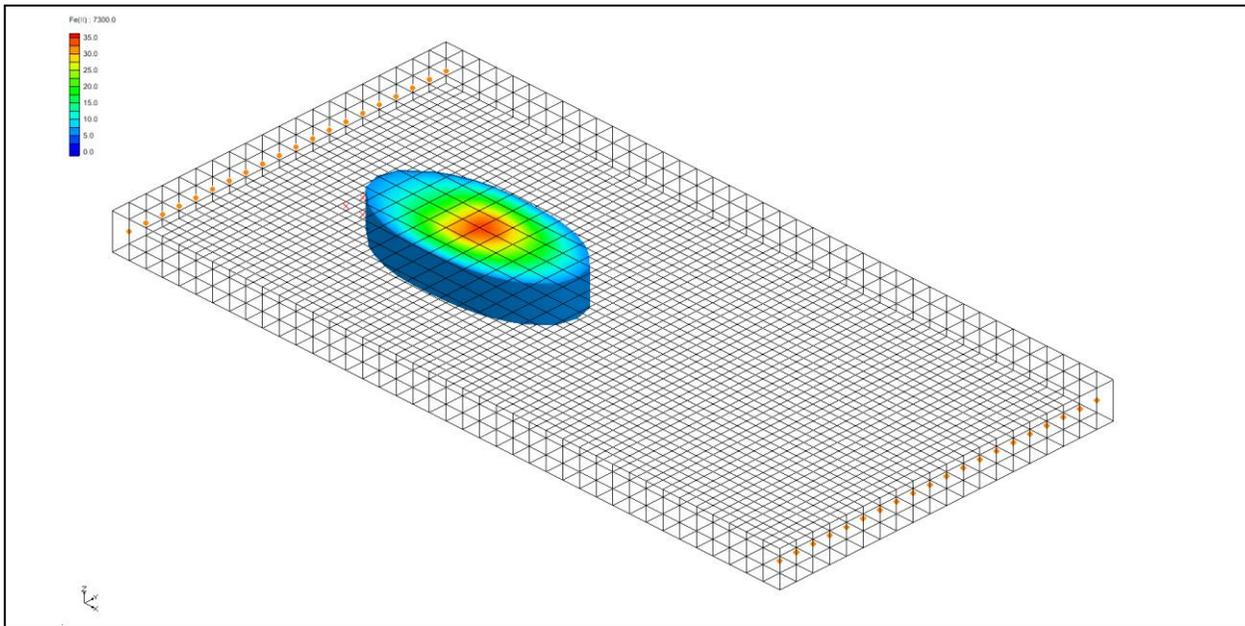


GMS 10.5 Tutorial

SEAM3D – Chlorinated Ethenes



Objectives

This tutorial illustrates how to use the Biodegradation, Reductive Dechlorination, and NAPL Dissolution packages to set up a transport problem for simulating reductive dechlorination under variable redox conditions along the groundwater flowpath.

Prerequisite Tutorials

- MT3DMS – Grid Approach

Required Components

- Grid Module
- Map Module
- MODFLOW
- SEAM3D

Time

- 25–40 minutes



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1 Introduction

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 Biodegradation 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.

The site in the sample 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.

Set up a SEAM3D simulation to simulate TCE degradation in an aerobic aquifer. With the introduction of the substrate, iron-reducing and 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.

