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RT3D Tutorials for GMS Users

T. P. Clement
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Printed in the United States of America

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PNNL-11805
February, 1998

RT3D Tutorials for GMS Users

By

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By Battelle

ACKNOWLEDGEMENTS

Funding Support

Funding support for RT3D code development research efforts was, in part, provided by the office of Technology Development, within the Department of Energy's Office of Environmental Management, under the "Plume Focus Area" and the "Subsurface Contamination Focus Area." The RT3D code was originally developed for the Remediation Technology Development Forum (RTDF) with the support from a DOE project that provided microbial characterization research and groundwater-modeling support to the bioremediation of chlorinated solvents consortium of the RTDF.

The Department of Defense Groundwater Modeling System (GMS) was developed by the Engineering Computer Graphics Laboratory of Brigham Young University in partnership with the U.S. Army Engineer Waterways Experiment Station.

Technical Support for RT3D Development Work

Dr. T. Prabhakar Clement, principal investigator of the RT3D project at PNNL, developed the initial concepts and design for the RT3D computer code. Dr. Clement also coded this version of RT3D (v1.0) from MT3D_DoD_1.5 (a public domain version of MT3D developed by Dr. Chunmiao Zheng at the University of Alabama). Several researchers at PNNL and other organizations provided technical support during various phases of this project: Dr. Yunwei Sun, Department of Chemical Engineering at Washington State University, provided debugging and coding support for developing a prototype version and a pre-processor MT2RT; Dr. Brian S. Hooker, Pacific Northwest National Laboratory, provided support for developing reaction expressions for hydrocarbon and chlorinated solvent degradation models; Christian D. Johnson, Pacific Northwest National Laboratory provided documentation and code testing support; Dr. James N. Petersen, Department of Chemical Engineering at Washington State University, provided debugging support for developing a prototype version and MT2RT; Dr. Chunmiao Zheng, Department of Geology, University of Alabama, provided support for solving MT3D (DoD_1.5) interfacing problems. In addition, Dr. Clement also benefited from helpful discussions with several other researchers-- suggestions of Dr. Ashok Chilakapati (at PNNL), Dr. Rodney Skeen (at PNNL), and Dr. Norman Jones (at BYU) are particularly acknowledged.

NOTICE:

The RT3D(v1.0) code is provided without any warranty. No author or distributor accepts any responsibility to anyone for the consequences of using it or for whether it serves any particular purpose.

For recent updates:

Visit:

<http://etd.pnl.gov:2080/bioprocess/rt3d.htm>

<http://www.ecgl.byu.edu/software/gms/gms.html>

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Introduction

RT3D (Reactive Transport in 3-Dimensions) is a computer code that solves coupled partial differential equations that describe reactive-flow and transport of multiple mobile and/or immobile species in a three dimensional saturated porous media. RT3D was developed from the single-species transport code, MT3D (DoD_1.5, 1997 version). As with MT3D, RT3D also uses the USGS groundwater flow model MODFLOW for computing spatial and temporal variations in groundwater head distribution.

This report presents a set of tutorial problems that are designed to illustrate how *RT3D* simulations can be performed within the Department of Defense Groundwater Modeling System (*GMS*). *GMS* serves as a pre- and post-processing interface for *RT3D*. *GMS* can be used to define all the input files needed by *RT3D* code, and later the code can be launched from within *GMS* and run as a separate application. Once the *RT3D* simulation is completed, the solution can be imported to *GMS* for graphical post-processing.

RT3D v1.0 supports several reaction packages that can be used for simulating different types of reactive contaminants. Each of the tutorials, described below, provides training on a different *RT3D* reaction package. Each reaction package has different input requirements, and the tutorials are designed to describe these differences. Furthermore, the tutorials illustrate the various options available in *GMS* for graphical post-processing of *RT3D* results. Users are strongly encouraged to complete the tutorials before attempting to use *RT3D* and *GMS* on a routine basis.

1.1 Other Documents

There are several other documents describing *GMS* and *RT3D*. The *GMS Reference Manual* is a complete reference on *GMS* and includes a chapter describing the *RT3D* interface. The *RT3D Reference Manual* provides a detailed discussion of the equations, numerical methods, file formats, and other issues related to the *RT3D* model.

In addition to the *GMS* and *RT3D* manuals, the *GMS Tutorials* document contains a set of tutorials similar to the tutorials described in this document. These tutorials describe basic operation of *GMS* and include tutorials on *MODFLOW*, *MT3D*, *MODPATH*, *FEMWATER*, and *SEEP2D*. While it is not essential, it is recommended that the new user complete the *MODFLOW* and *MT3D* tutorials before beginning the *RT3D* tutorials contained in this document. The *GMS Tutorials* document does not contain *RT3D* tutorials. All *RT3D* tutorials are contained in this document.

1.2 Organization

The first tutorial (*Chapter 2 - Instantaneous Aerobic Degradation*) includes a description of how to build both the flow and the transport model within *GMS*. The remaining tutorials use a pre-defined flow model and only describe the construction of the transport model. Although the tutorials may be completed in any order, it is generally best to complete the first tutorial before attempting to complete any of the remaining tutorials.

1.3 Demo vs. Normal Mode

GMS utilizes a copy protection system wherein different components of the *GMS* interface may be licensed and activated separately. Modules and interfaces that have been licensed are enabled using the *Register* command in the *File* menu. The icons for the unlicensed modules or the menus for model interfaces are dimmed and cannot be accessed.

GMS provides two modes of operation: demo and normal. In normal mode, the modules and interfaces you have licensed are undimmed and fully functional and the items you have not licensed are dimmed and inaccessible. In demo mode, all modules and interfaces are undimmed and functional regardless of which items have been licensed. However, all of the print and save commands are disabled. While some of the tutorials in the *GMS Tutorials* document can be completed in demo mode, all of the tutorials in this document must be completed in normal mode.

Instantaneous Aerobic Degradation

This tutorial illustrates the steps involved in performing a reactive transport simulation using the *RT3D* model. *RT3D* is a modified version of *MT3D* that can be used to perform multi-species reactive transport modeling. Several types of reactions can be simulated with *RT3D*. The reaction simulated in this tutorial is instantaneous aerobic degradation of hydrocarbons.

2.1 Description of Problem

The problem we will be solving in this tutorial is shown in Figure 2.1. 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 hydrocarbons is 1000 mg/L and the spill may be assumed to be devoid of oxygen. Details of the aquifer hydrology and geometry are given below. Initial levels of hydrocarbon and oxygen in the aquifer are 0.0 and 9.0 mg/L, respectively. We will simulate a continuous spill event and compute the resulting hydrocarbon and oxygen contours after one year using instantaneous degradation kinetics.

The first part of the problem will be to compute a flow model of the site using *MODFLOW*. Using the flow field computed by *MODFLOW*, a reactive transport model will be then be defined using *RT3D*.

Figure 2.1 Sample Problem to be Modeled with RT3D.

2.2 Description of Reaction

The reaction model we will be using simulates the instantaneous degradation of fuel hydrocarbons under aerobic conditions based on the following reaction (benzene basis):

Therefore, the mass ratio of benzene to oxygen, F , is 3.08. The instantaneous removal of either contaminant (H) or oxygen (O) is dictated by the following algorithm, where t refers to a particular time step:

$$H(t+1) = H(t) - O(t) / F \text{ and } O(t+1) = 0, \text{ when } H(t) > O(t) / F \dots\dots (2.2)$$

$$O(t+1) = O(t) - H(t) \cdot F \text{ and } H(t+1) = 0, \text{ when } O(t) > H(t) \cdot F \dots\dots (2.3)$$

Given this algorithm, either hydrocarbon or oxygen concentration in a given grid cell will be reduced to zero at each time step, depending on which component is stoichiometrically limiting in the prior time step.

2.3 Launching GMS

Before launching *GMS*, you should have installed *GMS*. If you have not yet installed *GMS*, please do so before continuing.

To launch the PC version of *GMS*:

Select the *GMS* shortcut from the Programs in the Start menu (Windows 95, Windows NT 4.0), or double-click on the *GMS* icon in the *GMS* program group (Windows 3.1).

