

GMS 7.0 TUTORIALS

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

This tutorial illustrates the steps involved in modeling sequential anaerobic degradation of PCE using the RT3D model. Since the flow model used in this simulation is the same as the flow model used in *RT3D – Instantaneous Aerobic Degradation*, the steps involved in building the flow model will not be described in this tutorial. A pre-defined version of the flow model will be used.

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1.2 Outline

This is what you will do:

1. Import a MODFLOW model.
2. Define conditions.
3. Run MODFLOW.
4. Run RT3D.
5. Create a time series plot.

1.3 Required Modules/Interfaces

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

- Grid
- MODFLOW
- RT3D

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

2 Description of Problem

The problem we will be solving in this tutorial is similar to the problem described in the first tutorial (*RT3D – Instantaneous Aerobic Degradation*). 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 m³/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) 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. We 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, a reactive transport model will then be defined using RT3D.

3 Description of Reaction

The reaction we will be simulating 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.



The following set of equations describes the reaction kinetics framework.

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

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

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

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

Kinetic Constants (to be input by the user):

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

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.

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 and open the file entitled
tutfiles\RT3D\flowmod\flowmod.gpr.



At this point, you should see a grid 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, we will 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  item.
2. Right-click on the grid  and select the *New RT3D* command from the pop-up menu.

8 The BTN Package

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

1. In the *Model* section, select the *RT3D* option.
2. Select the *Packages* button.
3. Turn on the following packages:
 - *Advection package*
 - *Dispersion package*
 - *Source/Sink Mixing package*
 - *Chemical reaction package*
4. For the *RT3D reactions*, 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 we are modeling 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, we will simply accept the default values for starting concentrations.

8.2 Porosity

Next, we will define the porosity as 0.3. Since this is the default supplied by GMS, no changes need to be made.

8.3 Stress Periods

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

1. Select the *Stress Periods* button.
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, we will 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 we need for the simple post-processing we intend to do, we will specify that a solution be saved every 73 days (every time step).

5. Select the *Output Control* button.
6. Select the *Print or save at specified times* button.
7. Select the *Times* button.
8. Select the *Initialize Values* button.
9. Enter **73.0** for the *Initial time step size*.
10. Enter **73.0** for the *Maximum time step size*.
11. Enter **730.0** for the *Maximum simulation time*.
12. Select the *OK* button to exit the *Initialize Time Steps* dialog
13. Select the *OK* button to exit the *Variable Time Steps* dialog.
14. Select the *OK* button to exit the *Output Control* dialog.

This completes the input for the Basic Transport package.

15. 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 *MT3D | Advection Package* command.
2. Select the *Standard finite difference method* solution scheme.
3. Select the *OK* button.

10 The Dispersion Package

Next, we will 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 *MT3D | Dispersion Package* command.
2. Enter a value of **0.3** for the *TRPT* value.
3. Select the *Longitudinal Dispersivity* button.
4. Select the *Constant* → *Grid* button.
5. Enter a value of **10.0** and select *OK*.
6. Select the *OK* button to exit the *Longitudinal Dispersivity* dialog.
7. Select the *OK* button to exit the *Dispersion Package* dialog.

11 The Source/Sink Mixing Package

Next, we will initialize the Source/Sink Mixing package and define the concentration at the spill location. We will 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 *MT3D | Source/Sink Mixing Package* command.
2. In the *Initialize point source/sinks from MODFLOW* section, select the *Well* button.
3. Using the horizontal scroll bar below the spreadsheet section, scroll over until the *PCE* column is visible.

4. Change the *PCE* value to **1000.0**.
5. Select the *OK* button to exit the *Source/Sink Mixing Package* dialog.

12 The Chemical Reaction Package

Next, we will initialize the chemical reaction package and define appropriate reaction rate constants.

1. Select the *MT3D | Chemical Reaction Package* command.
2. In the *Reaction Parameters* section, change the K_{pce} value to **0.005**.
3. Likewise, 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, we will regenerate the MODFLOW solution.

1. Select the *File | Save As* command.
2. In the *Save As* dialog, locate and open the directory entitled **tutfiles\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, close the window.

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

14 Running RT3D

At this point, we are ready to save the model and run RT3D.


To run RT3D:

1. Select the *MT3D* | *Run RT3D* command.
2. Select *Yes* at the prompt to save your changes.
3. When the simulation is finished, select the *Close* button.


GMS automatically reads in the RT3D solution.

15 Viewing the Results




First, we will view the PCE solution at 730 days.

1. Select the *PCE* data set  from the *Project Explorer*. (You may need to 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.
4. Change the *Contour method* to **Color Fill**.
5. Select the *OK* button to exit the *Contour Options* dialog.

Next, we will view the other solutions at 730 days.

6. Select the *TCE* data set  from the *Project Explorer*.
7. If necessary, select the **730.0** time step from the *Time Steps Window*.
8. Select the *DCE* data set  from the *Project Explorer*.
9. Select the *VC* data set  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 Data Set Time Series* option.
3. Select the *Finish* button.
4. Select the *Select Cell* tool .

5. Select any cell of the grid
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, you may wish to experiment with the other post-processing options, including film loop animation. This concludes the tutorial.