GMS TUTORIALS

SEAM3D – Chlorinated Ethenes

SEAM3D also simulates the transport and attenuation of chlorinated ethenes in groundwater systems in which either tetrachloroethene (PCE) or trichloroethene (TCE) are source compounds. Because the rate and extent of the biodegradation of chlorinated ethenes is dependent on the redox condition, SEAM3D is ideally suited to simulate this problem by combining the features of the *Biodegration* package with the *Reductive Dechlorination* package. The source compounds (PCE and/or TCE) serve as electron acceptors, and the daughter products of reductive dechlorination, cis-1,2-dichloroethene (cis-DCE) and vinyl chloride (VC), may serve as either electron acceptors or electron donors. Source terms for chlorinated ethene problems may be implemented using the SEAM3D *NAPL Dissolution* package. This tutorial illustrates how to use these three packages to set up a transport problem for simulating reductive dechlorination under variable redox conditions along the groundwater flowpath.

1 Description of Problem

The site in this problem 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 source is comprised of 15% TCE, 15% non-reactive tracer, 25% biodegradable substrate, and 45% inert substances. The tracer, substrate, and TCE are dissolving into the ground water and are transported downgradient.

We will set up a SEAM3D simulation to simulate TCE degradation in an aerobic aquifer. With the introduction of the substrate, iron-reducing and also methanogenic conditions will develop. The model will include biodegradation, dispersion, and retardation due to sorption. The electron acceptors (oxygen and Fe(III)) and end products (Fe(II) and methane) will be modeled using the *Biodegradation* package. The gradual release of mass from the NAPL plume will be modeled as a source term using the *NAPL Dissolution* package. The degradation of TCE resulting from reductive dechlorination and the subsequent generation and biodegradation of cis-DCE and VC will be modeled using the *Reductive Dechlorination* package.

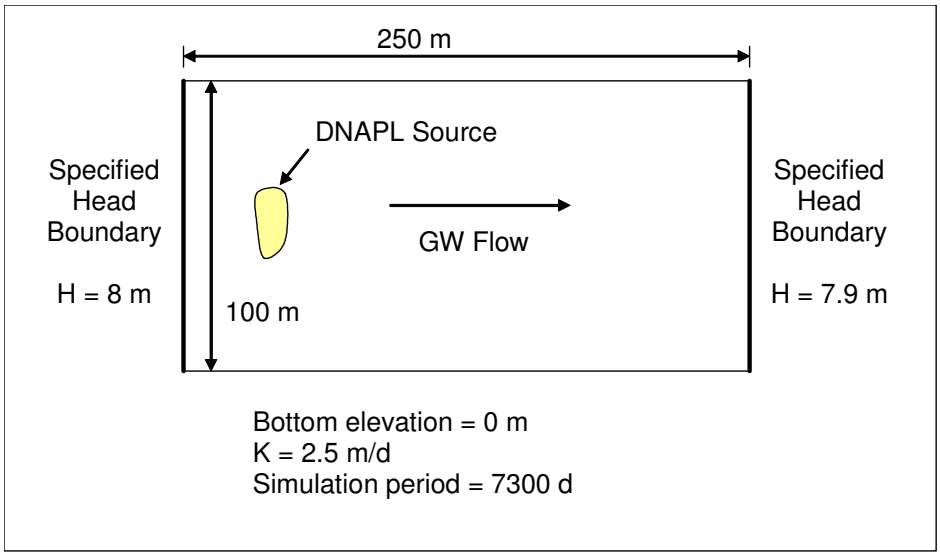

Figure 1-1 Problem to be Solved in SEAM3D *Tutorial.*

2 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.

3 Required Modules/Interfaces

The license registration system used by GMS allows the components of GMS to be licensed individually, depending on the needs of the user. Before continuing, you may wish to check whether or not the GMS components used in this tutorial have been enabled in the copy of GMS you are using. This can be accomplished by selecting the *Register* command in the *File* menu. On the left side of the *Register* dialog, the following components should have "ENABLED" displayed in the *Status* column to the right of each of the following components:

- Grid
- Map
- MODFLOW
- SEAM3D

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\TCE-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. Select the MT3D | New Simulation 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 length of 7300 days. For the transport step size, we will use 36.5 days. 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 **7300**.
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*
- *Reductive dechlorination package*

3. Select the *Next* button.

6.3 Defining the Species

Next, we will define the species used in the simulation.

1. Set the Number of nondegradable tracers to **1**.
2. In the Microbial Processes section of the dialog turn on the Fe(III) reduction and Methanogenesis options.
3. In the Products to track section of the dialog turn on the Fe(II) option.
4. 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 182.5 days for a total of 20 time steps over each 3650-day stress period.

