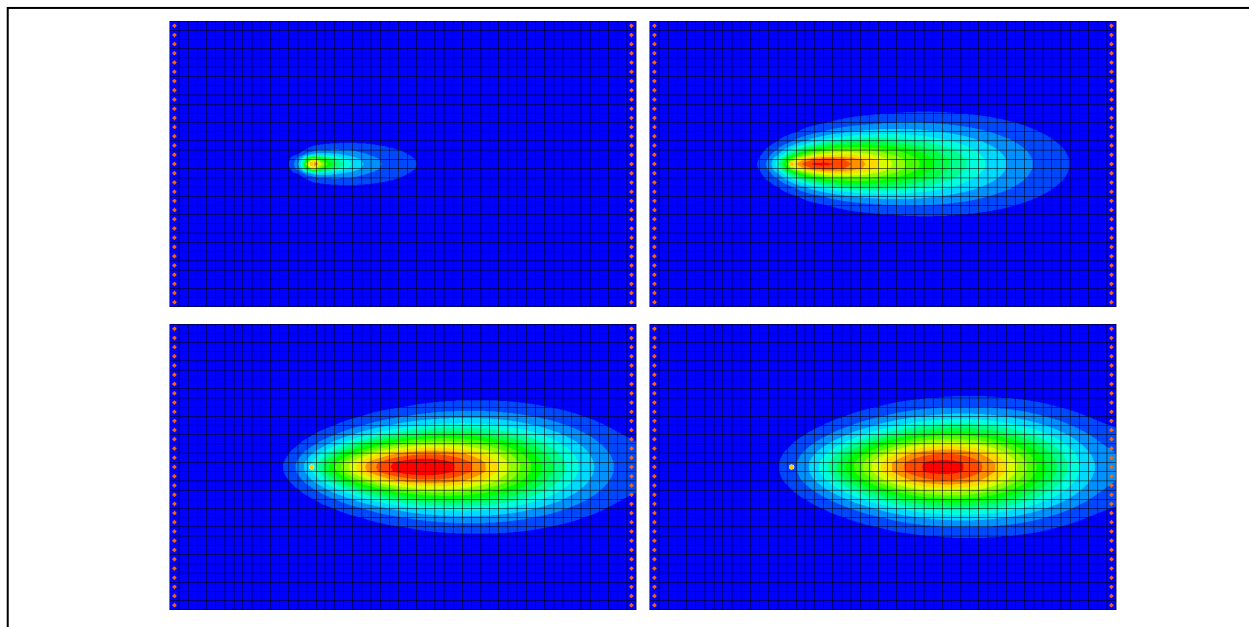*GMS 10.4 Tutorial*

RT3D – Sequential Anaerobic Degradation: PCE → TCE → DCE → VC

Objectives

Illustrate the steps involved in modeling sequential anaerobic degradation of tetrachloroethene (PCE) using the RT3D model.

Prerequisite Tutorials	Required Components	Time
• RT3D – Instantaneous Aerobic Degradation	• Grid Module • MODFLOW • RT3D	• 10–25 minutes

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1   Introduction

This tutorial will use the problem described below. It will start with importing a MODFLOW model. Then the RT3D inputs and boundary conditions will be defined followed by running simulations for both MODFLOW and RT3D. Finally, a time series plot will be created to review the results.

1.1   Description of Problem

The problem in this tutorial is similar to the problem described in the "RT3D – Instantaneous Aerobic Degradation" tutorial. The site is a 510 m x 310 m section of a confined aquifer with a flow gradient from left to right. An underground storage tank is leaking fuel hydrocarbon contaminants at 2 m^3/day at the location shown. Concentration of tetrachloroethene (PCE) is 1000 mg/L. This high hypothetical concentration was selected to simulate a plume with considerable PCE mass and with a relatively low injection flow rate. Initial levels of PCE and its degradation products in the aquifer are assumed to be 0.0 mg/L. The tutorial will simulate a continuous spill event and compute the resulting PCE, trichloroethene (TCE), dichloroethene (DCE), and vinyl chloride (VC) contours after two years.

The first part of the problem will be to import a previously computed MODFLOW flow model of the site. Using this flow field, RT3D will then define a reactive transport model.