To launch the Unix version of *GMS*:

1. Bring up an xterm window.
2. Change to the directory containing the *GMS* executable.
3. Type **gms** at the command line.

2.4 Required Modules/Interfaces ---

This tutorial utilizes the following components of the *GMS* interface:

- The *3D Grid* module
- The *MODFLOW* interface
- The *RT3D* interface

You can confirm whether each of these components has been enabled on your copy of *GMS* by selecting the *Register* command from the *File* menu. If you have licensed and enabled each of the listed items on your version of *GMS*, you can proceed to complete the tutorial in normal mode. If not, you will need to obtain an updated password or hardware lock before continuing.

2.5 Building the MODFLOW Model ---

The first part of the simulation is to build a *MODFLOW* flow model. In this case, a steady state flow model will be used with the transport simulation.

2.5.1 Conceptual Model Approach vs. Grid Approach ---

In many cases, the most efficient way to create a *MODFLOW* simulation is to build a conceptual model of the site using the feature objects in the *Map* module. However, since this problem is a simple rectangular model, we will use the grid approach and edit values directly on the cells.

2.5.2 Creating the Grid

The first step in defining the *MODFLOW* simulation is to create a single layer grid.

1. Switch to the *3D Grid Module* .
2. Select the *Create Grid* command in the *Grids* menu.
3. In the *X dimension* section, enter 510 for the length and 51 for the number of cells.
4. In the *Y dimension* section, enter 310 for the length and 31 for the number of cells.
5. In the *Z dimension* section, enter 1 for the number of cells (the length in Z does not matter).
6. Select the *OK* button.

At this point, you should see a grid appear.

2.5.3 The Basic Package

The next step is to define the data in the *MODFLOW* Basic Package. First, we will initialize the *MODFLOW* data.

1. Select the *Basic Package* command from the *MODFLOW* menu.
2. Select the *New* button.
3. In the *Time Units* section, select the *Days* option.

Next, we will define an initial condition of 100 m everywhere in the grid.

1. Select the *Starting Heads* button.
2. Select the *Constant -> Grid* button.
3. Select *OK* at the prompt.
4. Enter a value of 100.
5. Select the *OK* button.
6. Select the *OK* button to exit the *Starting Heads* dialog.

We need to change some values in the IBOUND array to designate the constant head boundaries. However, we will do this later by selecting the cells and using the *Cell Attributes* command. Thus, we are finished with this dialog.

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

2.5.4 The BCF Package

Next, we will define the data in the BCF package. First, we will select the steady state option.

1. Select the *BCF Package* command from the *MODFLOW* menu.
2. Select the *Steady State* option.

Next, we will define the layer data. Since we have one confined layer, the only value we need to enter is transmissivity.

1. In the *Layer* section, select the *Confined* option.
2. Select the *Transmissivity* button.
3. Select the *Constant -> Grid* button.
4. Enter a value of 500.
5. Select the *OK* button.
6. Select the *OK* button to exit the *Transmissivity* dialog.

The rest of the default options in the package should be sufficient.

Select the *OK* button to exit the *BCF Package* dialog.

2.5.5 Defining the Spill Well

The spill will be simulated by defining an injection well at the location of the spill with a small injection rate. During the transport simulation, a concentration will be assigned to the well. To define the well:

1. Select the *Select Cell* tool .
2. While watching the I,J fields in the *Edit Window*, locate and select the cell at I=16, J=16, K=1.
3. Select the *Point Sources/Sinks* command from the *MODFLOW* menu.

4. Select the *Add* button in the *Well* section.
5. Enter a value of 2.0 for *Q*.
6. Select the *OK* button to exit the *Point Source/Sink* dialog.

2.5.6 Assigning the Head BC

The final step before running *MODFLOW* is to assign the constant head boundary conditions on the left and right sides of the model. First, we will assign the head BC on the left side.

1. Select the *Select J* tool .
2. Select the leftmost column in the grid by clicking in any of the cells in the column.
3. Select the *Cell Attributes* command in the *MODFLOW* menu.
4. Enter -1 for the *IBOUND* value and leave the *Starting Head* at 100.0.
5. Select the *OK* button.

Next, we will assign the head BC on the right side.

1. Select the rightmost column in the grid by clicking in any of the cells in the column.
2. Select the *Cell Attributes* command in the *MODFLOW* menu.
3. Enter -1 for the *IBOUND* value and enter 99 for the *Starting Head* value.
4. Select the *OK* button.

2.5.7 Running MODFLOW

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

1. Select the *Save Simulation* command from the *MODFLOW* menu.
2. At the top of the dialog, enter "flowmod" for the prefix.
3. To the right of the prefix, select the *Update* button.
4. At the top of the dialog, select the *File Browser* button .

5. In the *Save File* dialog, locate and open the directory entitled *gms/tutorial/rt3d/btexins1*.
6. Select the *Save* button to exit the *Save File* dialog.
7. Select the *Save* button to save the files.

To run *MODFLOW*:

1. Select the *Run MODFLOW* command from the *MODFLOW* menu.
2. Select *OK* at the prompt.
3. When the simulation is finished, select the *Yes* button to return to *GMS*.

2.5.8 Viewing the Results

Next, we will read in the computed head file and view the head contours to ensure the validity of the solution.

1. Select the *Data Browser* command from the *Data* menu.
2. Select the *Import* button on the left side of the dialog.
3. Select the *MODFLOW scalar file* option and select *OK*.
4. Select and open the file titled "flowmod.hed".
5. Select the *Done* button to exit the *Data Browser*.

To turn on the display of contours:

1. Select the *Display Options* command in the *Display* menu.
2. Turn on the *Layer Contours* option.
3. Select the *OK* button.

You should see a series of contours indicating a flow from left to right.

2.6 Building the Transport Model

Now that the flow model is established, 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.

2.6.1 The BTN Package

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

1. Select the *Basic Transport Package* command from the *MT3D/RT3D* menu.
2. Select the *New* button.
3. Select the *RT3D* option.
4. Select the *Packages* button.
5. Select the *Advection Package*, the *Source/Sink Mixing Package*, the *Dispersion Package*, and the *Chemical Reaction Package*.
6. For the reaction type, select the *Inst. Aerobic Deg. of BTEX* option.
7. Select the *OK* button to exit the *Packages* dialog.

Note that in the *Starting Concentration* 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. This is the correct concentration for BTEX. For oxygen, we will define an ambient concentration of 9.0 mg/L.

1. Select the *Oxygen* species in the list above the *Starting Concentration* button.
2. Select the *Starting Concentration* button.
3. Select the *Constant -> Grid* button.
4. Enter a value of 9.0 and select *OK*.
5. Select the *OK* button to exit the *Starting Concentration* dialog.

Next, we will define the layer parameters. The aquifer is a uniform horizontal aquifer with a top elevation of 10 m, a thickness of 10 m, and a porosity of 0.3.

1. Select the *HTOP* button.
2. Select the *Constant -> Grid* button.
3. Enter a value of 10 and select *OK*.

4. Select the *OK* button to exit the *HTOP* dialog.
5. Select the *Thickness* button.
6. Select the *Constant -> Grid* button.
7. Enter a value of 10 and select *OK*.
8. Select the *OK* button to exit the *Thickness* dialog.
9. Select the *Porosity* button.
10. Select the *Constant -> Grid* button.
11. Enter a value of 0.3 and select *OK*.
12. Select the *OK* button to exit the *Porosity* dialog.

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.

Since there is already one stress period by default, we will simply change the length of the stress period

1. Enter a value of 730 for the *Length*.
2. Enter a value of 10 for the *No. of time steps*.
3. Select the *OK* button to exit the *Stress Periods* dialog.

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).

1. Select the *Output Control* button.
2. Select the *Print at specified times* button.
3. Select the *Times* button.
4. Select the *Initialize Values* button.
5. Enter 73.0 for the *Initial time step size*.

6. Enter 73.0 for the *Maximum delta time step*.
7. Enter 730.0 for the *Maximum simulation time*.
8. Select the *OK* button to exit the *Variable Time Steps* dialog.
9. Select the *OK* button to exit the *Output Control* dialog.

This completes the input for the Basic Transport package.