1. Select the *Output Control* button.
2. Enter **20** for the *Print or save at specified interval*.
3. 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 tracer, substrate, chlorinated compounds, ethene, and methane. However, we must set the starting concentrations of the O2, Fe(II), and chloride 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 **4.0** (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 concentrations:

- *Fe(II)* = **0.001** mg/L
- *Chloride* = **0.2** 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 5 m and a transverse (horizontal) dispersivity of 0.50 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 **0.10** 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*, *Fe(II)*, and *Chloride*.

5. Select *O2 (mobile)* from the text window containing the species names.
6. Enter a value of **4.0** in the *All* row of the *Constant head* column.
7. Repeat this process to enter the following concentrations:

- Fe(II) (mobile) = **0.001** mg/L
- *Chloride* = **0.2** mg/L

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.
3. Enter the values shown in Figure 10-2 for *Bulk Density* and *1st sorption const.* values for TCE, DCE, and VC.

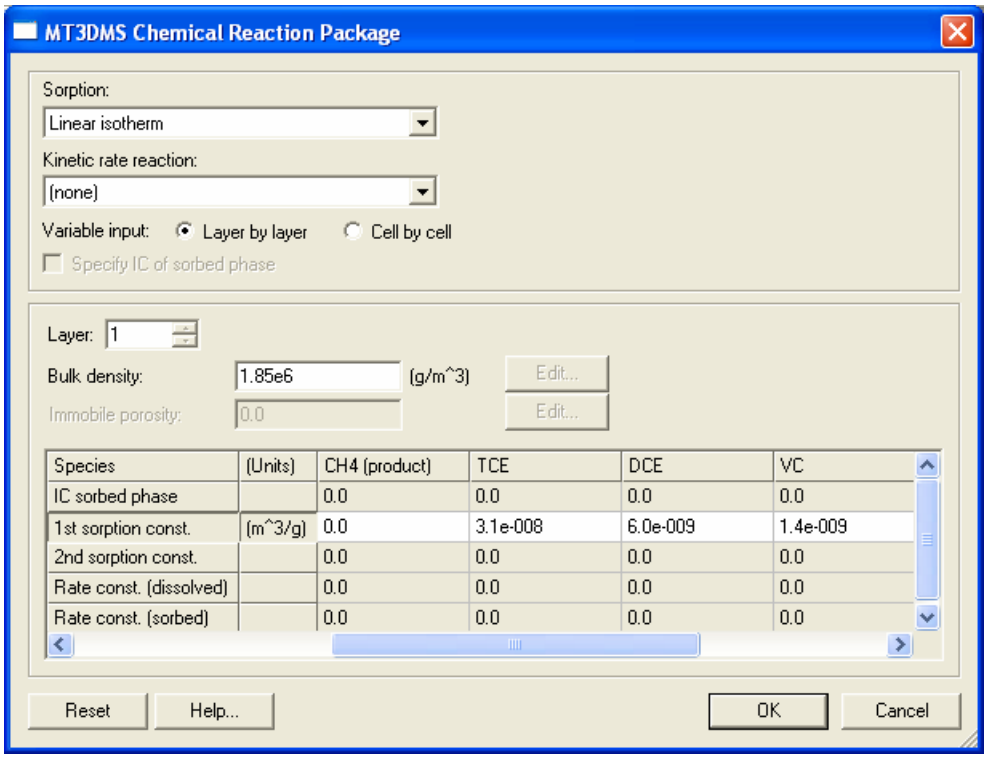

Figure 10-2 MT3DMS Chemical Reaction Package Dialog

4. Select *OK* to exit the *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 NAPL source and enter the initial concentration and dissolution rate. We also enter the initial mass fraction and solubility of *TCE*. 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 **9**, **5**, and **1** for the *I*, *J*, *K* value respectively and select *OK*.

4. Drag a rectangle to select a 4X2 rectangular region of cells as shown in Figure 11-3. The currently selected cell represents the cell in the upper left corner of the grid of cells.