1.2 Description of Reaction

The reaction being simulated is anaerobic PCE dechlorination with sequential, first-order, degradation kinetics. Degradation of PCE all the way to VC is assumed to be anaerobically favorable and the degradation kinetics are assumed to be first order in nature.

$$PCE \rightarrow TCE \rightarrow DCE \rightarrow VC$$ .... (1)
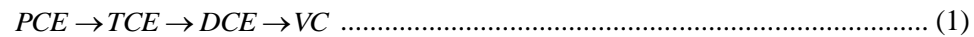
The following set of equations describes the reaction kinetics framework:

$$r_{PCE} = -k_1[PCE]$$ .... (2)

$$r_{TCE} = k_1 Y_{TCE/PCE}[PCE] - k_2[TCE]$$ .... (3)

$$r_{DCE} = k_2 Y_{DCE/TCE}[TCE] - k_3[DCE]$$ .... (4)

$$r_{DCE} = k_3 Y_{VC/DCE}[DCE] - k_4[VC]$$ .... (5)

Kinetic Constants (to be manually entered):

Constant	Value	Designation
k_1	0.005 day^{-1}	PCE anaerobic constant
k_2	0.003 day^{-1}	TCE anaerobic constant
k_3	0.002 day^{-1}	DCE anaerobic constant
k_4	0.001 day^{-1}	VC anaerobic constant

The following constants (yields in mg/mg basis) are fixed internally:

Constant	Value	Designation
$Y_{TCE/PCE}$	0.7920	TCE:PCE stoichiometric yield
$Y_{DCE/TCE}$	0.7377	DCE:TCE stoichiometric yield
$Y_{VC/DCE}$	0.6445	VC:DCE stoichiometric yield

1.3 Getting Started

Do the following to get started:

1. If GMS is not running, launch GMS.

2. If GMS is already running, select the *File* | **New** command to ensure the program settings are restored to the default state.

2 Importing the MODFLOW Model

The first part of the 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 *File* | **Open** command to bring up the *Open* dialog.

2. Navigate to *flowmod\flowmod*.

3. Select the file entitled "flowmod.gpr".

4. Click **Open** to import the project file and exit the *Open* dialog.
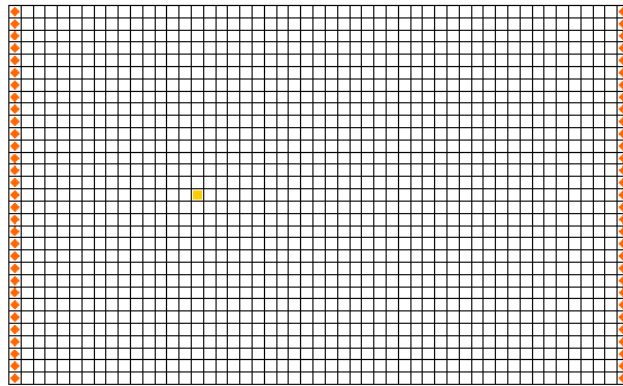
At this point, a grid will appear.

*Figure 1   The MODFLOW grid*

3   Building the Transport Model

Now that the flow model is imported, the next step is to perform the RT3D simulation. For this part of the simulation, select the reaction, define the reaction data, define the supplemental layer data needed by RT3D, and assign concentrations to the well.

4   Initializing the Model

The first step is to initialize the RT3D data.

1. In the Project Explorer, expand the " 3D Grid Data" folder.

2. Right-click on the " grid" item.

3. Select the **New MT3DMS…** command from the pop-up menu to open the *Basic Transport Package* dialog.

5   The Basic Transport Package

The next step is to initialize the data in the Basic Transport Package. First, it is necessary to select RT3D as the transport model and to select the appropriate packages.

1. In the *Model* section, select the *RT3D* option.

2. Select the **Packages…** button to open the *MT3DMS/RT3D Packages* dialog.

3. Turn on the following packages:

   - *Advection package*

   - *Dispersion package*

   - *Source/sink mixing package*

   - *Chemical reaction package*

4. For the *RT3D reactions* drop-down menu, select the "Sequential Decay Reactions" option.

5. Select the **OK** button to exit the *MT3DMS/RT3D Packages* dialog.

5.1   Starting Concentrations

Note that in the *Layer Data* section of the dialog, the species associated with the reaction being modeled are listed by name. The next step is to define the starting concentration for each of these species. By default, all of the starting concentrations are zero. Since the aquifer is assumed to be initially clean, simply accept the default values for starting concentrations.