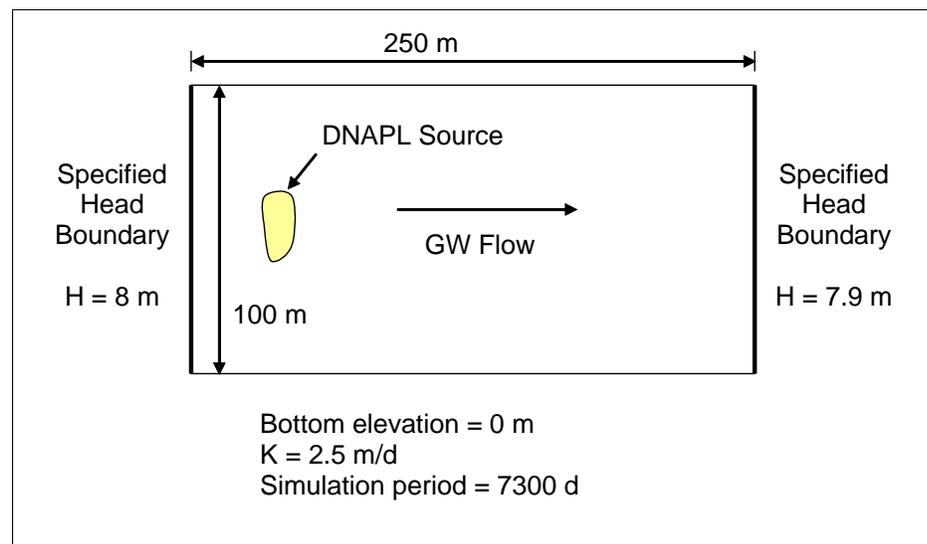


Figure 1 Problem to be solved in SEAM3D tutorial

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. Find the directory entitled *Chlorinated_Ethenes\Chlorinated_Ethenes*.
3. Select the file entitled “tce-flowmod.gpr”.
4. Click **Open** to import the project file and 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.

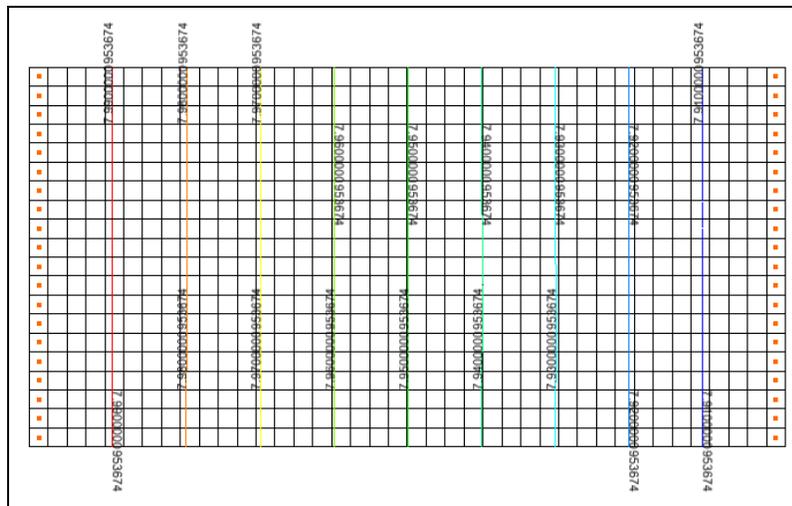


Figure 2 Grid with uniform flow field

3 Defining the Units

The first step is to define the units. The length and time units will already be set by the MODFLOW model, all that is needed is to specify the mass and concentration units.

1. Select the *Edit* / **Units...** command to open the *Units* dialog.
2. Ensure that the following units are selected:

Length	m
--------	---

<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 entered units 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 necessary to enter consistent units.

4 Initializing the SEAM3D Simulation

Do the following to create a new SEAM3D simulation:

1. Expand the “ 3D Grid Data” folder in the Project Explorer.
2. Right-click on the “ grid” item in the Project Explorer and select the **New MT3DMS...** command to open the *Basic Transport Package* dialog.
3. 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 length of 7300 days. For the transport step size, 36.5 days will be used. 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 “7300”.
3. Select the **OK** button to exit the *Stress Periods* dialog.

4.2 Package Selection

Next, select the packages to use in 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*
 - *Reductive dechlorination package*
3. Select the **Next** button to open the *Define Species* dialog.

4.3 Defining the Species

Next, 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 to exist the *Define Species* dialog.

4.4 Output Control

The next step is to edit the Output Control data to specify how frequently the solution data should be saved for post-processing. This tutorial 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 to open the *Output Control* dialog.
2. Enter “20” for *Print or save at specified interval*.
3. 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, do as follows:

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 tracer, substrate, chlorinated compounds, ethene, and methane. However, it's necessary to set the starting concentrations of the O₂, Fe(II), and chloride to the correct background values.