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

2.6.2 Assigning Concentrations to the Left Boundary

The left boundary of the model is a constant head boundary. Since the head at the left boundary is greater than the head at the right boundary, the left boundary acts as a source and water enters the model from the left. Thus, we must define the concentrations of our species at the left boundary. Otherwise, the water entering the model will have the default concentration (zero) for each of the species. This is often true for most species, but there are exceptions. For our model, the incoming fluid should have an ambient oxygen concentration of 9.0 mg/L. The oxygen concentration can be assigned one of two ways:

1. The cells at the boundary can be marked as specified concentration cells by changing the ICBUND value at the cells to -1.
2. The concentration of the incoming fluid at the boundary can be defined using the Source/Sink Mixing package.

The first method requires the fewest number of steps to set up. As long as the boundary acts as a source throughout the simulation, either of these approaches will achieve the same result. However, if the boundary acts as a sink during any part of the simulation, the second option should be used. With the second option, if the boundary switches to a sink due to changing heads in the interior of the model, the concentrations at the cells would be computed by RT3D. With the first option, the concentrations at the cells are fixed, regardless of the flow direction.

For our problem, the flow field is steady state and we know that the boundary acts as a source. Thus, we will use the first option. To mark the cells as specified concentration cells:

1. Select the *Select Cell* tool .
2. Select the cells on the left boundary by dragging a box that just surrounds the cells.

3. Select the *Cell Attributes* command in the *MT3D/RT3D* menu.
4. Change the *ICBUND* value to -1.
5. Select the *OK* button.

Note that we do not need to assign a value, since the values are already assigned via the starting concentration arrays.

2.6.3 The Advection Package

The next step is to initialize the data for the Advection package. We will be using the MOC method. Since this is the default method, no changes need to be made.

2.6.4 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 dispersivity of 3.0 m. The vertical dispersivity is assumed equal to the longitudinal dispersivity.

1. Select the *Dispersion Package* command in the *MT3D/RT3D* menu.
2. Select the *Longitudinal Dispersivity* button.
3. Select the *Constant -> Grid* button.
4. Enter a value of 10.0 and select *OK*.
5. Select the *OK* button to exit the *Longitudinal Dispersivity* dialog.
6. Enter a value of 0.3 for the *Ratio of the transverse dispersivity to long. dispersivity* value.
7. Select the *OK* button to exit the *Dispersion Package* dialog.

2.6.5 The Source/Sink Mixing Package

Next, we will initialize the Source/Sink Mixing package and define the concentration at the spill location.

1. Select the *Source/Sink Mixing Package* command in the *MT3D/RT3D* menu.
2. In the *Initialize Point Source/Sinks from MODFLOW* section in the lower right corner of the dialog, select the *Well* button.

At this point, the concentrations at the well can be edited directly from this dialog or by exiting the dialog and selecting the cell containing the well and selecting the *Point Source/Sink* command. Since there is only one well, the easiest approach in this case is to edit the concentration in this dialog. We will assign a concentration of 1000 mg/L for the BTEX and leave the oxygen at the default value of 0.0.

1. Using the horizontal scroll bar below the spreadsheet section, scroll over until the BTEX column is visible.
2. Change the BTEX value to 1000.0.
3. Select the *OK* button to exit the *Source/Sink Mixing Package* dialog.

2.6.6 The Chemical Reactions Package

The next step is to initialize the data for the Chemical Reactions package. In this case, the default values are adequate and no changes are necessary.

2.6.7 Running RT3D

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

1. Select the *Save Simulation* command from the *MT3D/RT3D* menu.
2. At the top of the dialog, enter "btexmod" for the prefix.
3. To the right of the prefix, select the *Update* button.
4. At the top of the dialog, select the *File Browser* button .
5. In the *Save File* dialog, locate and open the directory entitled *gms/tutorial/rt3d/btexins1/*.
6. Select the *Save* button to exit the *Save File* dialog.
7. Select the *OK* button to save the files.

To run *RT3D*:

1. Select the *Run RT3D* command from the *MT3D/RT3D* menu.
2. Select *OK* at the prompt.
3. When the simulation is finished, return to *GMS*.

2.6.8 Viewing the Results

Now, we will read in the concentration files and view the results. A separate concentration file is created by RT3D for each of the species. A data set super file containing the names of the concentration files is also created. All of the concentration files can be read at once simply by opening this file.

1. Select the *Open* command from the *File* menu.
2. Select and open the file titled "btexmod.dss".
3. Select the *Data Browser* command in the *Data* menu.

Note that all of the species names are listed in the *Data Browser*. Each species is saved to a separate data set file. The *.dss file is a "data set super file" which contains the names of each of the species files. By reading in the *.dss file, we effectively read in all of the files at once.

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

1. Select the *Oxygen* data set.
2. Scroll down and select the time step at $t=730$ days.
3. Select the *Done* button to exit the *Data Browser*.

To get a better plot of the concentration contours:

1. Select the *Contour Options* command in the *Data* menu.
2. Select the *Color fill between contours* option.
3. Select the *Color Ramp Opts* button.
4. Select the *Show color legend* option.
5. Select the *OK* button to exit the *Color Ramp Options* dialog.
6. Select the *OK* button to exit the *Contour Options* dialog.

Next, we will view the BTEX solution at 730 days.

1. Select the *Data Browser* command from the *Data* menu.
2. Select the *BTEX* data set.
3. Scroll down and select the time step at $t=730$ days.
4. Select the *Done* button to exit the *Data Browser*.

2.6.9 Viewing a Film Loop Animation

The most effective post-processing tool for transient data is a film loop animation. We will set up a film loop showing the fate of the BTEX through the entire duration of the simulation.

Before setting up the film loop, we will turn off the color legend.

1. Select the *Color Ramp Opts* command in the *Data* menu.
2. Turn off the *Show color legend* option.
3. Select the *OK* button.

To set up the film loop:

1. Select the *Film Loop* command in the *Data* menu.
2. Select the *Setup* button.
3. Turn on the *Display clock* option.
4. Select the *OK* button.

When the hourglass cursor disappears:

1. Select the *Play* button to begin the animation.
2. After viewing the animation, select the *Stop* button to stop the animation.
3. Select the *Step* button to move the animation one frame at a time.
4. You may wish to experiment with some of the other playback controls. When you are finished, select the *Done* button to exit the *Film Loop* dialog.

2.7 Conclusion

This concludes the *Instantaneous Aerobic Degradation* tutorial. If you wish to exit *GMS* at this time:

1. Select the *Exit* command from the *File* menu.
2. Select the *OK* button at the prompt.

BTEX Degradation with Multiple Electron Acceptors

This tutorial illustrates the steps involved in using *GMS* and *RT3D* to model BTEX degradation using a multiple electron acceptor model. Since the flow model used in this simulation is similar to the flow model used in Chapter 2 *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.

3.1 Description of the Reaction Model

The reaction we will be simulating is biodegradation of BTEX compounds via different aerobic/anaerobic pathways using multiple electron acceptors. Five different processes, considered in this model, include Aerobic Respiration (AR), Denitrification (DN), Iron (III) Reduction (IR), Sulfate Reduction (SR), and Methanogenesis (MG). All of these bio/chemical reactions are assumed to occur at the aqueous phase, mediated the existing subsurface microbes, and are expected to happen in the following sequence:

The following reaction kinetic framework is used to model the degradation of rate of hydrocarbon via different electron acceptor pathways:

$$r_{\text{HC},\text{O}_2} = -k_{\text{HC},\text{O}_2} [\text{HC}] \frac{[\text{O}_2]}{K_{\text{O}_2} + [\text{O}_2]} \dots\dots\dots (3.2)$$

$$r_{\text{HC},\text{NO}_3} = -k_{\text{HC},\text{NO}_3} [\text{HC}] \frac{[\text{NO}_3]}{K_{\text{NO}_3} + [\text{NO}_3]} \cdot \frac{K_{\text{i},\text{O}_2}}{K_{\text{i},\text{O}_2} + [\text{O}_2]} \dots\dots\dots (3.3)$$

$$r_{\text{HC},\text{Fe}^{3+}} = -k_{\text{HC},\text{Fe}^{3+}} [\text{HC}] \frac{[\text{Fe}^{3+}]}{K_{\text{Fe}^{3+}} + [\text{Fe}^{3+}]} \cdot \frac{K_{\text{i},\text{O}_2}}{K_{\text{i},\text{O}_2} + [\text{O}_2]} \dots\dots\dots (3.4)$$

$$\cdot \frac{K_{\text{i},\text{NO}_3}}{K_{\text{i},\text{NO}_3} + [\text{NO}_3]}$$

$$r_{\text{HC},\text{SO}_4} = -k_{\text{HC},\text{SO}_4} [\text{HC}] \frac{[\text{SO}_4]}{K_{\text{SO}_4} + [\text{SO}_4]} \cdot \frac{K_{\text{i},\text{O}_2}}{K_{\text{i},\text{O}_2} + [\text{O}_2]} \dots\dots\dots (3.5)$$

$$\cdot \frac{K_{\text{i},\text{NO}_3}}{K_{\text{i},\text{NO}_3} + [\text{NO}_3]} \cdot \frac{K_{\text{i},\text{Fe}^{3+}}}{K_{\text{i},\text{Fe}^{3+}} + [\text{Fe}^{3+}]}$$

$$r_{\text{HC},\text{CH}_4} = -k_{\text{HC},\text{CH}_4} [\text{HC}] \frac{[\text{CO}_2]}{K_{\text{CH}_4} + [\text{CO}_2]} \cdot \frac{K_{\text{i},\text{O}_2}}{K_{\text{i},\text{O}_2} + [\text{O}_2]} \dots\dots\dots (3.6)$$

$$\cdot \frac{K_{\text{i},\text{NO}_3}}{K_{\text{i},\text{NO}_3} + [\text{NO}_3]} \cdot \frac{K_{\text{i},\text{Fe}^{3+}}}{K_{\text{i},\text{Fe}^{3+}} + [\text{Fe}^{3+}]} \cdot \frac{K_{\text{i},\text{SO}_4}}{K_{\text{i},\text{SO}_4} + [\text{SO}_4]}$$

where r_{HC,O_2} is the rate at which hydrocarbon is destroyed by utilizing oxygen, $r_{\text{HC},\text{NO}_3}$ is the rate at which hydrocarbon is destroyed by utilizing Nitrate, $r_{\text{HC},\text{Fe}^{2+}}$ is the rate at which hydrocarbon is destroyed by producing Fe^{2+} (or utilizing Fe^{3+}), $r_{\text{HC},\text{SO}_4}$ is the rate at which hydrocarbon is destroyed by utilizing sulfate, $r_{\text{HC},\text{CH}_4}$ is the rate at which hydrocarbon is destroyed by producing methane, $[\text{O}_2]$ is the oxygen concentration $[\text{ML}^{-3}]$, k_{O_2} is the first-order rate constant $[\text{T}^{-1}]$, K_{O_2} is the Monod half saturation constant $[\text{ML}^{-3}]$ (by setting all the half-saturation constants to a small value we can simulate zero-order dependency with respect electron donor and hence a first-order degradation model with respect to hydrocarbon; the default values simulate this option), and K_{i,O_2} is the oxygen inhibition constant $[\text{ML}^{-3}]$ (by setting all inhibition constants to a small value we can force the reactions to occur in a sequential fashion; the default values simulate this process). Similar nomenclature is used to identify other Monod constants and inhibition coefficients.

Since the concentrations of Fe^{3+} and CO_2 are not readily measurable under normal field conditions, these terms were replaced with the "assimilative capacity" for iron reduction and methanogenesis, defined as:

$$[\text{Fe}^{3+}] = [\text{Fe}^{2+}_{\text{max}}] - [\text{Fe}^{2+}] \dots\dots\dots (3.7)$$

$$[\text{MC}] = [\text{CO}_2] = [\text{CH}_{4,\text{max}}] - [\text{CH}_4] \dots\dots\dots (3.8)$$

where $[\text{Fe}^{2+}_{\text{max}}]$ and $[\text{CH}_{4,\text{max}}]$ are the maximum possible aquifer levels of these species that represent the aquifer's maximum capacity for iron reduction and methanogenesis. Note, the concentration of CO_2 used here is the CO_2 evolved while the hydrocarbon is destroyed via methanogenesis which may be thought of as the "Methanogenic Capacity" (MC) of the aquifer. Using these relations, iron (III) reduction and methanogenesis processes may be related back to measurable Fe^{2+} and CH_4 concentration levels.

The total rate of hydrocarbon destruction, via all the above described processes, is the sum of each individual rates and is given as:

$$\frac{d[\text{HC}]}{dt} = r_{\text{HC},\text{O}_2} + r_{\text{HC},\text{NO}_3} + r_{\text{HC},\text{Fe}^{2+}} + r_{\text{HC},\text{SO}_4} + r_{\text{HC},\text{CH}_4} \dots\dots\dots (3.9)$$

Rates of electron acceptor utilization are given as the corresponding rate of hydrocarbon destruction multiplied by the appropriate yield coefficient (Y):

$$\frac{d[\text{O}_2]}{dt} = Y_{\text{O}_2/\text{HC}} r_{\text{HC},\text{O}_2} \dots\dots\dots (3.10)$$

$$\frac{d[\text{NO}_3]}{dt} = Y_{\text{NO}_3/\text{HC}} r_{\text{HC},\text{NO}_3} \dots\dots\dots (3.11)$$

$$\frac{d[\text{Fe}^{2+}]}{dt} = -Y_{\text{Fe}^{2+}/\text{HC}} r_{\text{HC},\text{Fe}^{2+}} \dots\dots\dots (3.12)$$

$$\frac{d[\text{SO}_4]}{dt} = Y_{\text{SO}_4/\text{HC}} r_{\text{HC},\text{SO}_4} \dots\dots\dots (3.13)$$

$$\frac{d[\text{CH}_4]}{dt} = -Y_{\text{CH}_4/\text{HC}} r_{\text{HC},\text{CH}_4} \dots\dots\dots (3.14)$$

The yield values (the mass ratio of electron acceptors removed or metabolic byproducts produced to total BTEX degraded) are: $Y_{\text{O}_2/\text{HC}} = 3.14$, $Y_{\text{NO}_3/\text{HC}} = 4.9$, $Y_{\text{Fe}^{2+}/\text{HC}} = 21.8$, $Y_{\text{SO}_4/\text{HC}} = 4.7$, and $Y_{\text{CH}_4/\text{HC}} = 0.78$.

3.2 Description of Problem

The problem we will be solving in this tutorial is similar to the problem described in the first tutorial (Figure 2.1). 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 BTEX is 1000 mg/L. Initial levels of hydrocarbon, oxygen, nitrate, Fe²⁺, sulfate, and methane in the aquifer are assume to be: 0.0, 4.0, 20.0, 0.0, 10.0, and 0.0 mg/L, respectively. The reaction constants to be used are as follows:

Constant	Value
Max Fe2+	25.0 mg/L
Max Methane	30.0 mg/L
k _{HC,O2}	0.1 day ⁻¹
k _{HC,NO3}	0.008 day ⁻¹
k _{HC,Fe3+}	0.0005 day ⁻¹
k _{HC,SO4}	0.00025 day ⁻¹
k _{HC,CH4}	0.0001 day ⁻¹

Values of all inhibition coefficients are assumed to be 0.01 mg/L and all Monod constants are assumed to 0.5 mg/L. The yield values are same as those described in the previous section.

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 be then be defined using *RT3D*.

3.3 Launching GMS

Before launching *GMS*, you should have installed *GMS*. If you have not yet installed *GMS*, please do so before continuing.

To launch the PC version of *GMS*:

Select the *GMS* shortcut from the Programs in the Start menu (Windows 95, Windows NT 4.0), or double-click on the *GMS* icon in the *GMS* program group (Windows 3.1).

To launch the Unix version of *GMS*:

1. Bring up an xterm window.
2. Change to the directory containing the *GMS* executable.
3. Type **gms** at the command line.