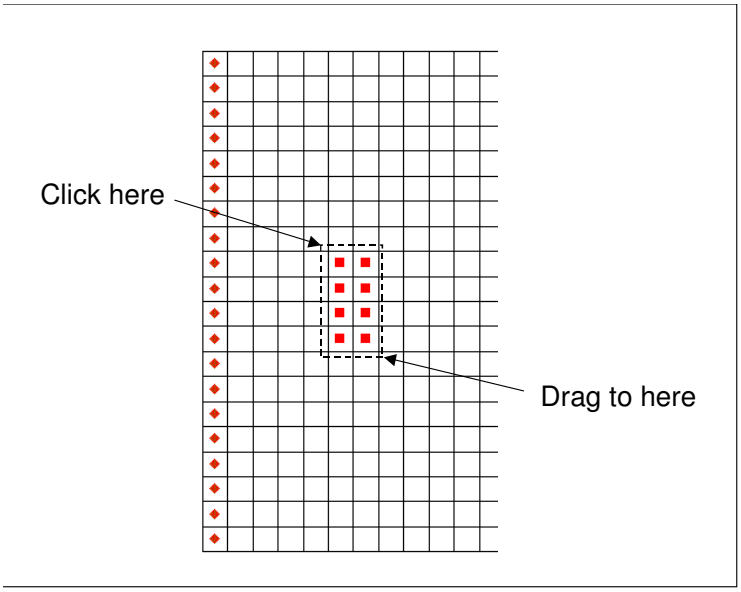

Figure 11-3 Selecting the Cells Defining the Plume.

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 **0.1** for the *Initial conc.* for all cells
4. Enter a value of **1.0** for the *Rate dissolved* 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. Enter the values shown in Figure 10-4.

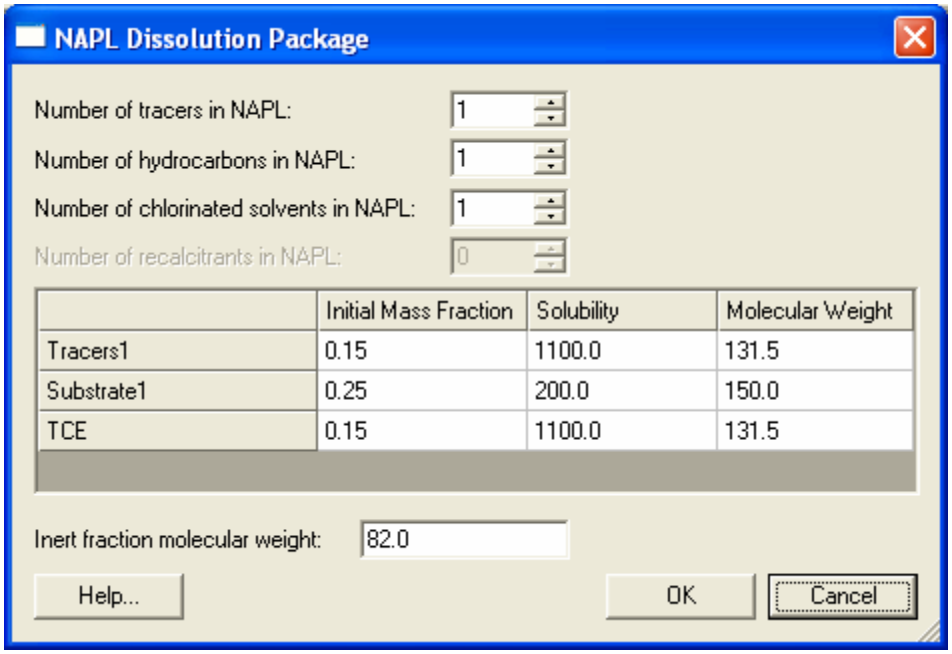

Figure 10-4 NAPL Dissolution Package dialog.

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

12 Biodegradation Package

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

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. The default concentration is zero. This will be the correct starting concentration for *O2* and *Substrate1*.

1. Select the *Min. Conc.* tab.
2. Enter **2** for the *Number of bio steps per transport step*.
3. Enter **0.001** for the *Microcolony minimum concentration*.
4. Enter **5.0** for the *Minimum Concentration of Fe(III)*.

12.2 Electron Acceptor Coefficients

Next, we will enter the Electron Acceptor data.

1. Select the Elec. Acc. tab in the Biodegradation Package dialog.
2. For Inhibition Coefficient enter the following values:

Fe-O2	**0.1**
Methane-O2	**0.1**
Methane-Fe	**25**

3. Enter the following values for the *Yield Coefficient*:

O2-Substrate1	**0.1**
Fe(III)-Substrate1	**0.02**
Methane-Substrate1	**0.01**

12.3 Generation Coefficients

To enter the Generation Coefficient for *Fe(II)* and *Methane*:

1. Select the *Gen. Coeff.* tab.
2. Enter **0.10** in the *Product Coefficient* value for *Fe(II).*
3. Enter **0.7** in the *Methane Coefficient* for *Substrate1*.

