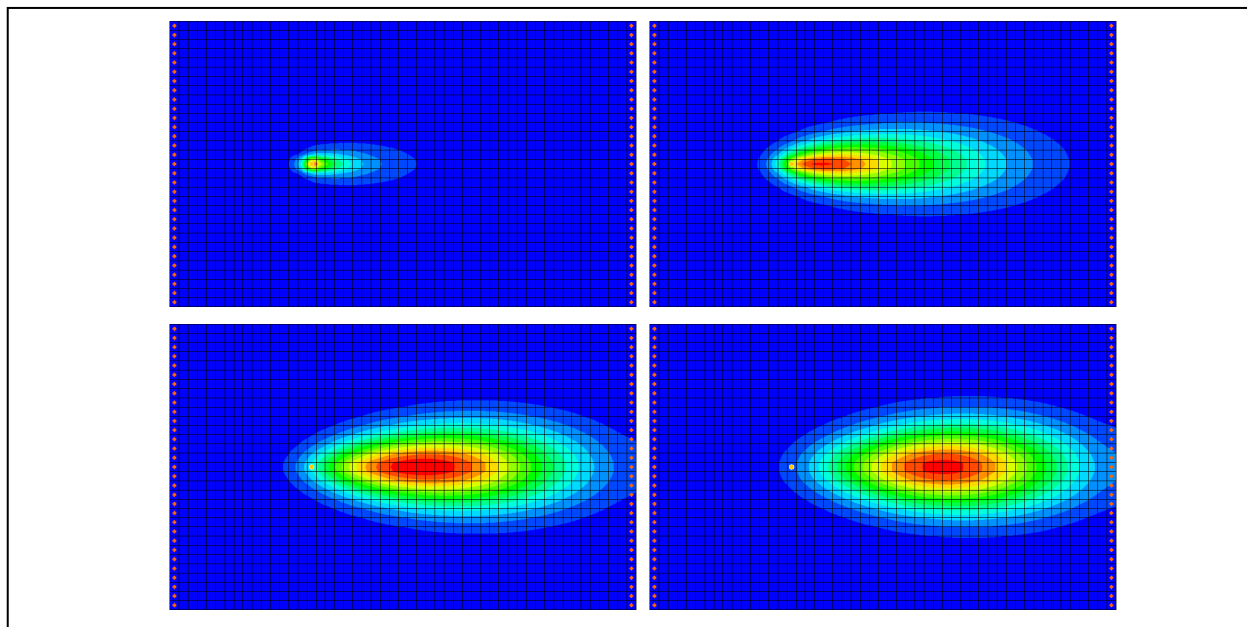*GMS 10.1 Tutorial*

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

Objectives

Illustrates the steps involved in modeling sequential anaerobic degradation of PCE using the RT3D model.

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

AQUAVEO™

1   Outline

Here are the steps for this tutorial:

1. Import a MODFLOW model.

2. Define RT3D inputs and boundary conditions.

3. Run MODFLOW.

4. Run RT3D.

5. Create a time series plot.

2   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 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, TCE, DCE and 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.

3   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.

$$PCE \rightarrow TCE \rightarrow DCE \rightarrow VC \quad \text{..} \quad (1)$$

The following set of equations describes the reaction kinetics framework:

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

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

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

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

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

4   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.

5   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.

2. In the *Open* dialog, locate the directory entitled *Tutorials\RT3D\flowmod.*

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

4. Click **Open**.

At this point, a grid should appear.

6   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.

7   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 MT3D** command from the pop-up menu.

8   The BTN 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 *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 *Packages* dialog.

8.1   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.

8.2   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.

8.3   Stress Periods

Next, define the stress periods. Since the injection rate and the boundary conditions do not change, use a single stress period with a length of 730 days (two years).

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.

8.4   Output Options

Finally, 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 are needed for the simple post-processing the tutorial intends to do, 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.

9   The Advection Package

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

1. Select the *RT3D |* **Advection Package** command.

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

3. Select the **OK** button.

10   The Dispersion Package

Next, 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.

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**.

7. Select the **OK** button to exit the *Longitudinal Dispersivity* dialog.

8. Select the **OK** button to exit the *Dispersion Package* dialog.

11   The Source/Sink Mixing Package

Next, define the concentration at the spill location. Assign a concentration of 1000 mg/L for PCE and leave TCE, DCE, and VC concentrations at the default value of 0.0

1. 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.

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 dialog.

12   The Chemical Reaction Package

Next, 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 K_{pce} value to "0.005".

3. Set the value of K_{tce} to "0.003".

4. Set the value of K_{dce} to "0.002".

5. Set the value of K_{vc} to "0.001".

6. Select the **OK** button.

13   Run MODFLOW

Before running RT3D, regenerate the MODFLOW solution.

1. Select the *File* | **Save As** command.

2.   In the *Save As* dialog, locate and open the directory entitled
     Tutorials\RT3D\pce1.

3.   Enter "rtmod" for the file name.

4.   Select the **Save** button to save the files.

To run MODFLOW:

5.   Select the *MODFLOW |* **Run MODFLOW** command.

6.   When the simulation is finished, select the **Close** button.

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

14   Running RT3D

At this point, it is time to save the model and run RT3D.

To run RT3D:

1.   Select the *RT3D |* **Run RT3D** command.

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

3.   When the simulation is finished, select the **Close** button.

GMS automatically reads in the RT3D solution.

15   Viewing the Results

First, view the PCE solution at 730 days.

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 dialog.

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.

15.1   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.

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

3. Select the **Finish** button.

4. Select the **Select Cell** 🔳 tool.

5. Select any cell in the grid downstream from the contaminant source.

6. 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.

15.2   Other Post-Processing Options

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

16   Conclusion

This concludes the tutorial.