3.4 Required Modules/Interfaces

This tutorial utilizes the following components of the *GMS* interface:

- The *3D Grid* module
- The *MODFLOW* interface
- The *RT3D* interface

You can confirm whether each of these components has been enabled on your copy of *GMS* by selecting the *Register* command from the *File* menu. If you have licensed and enabled each of the listed items on your version of *GMS*, you can proceed to complete the tutorial in normal mode. If not, you will need to obtain an updated password or hardware lock before continuing.

3.5 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. Switch to the *3D Grid Module* .
2. Select the *Read Simulation* command in the *MODFLOW* menu.
3. In the *Open* dialog, locate and open the file entitled *gms/tutorial/rt3d/flowmod/flowmod1.mfs*.

At this point, you should see a grid appear.

3.6 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.

3.7 The BTN Package

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

1. Select the *Basic Transport Package* command from the *MT3D/RT3D* menu.
2. Select the *New* button.
3. Select the *RT3D* option.
4. Select the *Packages* button.
5. Select the *Advection Package*, the *Source/Sink Mixing Package*, the *Dispersion Package*, and the *Chemical Reaction Package*.
6. For the reaction type, select the *Kinetic-Limited Deg. of BTEX w/ MEA* option.
7. Select the *OK* button to exit the *Packages* dialog.

Note that in the *Starting Concentration* 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. The default starting concentration is zero. We will use the default value for BTEX, Fe^{2+} , and methane, but we use non-zero values for oxygen (4.0 mg/L), nitrate (20.0 mg/L), and sulfate (10.0 mg/L).

1. Select oxygen from the list of species.
2. Select the *Starting Conc.'s* button.
3. Select the *Constant -> Grid* button.
4. Enter a value of 4.0.
5. Select the *OK* button.
6. Select the *OK* button to exit the *Starting Concentration* dialog.
7. Repeat these steps to enter a starting value of 20.0 for the nitrate and 10.0 for the sulfate.

Next, we will define the layer parameters. The aquifer is a uniform horizontal aquifer with a top elevation of 10 m, a thickness of 10 m, and a porosity of 0.3.

1. Select the *HTOP* button.

2. Select the *Constant -> Grid* button.
3. Enter a value of 10 and select *OK*.
4. Select the *OK* button to exit the *HTOP* dialog.
5. Select the *Thickness* button.
6. Select the *Constant -> Grid* button.
7. Enter a value of 10 and select *OK*.
8. Select the *OK* button to exit the *Thickness* dialog.
9. Select the *Porosity* button.
10. Select the *Constant -> Grid* button.
11. Enter a value of 0.3 and select *OK*.
12. Select the *OK* button to exit the *Porosity* dialog.

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 *No. of time steps*.
4. Select the *OK* button to exit the *Stress Periods* dialog.

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).

1. Select the *Output Control* button.
2. Select the *Print at specified times* button.
3. Select the *Times* button.
4. Select the *Initialize Values* button.
5. Enter 73.0 for the *Initial time step size*.

6. Enter 73.0 for the *Maximum delta time step*.
7. Enter 730.0 for the *Maximum simulation time*.
8. Select the *OK* button to exit the *Variable Time Steps* dialog.
9. Select the *OK* button to exit the *Output Control* dialog.

This completes the input for the Basic Transport package.

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

3.8 Assigning Concentrations to the Left Boundary

The left boundary of the model is a constant head boundary. Since the head at the left boundary is greater than the head at the right boundary, the left boundary acts as a source and water enters the model from the left. Thus, we must define the concentrations of our species at the left boundary. The simplest way to do this is to mark the cells as specified concentration cells.

1. Select the *Select Cell* tool .
2. Select the cells on the left boundary by dragging a box that just surrounds the cells.
3. Select the *Cell Attributes* command in the *MT3D/RT3D* menu.
4. Change the *ICBUND* value to -1.
5. Select the *OK* button.

3.9 The Advection Package

The next step is to initialize the data for the Advection package. Select upstream finite-difference method and accept the default settings.

3.10 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 assumed equal to the longitudinal dispersivity.

1. Select the *Dispersion Package* command in the *MT3D/RT3D* menu.
2. Select the *Longitudinal Dispersivity* button.
3. Select the *Constant -> Grid* button.
4. Enter a value of 10.0 and select *OK*.
5. Select the *OK* button to exit the *Longitudinal Dispersivity* dialog.
6. Enter a value of 0.3 for the *Ratio of the transverse dispersivity to long. dispersivity* value.
7. Select the *OK* button to exit the *Dispersion Package* dialog.

3.11 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 BTEX and leave other electron acceptor concentrations at the default value of 0.0.

1. Select the *Source/Sink Mixing Package* command in the *MT3D/RT3D* menu.
2. In the *Initialize Point Source/Sinks from MODFLOW* section in the lower right corner of the dialog, select the *Well* button.
3. Using the horizontal scroll bar below the spreadsheet section, scroll over until the BTEX column is visible.
4. Change the BTEX value to 1000.0.
5. Select the *OK* button to exit the *Source/Sink Mixing Package* dialog.

3.12 The Chemical Reaction Package

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

1. Select the *Chemical Reaction Package* command in the *MT3D/RT3D* menu.
2. In the *Reaction Constants* section, click on the *Max Fe²⁺* item and set its value to 25.0.

3. Likewise, set the value of *Max Methane* to 30.0.
4. Set the value of k_{HC,O_2} to 0.1.
5. Set the value of $k_{\text{HC},\text{NO}_3}$ to 0.008.
6. Set the value of $k_{\text{HC},\text{Fe}^{3+}}$ to 0.0005.
7. Set the value of $k_{\text{HC},\text{SO}_4}$ to 0.00025.
8. Set the value of $k_{\text{HC},\text{CH}_4}$ to 0.0001.

The monod constants, inhibition coefficients, and yield values will all be left at the default values.

Select the OK button.

3.13 Running RT3D

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

1. Select the *Save Simulation* command from the *MT3D/RT3D* menu.
2. At the top of the dialog, enter "btmod" for the prefix.
3. To the right of the prefix, select the *Update* button.
4. At the top of the dialog, select the *File Browser* button .
5. In the *Save File* dialog, locate and open the directory entitled *gms/tutorial/rt3d/btexkin/*.
6. Select the *Save* button to exit the *Save File* dialog.
7. Select the *OK* button to save the files.

To run *RT3D*:

1. Select the *Run RT3D* command from the *MT3D/RT3D* menu.
2. Select *OK* at the prompt.
3. When the simulation is finished, select the *Yes* button to return to *GMS*.

3.14 Viewing the Results

Now, we will read in the concentration files and view the results.

1. Select the *Open* command from the *File* menu.
2. Select and open the file titled "btmod.dss".
3. Select the *Data Browser* command in the *Data* menu.

Note that all of the species names are listed in the *Data Browser*. Each species is saved to a separate data set file. The *.dss file is a "data set super file" which contains the names of each of the species files. By reading in the *.dss file, we effectively read in all of the files at once.

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

1. Select the *BTEX* data set.
2. Scroll down and select the time step at $t=730$ days.
3. Select the *Done* button to exit the *Data Browser*.

To display the concentration contours:

1. Select the *Display Opts* command in the *Display* menu.
2. Turn off the *Cells* option.
3. Turn on the *Grid shell* option.
4. Turn on the *Layer contours* option.
5. Select the *OK* button.

3.14.1 Overlaying Contours

Next, we will view concentration contours for the other species. When working with multiple species, it is often convenient to overlay contours of one species on top of contours from another species. As an example, we will overlay the contours of the other species on top of the BTEX contours. To do this, we must save a copy of the BTEX contours to a DXF file, read the file in, and display the BTEX contours in the background.

Before saving the dxf file, we will turn off most of the display options other than the contours.

1. Select the *Display Opts* command in the *Display* menu.

2. Turn off all of the options but the *Layer contours* option.
3. Select the *OK* button.

To save the contours to a DXF file:

1. Select the *Export* command in the *File* menu.
2. Select the *DXF file* option.
3. Select the *OK* button.
4. If necessary, path to the *gms/tutorials/rt3d/btexkin* directory.
5. Enter "btexcont.dxf" for the file name.
6. Select the *Save* button.