5.2   Porosity

Next, consider the porosity, which should be set as 0.3. Since this is the default supplied by GMS, no changes need to be made.

5.3   Stress Periods

The next step is to define the stress periods. Since the injection rate of the well and the other boundary conditions do not change, a single stress period will be used.

1. Select the **Stress Periods…** button to open the *Stress Periods* dialog.

2. Enter a value of "730" for the *Length*.

3. Enter a value of "10" for the *Num time steps*.

4. Select the **OK** button to exit the *Stress Periods* dialog.

5.4   Output Options

The next step is to define the output options. One binary solution file is created by RT3D for each of the species. By default, RT3D saves a solution at each transport step for each species. Since this results in large files containing more solutions than needed for the

simple post-processing, it would be better to specify that a solution be saved every 73 days (every time step).

1. Select the **Output Control…** button to open the *Output Control* dialog.

2. Select the *Print or save at specified times* button.

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 "73.0" for the *Initial time step size*.

6. Enter "73.0" for the *Maximum time step size*.

7. Enter "730.0" 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.

This completes the input for the Basic Transport package.

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

6   The Advection Package

The next step is to initialize the data for the Advection package.

1. Select the *RT3D |* **Advection Package…** command to open the *Advection Package* dialog.

2. In the *Solution scheme* drop-down menu, select "Standard finite difference method".

3. Select the **OK** button to close the *Advection Package* dialog.

7   The Dispersion Package

The next step is to enter the data for the Dispersion package. The aquifer has a longitudinal dispersivity of 10.0 m and a transverse (horizontal) dispersivity of 3.0 m. The vertical dispersivity is not used since this is a one layer model.

1. Select the *RT3D |* **Dispersion Package…** command to open the *Dispersion Package* dialog.

2. Enter a value of "0.3" for the *TRPT* value.

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 a value of "10.0".

6. Select **OK** to exit 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.

8   The Source/Sink Mixing Package

Next, to define the concentration at the spill location:

1. Using the **Select Cells** 🔲 tool, select the cell containing the injection well (spill location) by clicking anywhere in the interior of the cell.

2. Select the *RT3D* | **Point Sources/Sinks…** command to open the *MODFLOW/RT3D Source/Sinks* dialog.

3. Click the **Add BC** button near the bottom of the dialog.

4. Change the *Type (ITYPE)* to "well (WEL)".

5. In the *PCE* column, enter a concentration of "500" (mg/L).

6. Select the **OK** button to exit the *MODFLOW/RT3D Source/Sinks* dialog.

9   The Chemical Reaction Package

Next, to initialize the chemical reaction package and define appropriate reaction rate constants:

1. Select the *RT3D* | **Chemical Reaction Package…** command to open the *RT3D Chemical Reaction Package* dialog.

2. In the *Reaction Parameters* section, change the *Kpce* value to "0.005".

3. Set the value of *Ktce* to "0.003".

4. Set the value of *Kdce* to "0.002".

5. Set the value of *Kvc* to "0.001".

6.   Select the **OK** button to exit the *RT3D Chemical Reaction Package* dialog.

10   Run MODFLOW

Before running RT3D, it is necessary to regenerate the MODFLOW solution.

1.   Select the *File |* **Save As…** command to open the *Save As* dialog.

2.   Enter "rtmod" for the *File name*.

3.   Select the **Save** button to save the files and exit the *Save As* dialog.

To run MODFLOW:

4.   Select the *MODFLOW |* **Run MODFLOW** command to launch the *MODFLOW* simulation.

5.   When the *MODFLOW* simulation is finished, select the **Close** button to exit the *MODFLOW* dialog.

The MODFLOW solution is imported and displayed as contours on the grid.

11   Running RT3D

It is now possible to save the model and run RT3D.