1. Select O₂ in the spreadsheet and enter a value of “4.0” for the *Starting Conc. (mg/l)*.
2. Repeat this process to enter the following *Starting Conc. (mg/l)*:
 - Fe(II) “0.001” mg/L
 - Chloride “0.2” 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, and 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 5 meters and a transverse (horizontal) dispersivity of 0.50 meters. 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. Ensure that a value of “0.10” is entered 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 necessary to enter the correct “background” concentrations for fresh water entering through this boundary.

1. Using the **Select j**  tool, 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. But it is necessary to change the values for *O2*, *Fe(II)*, and *Chloride*.

5. In the *O2* column, enter a concentration of “4.0” (mg/L) in the *All* row.
6. In the *Fe(II)* column, enter a concentration of “0.001” (mg/L) in the *All* row.
7. In the *Chloride* column, enter a concentration of “0.2” (mg/L) in the *All* row.
8. 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. Use 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.
3. Enter “1850000.0” for *Bulk density*.
4. Enter the values in the following table for the 1st *sorption const.*

	1 st <i>sorption const.</i>
TCE	3.1e-008
DCE	6.0e-009
VC	1.4e-009

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. For this problem, 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, identify the cells containing the NAPL source and enter the initial concentration and dissolution rate. Also the initial mass fraction and solubility of TCE will be entered. 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 “9” for *I*, “5” for *J*, and “1” for *K*.
4. Select **OK** to close the *Find Grid Cell* dialog.
5. Drag a rectangle to select a 2x4 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.

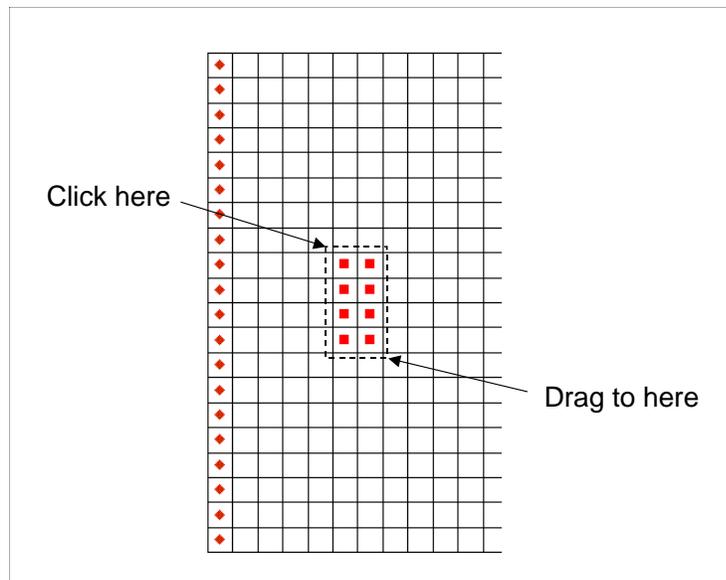


Figure 3 Selecting the cells defining the plume

9.2 Assigning the Concentration

With the plume cells 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 *SEAM3D: NAPL* in the left window.
3. Check the *All* row in the *NAPL* column in the right window.
4. Enter a value of “0.1” for the *Initial conc.(mg/l)* for all cells.
5. Enter a value of “1.0” for the *Rate dissolved (1/d)* for all cells.
6. Select the **OK** button 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. Enter “1” for *Number of tracers in NAPL*, *Number of hydrocarbons in NAPL*, and *Number of chlorinated solvents in NAPL*.

- Enter the values in the following table.

	<i>Initial Mass Fraction</i>	<i>Solubility</i>	<i>Molecular Weight</i>
<i>Tracers1</i>	0.15	1100.0	131.5
<i>Substrate1</i>	0.25	200.0	150.0
<i>TCE</i>	0.15	1100.0	131.5

- Enter “82.0” for the *Inert fraction molecular weight*.
- Select **OK** to exit the *NAPL Dissolution Package* dialog.

10 Biodegradation Package

The next package to set up is the Biodegradation package. It’s necessary to enter the yield coefficients, inhibition coefficients, and other reaction parameters controlling the degradation of the substrate.