Before reading the contours back in, we will reset the display options and view the oxygen solution at 730 days.

1. Select the *Display Opts* command in the *Display* menu.
2. Turn on the *Grid Shell* option.
3. Select the *OK* button.
4. Select the *Data Browser* command from the *Data* menu.
5. Select the *oxygen* data set.
6. Scroll down and select the time step at $t=730$ days.
7. Select the *Done* button to exit the *Data Browser*.
8. Select the *Contour Options* command in the *Data* menu.
9. Select the *Use color ramp* option.
10. Select the *Color Ramp Opts* button.
11. Select the *Show color legend* option.
12. Select the *OK* button to exit the *Color Ramp Options* dialog.
13. Select the *OK* button to exit the *Contour Options* dialog.

Now we are ready to import the BTEX contours.

1. Switch to the *Map* module .
2. Select the *Import* command in the *DXF* menu.
3. Select and open the "btexcont.dxf" file.

Next, we will view the nitrate solution at 730 days.

1. Switch to the *3D Grid* module .
2. Select the *Data Browser* command from the *Data* menu.
3. Select the *nitrate* data set.
4. Scroll down and select the time step at t=730 days.
5. Select the *Done* button to exit the *Data Browser*.

Finally, we will view the Fe^{2+} solution at 730 days.

1. Select the *Data Browser* command from the *Data* menu.
2. Select the Fe^{2+} data set.
3. Scroll down and select the time step at t=730 days.
4. Select the *Done* button to exit the *Data Browser*.

3.14.2 Other Post-Processing Options

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

3.15 Conclusion

This concludes the tutorial: *BTEX Degradation with Multiple Electron Acceptor*. If you wish to exit *GMS* at this time:

1. Select the *Exit* command from the *File* menu.
2. Select the *OK* button at the prompt.

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 similar to the flow model used in Chapter 2 *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.

4.1 Description of Problem

The problem we will be solving in this tutorial is similar to the problem described in the first tutorial (Figure 2.1). 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 (note, this high hypothetical concentration was selected to simulate a plume (with considerable PCE mass) with relatively low injection flow rate). Details of the aquifer hydrology and geometry are shown in Figure 2.1. 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 three 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 be then be defined using *RT3D*.

4.2 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.

$$r_{\text{PCE}} = -k_1 [\text{PCE}] \quad (4.2)$$

$$r_{\text{TCE}} = k_1 Y_{\text{TCE/PCE}} [\text{PCE}] - k_2 [\text{TCE}] \quad (4.3)$$

$$r_{\text{DCE}} = k_2 Y_{\text{DCE/TCE}} [\text{TCE}] - k_3 [\text{DCE}] \quad (4.4)$$

$$r_{\text{DCE}} = k_3 Y_{\text{VC/DCE}} [\text{DCE}] - k_4 [\text{VC}] \quad (4.5)$$

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
$Y_{\text{TCE/PCE}}$	0.7920	TCE:PCE stoichiometric yield
$Y_{\text{DCE/TCE}}$	0.7377	DCE:TCE stoichiometric yield
$Y_{\text{VC/DCE}}$	0.6445	VC:DCE stoichiometric yield

4.3 Launching GMS

Before launching *GMS*, you should have installed *GMS*. If you have not yet installed *GMS*, please do so before continuing.

To launch the PC version of *GMS*:

Select the *GMS* shortcut from the Programs in the Start menu (Windows 95, Windows NT 4.0), or double-click on the *GMS* icon in the *GMS* program group (Windows 3.1).

To launch the Unix version of *GMS*:

1. Bring up an xterm window.

2. Change to the directory containing the *GMS* executable.
3. Type **gms** at the command line.

4.4 Required Modules/Interfaces

This tutorial utilizes the following components of the *GMS* interface:

- The *3D Grid* module
- The *MODFLOW* interface
- The *RT3D* interface

You can confirm whether each of these components has been enabled on your copy of *GMS* by selecting the *Register* command from the *File* menu. If you have licensed and enabled each of the listed items on your version of *GMS*, you can proceed to complete the tutorial in normal mode. If not, you will need to obtain an updated password or hardware lock before continuing.

4.5 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. Switch to the *3D Grid Module* .
2. Select the *Read Simulation* command in the *MODFLOW* menu.
3. In the *Open* dialog, locate and open the file entitled *gms/tutorial/rt3d/flowmod/flowmod1.mfs*.

At this point, you should see a grid appear.

4.6 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.

4.7 The BTN Package

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

1. Select the *Basic Transport Package* command from the *MT3D/RT3D* menu.
2. Select the *New* button.
3. Select the *RT3D* option.
4. Select the *Packages* button.
5. Select the *Advection Package*, the *Source/Sink Mixing Package*, the *Dispersion Package*, and the *Chemical Reaction Package*.
6. For the reaction type, select the *Sequential Decay Reactions* option.
7. Select the *OK* button to exit the *Packages* dialog.

Note that in the *Starting Concentration* 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.

Next, we will define the layer parameters. The aquifer is a uniform horizontal aquifer with a top elevation of 10 m, a thickness of 10 m, and a porosity of 0.3.

1. Select the *HTOP* button.
2. Select the *Constant -> Grid* button.
3. Enter a value of 10 and select *OK*.
4. Select the *OK* button to exit the *HTOP* dialog.
5. Select the *Thickness* button.
6. Select the *Constant -> Grid* button.
7. Enter a value of 10 and select *OK*.
8. Select the *OK* button to exit the *Thickness* dialog.
9. Select the *Porosity* button.

10. Select the *Constant -> Grid* button.
11. Enter a value of 0.3 and select *OK*.
12. Select the *OK* button to exit the *Porosity* dialog.

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).

5. Select the *Stress Periods* button.
6. Enter a value of 730 for the *Length*.
7. Enter a value of 10 for the *No. of time steps*.
8. Select the *OK* button to exit the *Stress Periods* dialog.

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).

1. Select the *Output Control* button.
2. Select the *Print at specified times* button.
3. Select the *Times* button.
4. Select the *Initialize Values* button.
5. Enter 73.0 for the *Initial time step size*.
6. Enter 73.0 for the *Maximum delta time step*.
7. Enter 730.0 for the *Maximum simulation time*.
8. Select the *OK* button to exit the *Variable Time Steps* dialog.
9. Select the *OK* button to exit the *Output Control* dialog.

This completes the input for the Basic Transport package.

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

4.8 The Advection Package

The next step is to initialize the data for the Advection package. Select the upstream finite-difference method and accept the default settings.

4.9 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 assumed equal to the longitudinal dispersivity.

1. Select the *Dispersion Package* command in the *MT3D/RT3D* menu.
2. Select the *Longitudinal Dispersivity* button.
3. Select the *Constant -> Grid* button.
4. Enter a value of 10.0 and select *OK*.
5. Select the *OK* button to exit the *Longitudinal Dispersivity* dialog.
6. Enter a value of 0.3 for the *Ratio of the transverse dispersivity to long. dispersivity* value.
7. Select the *OK* button to exit the *Dispersion Package* dialog.

4.10 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 *Source/Sink Mixing Package* command in the *MT3D/RT3D* menu.
2. In the *Initialize Point Source/Sinks from MODFLOW* section in the lower right corner of the dialog, 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.

4.11 The Chemical Reaction Package

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

1. Select the *Chemical Reaction Package* command in the *MT3D/RT3D* menu.
2. In the *Reaction Constants* section, click on K_{pcc} and set its value to 0.005.
3. Likewise, set the value of K_{tcc} 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.

4.12 Running RT3D

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

1. Select the *Save Simulation* command from the *MT3D/RT3D* menu.
2. At the top of the dialog, enter "rtmod" for the prefix.
3. To the right of the prefix, select the *Update* button.
4. At the top of the dialog, select the *File Browser* button .
5. In the *Save File* dialog, locate and open the directory entitled *gms/tutorial/rt3d/pce1/*.
6. Select the *Save* button to exit the *Save File* dialog.
7. Select the *OK* button to save the files.

To run *RT3D*:

1. Select the *Run RT3D* command from the *MT3D/RT3D* menu.
2. Select *OK* at the prompt.
3. When the simulation is finished, return to *GMS*.