12.4 Use Coefficients

To enter the electron acceptor Use Coefficients:

1. Select the *Use Coeff.* tab.
2. Enter the following values for the *Electron Acceptor Use Coefficient*:

- *O2-Substrate1*: **3.5**
- *Fe(III)-Substrate1*: **35**

12.5 Saturation Constants

To enter the Saturation Constants:

1. Select the *Sat.Const.* tab.
2. Enter the following values for the *Hydro. Half Saturation Constant*:

- *O2-Substrate1*: **10**

- *Fe(III)-Substrate1*: **25**
- *Methane-Substrate1*: **50**

3. Enter the following values for the Electron Acceptor Half Saturation Constant:

- *O2*: **1.0**

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 the *Calculated by model* option is selected.
3. Enter the following values for the *Max. Specific Rate of Substrate Utilization*:

- *O2-Substrate1*: **0.5**
- *Fe(III)-Substrate1*: **0.05**
- *Methane-Substrate1*: **0.01**

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 the *Edit…* button next to *Fe(III).*
3. Select the *Constant* → *Grid* button.
4. Enter a value of **50** (mg/kg) and select the *OK* button.
5. Repeat steps 2-4 with the following values.

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

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

13 Reductive Dechlorination Package

The last package to set up is the *Reductive Dechlorination* package. We will enter the reaction parameters controlling the degradation of chlorinated ethenes (TCE, DCE and VC) and production of end products (ethene and chloride).

1. Select the MT3D | Reductive Dechlorination Package command.

13.1 Minimum and Starting 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 and starting concentrations. The default concentration is zero. This will be the correct minimum concentration for the chlorinated compounds, ethane, and chloride.

1. Select the *Concentrations* tab.
2. Enter **0.001** for the *Min. concentration for microbe populations*.
3. Select the *Edit…* button next to *PCE/TCE Reducers* in the *Starting Concentration* list.
4. Select the *Constant* → *Grid* button.
5. Enter a value of **0.25** (mg/kg) and select the *OK* button.
6. Repeat steps 3-5 for *DCE/VC Reducers* with a value of **0.025** (mg/kg).

13.2 Saturation Constants

Direct oxidation will not be simulated in this problem. To enter the saturation constants for reductive dechlorination:

1. Select the Saturation Constants tab.
2. Enter the following values for the Half Sat. Constant for Reductive Dechlorination:

- *TCE*: **10**
- *DCE*: **20**
- *VC*: **15**

13.3 Rates

To enter the Rate data for reductive dechlorination:

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 Reductive Dechlorination*:

- *TCE*: **0.1**
- *DCE*: **0.05**
- *VC*: **0.04**

13.4 Coefficients

The default values for the electron acceptor use and methane generation coefficients are zero. These default values will be used, and no data entry is required for these two parameter sets.

1. Select the *Coefficients* tab.

2. Enter the following values for the *Yield Coefficient*:

- *TCE*: **0.02**
- *DCE*: **0.01**
- *VC*: **0.01**

13.5 Reductive Dechlorination Factors

The chlorinated ethane stoichiometric factors are preset. Lastly, we will enter the chlorinated ethene data.

1. Select the Reductive Dechlorination Factors tab

2. Enter the following values for Chlorinated Ethene Inhibition terms:

TCE-O2	**0.1**
TCE-Fe(III)	**25**
DCE-O2	**0.1**
DCE-Fe(III)	**25**
DCE-TCE	**10**
VC-O2	**0.1**
VC-Fe(III)	**25**
VC-TCE	**10**
VC-DCE	**1**

3. Select the *OK* button to exit the *Reductive Dechlorination Package* dialog.

14 Saving the Simulation

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

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

15 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. When the simulation is finished, close the window and return to GMS. The solution is imported automatically.

16 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.

17 Setting the Contouring Options

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

1. Select the Data | Contour Options command.
2. Change the Contour method to Color fill.
3. Select the Color Ramp button.
4. Turn on the Legend option.

5. Select the OK button twice to exit both dialogs.

18 Viewing the Concentration Contours

First, we will view the Tracer solution at 7300 days.

1. Expand the *tce_run1 (SEAM3D)* folder in the *Project Explorer* and select the *Tracers1* data set .

2. Select the *Time Steps* list in the *Project Explorer*, select the time step at t=**7300** 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 *Tracers1* data set .

This plot (*Tracers1*) represents sorption but no reactions.

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

As you view the data sets, compare the travel distance of the tracer to TCE and the production of DCE, VC, ethane, and chloride, as well as the consumption of electron acceptors and generation of Fe(II) and Methane. You may wish to use the *Time Steps* list to view the solution at the initial and final time step.

19 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.

19.1 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.

20 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.

21 Conclusion

This concludes the tutorial.

