates the concentration contours corresponding to no sorption and no reactions. This is a useful benchmark to consider when viewing the other data sets. To quickly switch between data sets:

3. Click on the *MTBE* data set .

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

4. Use the down arrow key to view the other data sets.

As you view the data sets, note the relationship between the substrates and the electron acceptors. You may wish to use the *Time Steps* list to view the solution at different time steps.

# 18 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 Data Set Time Series" plot.

## 18.1 Creating a Time Series Plot

1. Select the *Plot Wizard* button .
2. Select the *Active Data Set Time Series* option for the plot type.

 

3. Select the *Finish* button.

4. Select a cell in the grid near the contaminant source. Notice that the plot shows the concentration v. time.

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

If you want to take the plot data and put it into Excel you can right click on the plot and select the view values option. This brings up a spreadsheet that you can copy and then paste into Excel.

## 19 Other Viewing Options

At this point, you may wish to experiment with other viewing options. For example, you may also wish to set up an animation using the animation command in the *Data* menu.

## 20 Conclusion

This concludes the tutorial.