4.13 Viewing the Results

Now, we will read in the concentration files and view the results.

1. Select the *Open* command from the *File* menu.
2. Select and open the file titled "rtmod.dss".
3. Select the *Data Browser* command in the *Data* menu.

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

1. Select the *PCE* data set.
2. Scroll down and select the time step at $t=730$ days.
3. Select the *Done* button to exit the *Data Browser*.

To view the concentration contours:

1. Select the *Display Options* command in the *Display* menu.
2. Turn off the *Cells* option.
3. Turn on the *Grid shell* option.
4. Turn on the *Layer contours* option.
5. Select the *OK* button.
6. Select the *Contour Opts* command in the *Data* menu.
7. Select the *Color fill between contours* option.
8. Select the *Color Ramp Opts* button.
9. Select the *Show color legend* option.
10. Select the *OK* button to exit the *Color Ramp Options* dialog.
11. Select the *OK* button to exit the *Contour Options* dialog.

Next, we will view the TCE solution at 730 days.

1. Select the *Data Browser* command from the *Data* menu.
2. Select the *TCE* data set.
3. Scroll down and select the time step at $t=730$ days.

4. Select the *Done* button to exit the *Data Browser*.

Next, we will view the DCE solution at 730 days.

1. Select the *Data Browser* command from the *Data* menu.
2. Select the *DCE* data set.
3. Scroll down and select the time step at $t=730$ days.
4. Select the *Done* button to exit the *Data Browser*.

Next, we will view the VC solution at 730 days.

1. Select the *Data Browser* command from the *Data* menu.
2. Select the *VC* data set.
3. Scroll down and select the time step at $t=730$ days.
4. Select the *Done* button to exit the *Data Browser*.

4.13.1 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. Time series plots are set up using an observation coverage in the *Map* module.

First, we will define an observation coverage.

1. Switch to the *Map* module .
2. Select the *Coverages* command in the *Feature Objects* menu.
3. In the *Attribute Set* section, select the *Observation* option.
4. Select the *Options* button to the right of the *Observation* option.
5. Turn on the *Interpolate in layer only* option.
6. Select the *OK* button to exit the *Observation Coverage Options* dialog.
7. Select the *OK* button to exit the *Coverages* dialog.

Next, we will create an observation point.

1. Select the *Create Point* tool

2. Click on a point somewhere in the grid downgradient of the well.

The final step is to create a time series plot.

1. Select the *Obs. Plot Options* command in the *Display* menu.
2. Select the *New* button to create a new plot.
3. Change the type of the plot to *Time series*.
4. Select the *OK* button.
5. Select the *Open/Close Plot Window* command in the *Display* menu.

Moving the Observation Point

At this point, you should see a plot of the active data set (VC) vs. time. The plot can easily be changed to display the variation in the data set at a different location.

1. Select the *Select Point/Node* tool

2. Click on the observation point and drag it to a new location (Note: you may need to reposition or resize the *Plot Window* to see the observation point).

Plotting Multiple Data Sets

By default, only the active data set is plotted. For *RT3D* solutions, it is often useful to include all of the species in the plot. This can be accomplished as follows:

1. Select the *Obs. Plot Options* command in the *Display* menu.
2. Select the *Options* button.
3. Select the *Use selected data set* option.
4. In the list of data sets, select each of the data sets that are not displayed and turn on the *Display* toggle.
5. Select the *OK* button to exit the *Time Series Plot Options* dialog.
6. Turn on the *Curve legend* option (this will help us distinguish which data set goes with which curve).

7. Select the *OK* button to exit the *Observation Plot Options* dialog.
8. Reselect the observation point if necessary.

Once again, note that you can move the point anywhere in the grid and the plot is updated.

4.13.2 Other Post-Processing Options

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

4.14 Conclusion

This concludes the tutorial: *Sequential Anaerobic Degradation: PCE->TCE->DCE->VC*. If you wish to exit *GMS* at this time:

1. Select the *Exit* command from the *File* menu.
2. Select the *OK* button at the prompt.

User-Defined Reactions

The objective of this chapter is to describe the steps involved in developing a user defined reaction module for simulating reactions that can not be simulated using a pre-defined *RT3D*-reaction package. Once developed, users can distribute the new reaction package to other interested modelers for applying the reaction model at different sites (i.e., it can be treated like a pre-defined reaction package).

5.1 Steps Involved in Creating a User-Defined Reaction

User-defined reaction packages can be created using one of two approaches: the dynamically linked library (DLL) option or the linked subroutine option. With the DLL option, the subroutine for the reaction package is compiled as a stand-alone DLL. The DLL is then copied to the same directory as the *RT3D* executable and the DLL is automatically launched by *RT3D* when *RT3D* is executed. The DLL can be recompiled or a new DLL can be used simply by copying the new DLL to the same directory as the *RT3D* executable and naming it appropriately. The *RT3D* executable does not need to be recompiled.

With the linked subroutine option, the code for the new reaction subroutine is compiled and linked with the rest of the *RT3D* source code (or the *RT3D* library made for a specific computer platform). In other words, the *RT3D* executable must be recompiled each time the reaction package is modified.

Because of the portability of the developed reaction package, the DLL option is the more convenient of the two options. However, the DLL option is only available on the *Windows 95/NT* platform. It is not available on *Unix*.

This tutorial describes the DLL approach for creating user-defined reaction packages. Special instructions for the *Unix* platform are contained in Section 5.16 on page 5-21.

5.2 Required Background

As a reaction module developer, you are considered an advanced user of the *RT3D* code. The required background is as follows:

- Should have a basic understanding of the functionality of *RT3D* code and understand how different types of components (mobile and immobile) are mathematically described within *RT3D*-modeling framework.
- Should be familiar with *GMS v2.1* and be able to create *MODFLOW* and *RT3D* input files with little effort.
- Should be familiar with the data structure of *RT3D* input files such as *BTN*, *SSM*, and *RCT* files.
- Should have a basic understanding of the *FORTRAN* language, and have access to *Microsoft FORTRAN Power Station* or *DEC Visual FORTRAN* compiler (or a *UNIX* system based *FORTRAN 90* compiler).
- Should have some background/understanding of biochemical reaction kinetics. Note inappropriate kinetic expressions and/or kinetic constants may lead to unpredictable code behavior.
- Should be familiar with contaminant transport equations, and coupled nonlinear differential equations.

5.3 Reaction Module Description

The flow and transport model we will be developing in this tutorial exercise is identical to the one described in the tutorial entitled: *Sequential Anaerobic Degradation: PCE->TCE->DCE->VC*.

Assuming first-order sequential biodegradation kinetics, the transformation of *PCE* and its decay products, along with its transport, can be predicted using the following set of partial differential equations:

$$R_p \frac{\partial [\text{PCE}]}{\partial t} = \frac{\partial}{\partial x_i} \left(D_{ij} \frac{\partial [\text{PCE}]}{\partial x_j} \right) - \frac{\partial (v_i [\text{PCE}])}{\partial x_i} + \frac{q_s}{\phi} [\text{PCE}]_s - K_{\text{PCE}} [\text{PCE}]$$

$$R_T \frac{\partial [\text{TCE}]}{\partial t} = \frac{\partial}{\partial x_i} \left(D_{ij} \frac{\partial [\text{TCE}]}{\partial x_j} \right) - \frac{\partial (v_i [\text{TCE}])}{\partial x_i} + \frac{q_s}{\phi} [\text{TCE}]_s + Y_{\text{Tce/Pce}} K_{\text{Pce}} [\text{PCE}] - K_{\text{Tce}} [\text{TCE}]$$

$$R_D \frac{\partial [\text{DCE}]}{\partial t} = \frac{\partial}{\partial x_i} \left(D_{ij} \frac{\partial [\text{DCE}]}{\partial x_j} \right) - \frac{\partial (v_i [\text{DCE}])}{\partial x_i} + \frac{q_s}{\phi} [\text{DCE}]_s + Y_{\text{Dce/Tce}} K_{\text{Tce}} [\text{TCE}] - K_{\text{Dce}} [\text{DCE}]$$