- 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. This tutorial will first, enter the data for the *Min. Conc.* section. The default concentration is zero. This will be the correct starting concentration for *O2* and *Substrate1*.

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

10.2 Electron Acceptor Coefficients

Next, to enter the Electron Acceptor data:

- Select the *Elec. Acc.* tab in the *Biodegradation Package* dialog.
- For the *Inhibition coefficient*, enter the following values:

<i>Fe-O2</i>	0.1
<i>Methane-O2</i>	0.1
<i>Methane-Fe</i>	25

- Enter the following values for the *Yield coefficient*:

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

10.3 Generation Coefficients

Do as follows 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*.

10.4 Use Coefficients

Do as follows 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”

10.5 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 value for the *Electron acceptor half saturation Constant*:
 - *O2*: “1.0”

10.6 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”

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. Select the **Edit...** button next to *Fe(III)* 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”.
5. Select the **OK** button to close the *Grid Value* dialog.
6. Select the **OK** button to close the *Starting Concentration Array* dialog.
7. Repeat steps 2–6 with the following values.
 - *Aerobes*: “0.25”
 - *Fe(III) Reducers*: “0.025”
 - *Methanogens*: “0.025”
8. Select the **OK** button to exit the *Biodegradation Package* dialog.

11 Reductive Dechlorination Package

The last package to set up is the Reductive Dechlorination package. It is necessary to 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 *SEAM3D / Reductive Dechlorination Package...* command to open the *Reductive Dechlorination Package* dialog.

11.1 Minimum and Starting Concentrations

Notice that the input for the dialog is broken up into a series of property sheets. This tutorial will first enter the data for the minimum starting concentrations. The default concentration is zero. This will be the correct minimum concentration for the chlorinated compounds, ethane, and chloride.

1. Make sure the *Concentrations* tab is selected.
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 to open the *Starting Concentration Array* dialog.
4. Select the **Constant** → **Grid** button to open the *Grid Value* dialog.
5. Enter a value of “0.25” (mg/kg).
6. Select the **OK** button to close the *Grid Values* dialog.
7. Select the **OK** button to exit the *Starting Concentration Array* dialog.
8. Repeat steps 3–7 for *DCE/VC Reducers* with a value of “0.025” (mg/kg).

11.2 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”

11.3 Rates

Do the following 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, 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”

11.4 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”

11.5 Reductive Dechlorination Factors

The chlorinated ethane stoichiometric factors are preset. The last parameter to enter is 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.

12 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. Enter “TCE-run1” for the *File name*.
3. Select the **Save** button to save the file and exit the *Save As* dialog.

13 Running MODFLOW

SEAM3D requires the HFF file generated by MODFLOW. Since the project has been saved in a different folder than the one where the MODFLOW simulation was opened from, 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 open the *MODFLOW* dialog.
2. When the simulation is finished, select the **Close** button to exit the *MODFLOW* dialog. The solution is imported automatically.

14 Running SEAM3D

To run SEAM3D:

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

15 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 – Tracers1* dialog.
2. Change the *Contour method* to “Color Fill”.
3. Make sure the *Legend* option is on.

4. Select the **OK** button to close the *Dataset Contour Options – 3D Grid – Tracers1* dialog.

16 Viewing the Concentration Contours

1. Expand the “ TCE-run1 (SEAM3D)” folder in the Project Explorer.
2. Select the “ Tracers1” dataset.
3. At the bottom of 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 datasets. To quickly switch between datasets, do the following:

4. Click on the “ Tracers1” dataset.

This plot (“Tracers1”) represents sorption but no reactions.

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

While viewing the datasets, 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. If desired, use the *Time Steps* list to view the solution at the initial and final time step.

17 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.

17.1 Creating a Time Series Plot

1. Select the **Plot Wizard**  button to open the *Plot Wizard* dialog.
2. Select the *Active Dataset Time Series* option for the *Plot Type*.
3. Select the **Finish** button.
4. Using the **Select Cells**  tool, 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 wanting 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.

18 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.

19 Conclusion

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