To run RT3D:

1.   Select the *RT3D |* **Run RT3D…** command to launch the *RT3D* simulation.

2.   Select **Yes** at the prompt to save the changes.

3.   When the *RT3D* simulation is finished, select the **Close** button to exit the *RT3D* dialog.

GMS automatically reads in the RT3D solution.

12   Viewing the Results

1.   Select the " PCE" dataset from the Project Explorer. (if needed, expand the "rtmod (RT3D)" solution)

2.   Select the "730.0" time step from the *Time Steps Window*.

To view color-fill contours:

3. Select the **Contour Options** ▣ button to open the *Dataset Contour Options – 3D Grid – PCE* dialog.

4. Change the *Contour method* to "Color Fill".

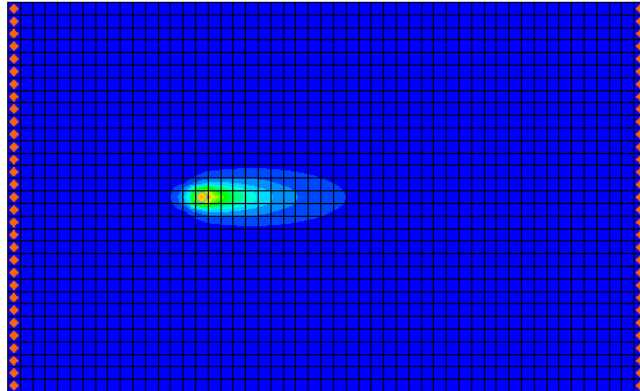5. Select the **OK** button to exit the *Dataset Contour Options – 3D Grid – PCE* dialog.

Figure 2   The PCE solution at 730 days

Next, view the other solutions at 730 days.

6. Select the "▤ TCE" dataset from the Project Explorer. If necessary, select the 730.0 time step from the *Time Steps Window*.

7. Select the "▤ DCE" dataset from the Project Explorer.

8. Select the "▤ VC" dataset from the Project Explorer.

12.1   Creating a Time Series Plot

Another highly effective tool for viewing RT3D solutions is a time series plot. A time series plot is used to display the variation of concentration vs. time for one or more species at a particular point in the model.

1. Select the **Plot Wizard** ▥ macro to open the *Plot Wizard*.

2. Select the *Active Dataset Time Series* option.

3. Select the **Finish** button to close the *Plot Wizard* and open a plot window.

4. Use the **Select Cells** ▥ tool to select any cell in the grid downstream from the contaminant source.

5. The plot now shows the variation of *VC* concentration vs. time at the specified location in the grid. To view the concentrations for any contaminant at a

different location, change the active dataset in the Project Explorer and the selected grid cell.
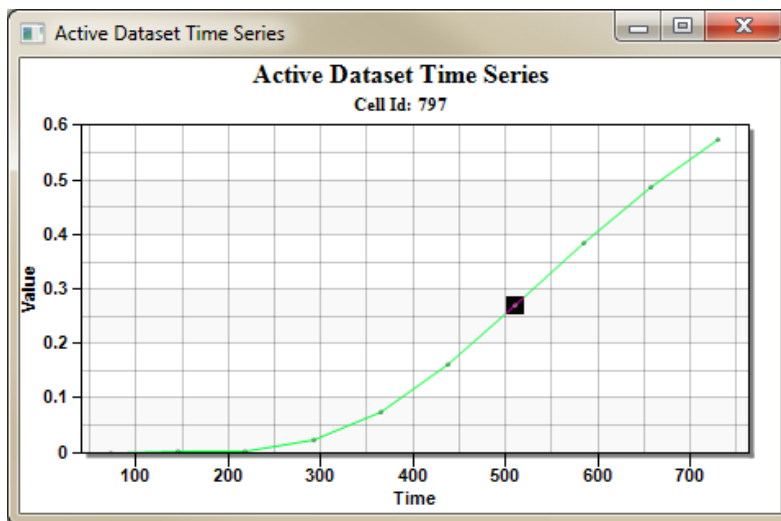

Figure 3   Active dataset time series plot for the VC solution

12.2   Other Post-Processing Options

At this point, feel free to experiment with the other post-processing options, including film loop animation.

13   Conclusion

This concludes the tutorial. Continue to explore the RT3D model or exit the program.