$$R_v \frac{\partial [\text{VC}]}{\partial t} = \frac{\partial}{\partial x_i} \left(D_{ij} \frac{\partial [\text{VC}]}{\partial x_j} \right) - \frac{\partial (v_i [\text{VC}])}{\partial x_i} + \frac{q_s}{\phi} [\text{VC}]_s + Y_{\text{Vc/Dce}} K_{\text{Dce}} [\text{DCE}] - K_{\text{Vc}} [\text{VC}]$$

where [PCE], [TCE], [DCE], and [VC] are the concentrations of the respective contaminants in mg/L; K_{PCE} , K_{TCE} , K_{DCE} , and K_{VC} are first-order degradation rates, R_p , R_T , R_D , R_v are retardation coefficients; and $Y_{\text{Tce/Pce}}$, $Y_{\text{Dce/Tce}}$, and $Y_{\text{Vc/Dce}}$ are yield coefficients whose values can be computed from stoichiometric relations as 0.79, 0.74, and 0.64, respectively [for example, based the chemical reaction stoichiometry, one mole of PCE will yield one mole of TCE (or 165.8 grams of PCE will yield 131.36 grams of TCE), therefore the yield value for $Y_{\text{Tce/Pce}} = 131.36/165.8 = 0.79$]. The kinetic model formulation presented assumes that the biological degradation reactions occur only in the liquid phase (a more conservative assumption).

Using the reaction operator-split strategy, the biological reaction kinetics can be separated from the transport equations and assembled together into a set differential equations:

$$\frac{d[\text{PCE}]}{dt} = - \frac{K_{\text{Pce}} [\text{PCE}]}{R_p}$$

$$\frac{d[\text{TCE}]}{dt} = \frac{Y_{\text{Tce/Pce}} K_{\text{Pce}} [\text{PCE}] - K_{\text{Tce}} [\text{TCE}]}{R_T}$$

$$\frac{d[\text{DCE}]}{dt} = \frac{Y_{\text{Dce/Tce}} K_{\text{Tce}} [\text{TCE}] - K_{\text{Dce}} [\text{DCE}]}{R_D}$$

$$\frac{d[\text{VC}]}{dt} = \frac{Y_{\text{Vc/Dce}} K_{\text{Dce}} [\text{DCE}] - K_{\text{Vc}} [\text{VC}]}{R_v}$$

The above set of coupled differential equations describes the kinetics of PCE degradation and its daughter products.

5.4 Coding a New Reaction Package

Three different methods can be used for coding a new user-defined reaction package. Each method treats the reaction parameter information (values of K_{ice} , K_{pcc} , etc.) in a different fashion.

1. In the first method, all reaction parameter values are explicitly assigned within the reaction module prior to compilation. This is not an efficient method since it requires recompilation of the reaction routine whenever a reaction parameter value is modified. However, this method is recommended for testing a new reaction module with the BATCHRXN utility.
2. In the second method, all the reaction parameter values are spatially constant but are assigned/modified externally, as input data, via the *.RCT file (to run RT3D) or batch.in file (to run BATCHRXN).
3. In the third method, some or all of the reaction parameters are treated as spatially variable (i.e. a different value may be assigned to each cell). The parameter values should be externally assigned/modified as input data, via the *.RCT file. This option should be used with caution because it may require significant computer resources, both execution time and memory!

We will first use method #1 in this tutorial; later, we will modify the code to demonstrate method #3.

5.4.1 Editing the Source Code of Reaction Module

The complete listing of the FORTRAN subroutine (using method-#1) that describes the PCE degradation reactions is given below:

```

SUBROUTINE rxns(ncomp,nvrndata,j,i,k,y,dydt,
&      poros,rhob,reta,rc,nlay,nrow,ncol,vrc)
c ***** Block 1: Comments block *****
c23456789012345678901234567890123456789012345678901234567890123456789012
c ncomp - Total number of components
c nvrndata - Total number of variable reaction parameters to be input via RCT file
c J, I, K - node location (used if reaction parameters are spatially variable)
c y - Concentration value of all component at the node [array variable y(ncomp)]
c dydt - Computed RHS of your differential equation [array variable dydt(ncomp)]
c poros - porosity of the node
c reta - Retardation factor [array variable reta(ncomp)]
c rhob - bulk density of the node
c rc - Stores spatially constant reaction parameters (up to 100 values)
c nlay, nrow, ncol - Grid size (used only for dimensioning purposes)
c vrc - Array variable that stores spatially variable reaction parameters
c ***** End of Block 1 *****

c *** Block 2: Please do not modify this standard interface block ***
!MS$ATTRIBUTES DLLEXPORT :: rxns
IMPLICIT NONE
INTEGER ncol,nrow,nlay
INTEGER ncomp,nvrndata,j,i,k
INTEGER First_time
DATA First_time/1/
DOUBLE PRECISION y,dydt,poros,rhob,reta
DOUBLE PRECISION rc,vrc
DIMENSION y(ncomp),dydt(ncomp),rc(50)
DIMENSION vrc(ncol,nrow,nlay,nvrndata),reta(50)

```



```

C ***** End of block 2 *****

C *** Block 3: Declare your problem-specific new variables here ***
C      INTEGER
C      DOUBLE PRECISION pce,tce,dce,vc,kpce,ktce,kdce,kvc
C      DOUBLE PRECISION ytcepcce,ydcetce,yvcdce
C ***** End of Block 3 *****

C *** Block 4: Initilize reaction parameters here, if required ***
C      IF (First_time .EQ. 1) THEN
C          kpce = 0.005 !PCE first-order degradation rate
C          ktce = 0.003 !TCE first-order degradation rate
C          kdce = 0.002 !DCE first-order degradation rate
C          kvc = 0.001 !VC first-order degradation rate
C          ytcepcce = 131.36/165.8
C          ydcetce = 96.9/131.36
C          yvcdce = 62.45/96.9
C          First_time = 0 !reset First_time to skip this block later
C      END IF
C ***** End of Block 4 *****

C *** Block 5: Definition of other variable names ***
C      pce = y(1)
C      tce = y(2)
C      dce = y(3)
C      vc = y(4)
C ***** End of Block 5 *****

C *** Block 6: Definition of Differential Equations ***
C      dydt(1) = -kpce*pce/reta(1)
C      dydt(2) = (-ktce*tce + kpce*pce*ytcepcce)/reta(2)
C      dydt(3) = (-kdce*dce + ktce*tce*ydcetce)/reta(3)
C      dydt(4) = (-kvc*vc + kdce*dce*yvcdce)/reta(4)
C ***** End of Block 6 *****
C      RETURN
C      END

```

Note that the reaction subroutine listed above is organized into the following six distinct blocks of FORTRAN code:

1. The comment block

This block contains a definition for all the variables that are passed into the rxns routine from the *RT3D* main program.

2. The interfacing block

This block contains FORTRAN statements that define the type of passed variables. This block should not be altered under any circumstances.

3. The local variable definition block

This block is used define all the new local variables that are used exclusively in the rxns subroutine.

4. The reaction parameter initialization block

This block is used to specify values for all the reaction parameters (such as K_{TCE} , K_{PCE} , etc.). Note that this initialization block is executed only when the subroutine is called for the first time.

5. Variables naming block

This block is typically used to transfer certain passed variables into meaningful names (this is required for code clarity purposes only).

6. The differential equations block

This block is used to describe the PCE degradation reaction equations in FORTRAN language.

The FORTRAN subroutine presented above is provided with the *GMS* files in the following location:

```
gms\tutorial\rt3d\userdef\rxns_1.f
```

You may wish to open and view this file using your favorite ASCII editor (such as *Notepad* or *WordPad*).

5.4.2 Compiling the Source Code

Now the reaction module is ready for compilation. To create a dynamic link library (RXNS.DLL file), open a DOS window and go to the subdirectory where RXNS.F was saved and type the following command (this assumes that you have previously installed the *Microsoft FORTRAN Power Station* or *DVF* compiler):

```
f132 /LD rxns_1.f
```

At this stage, the compiler will display all the syntax errors. If no changes have been made to the code, there shouldn't be any errors. If there are errors, fix them and recompile the code. After a successful compilation step, the compiler will create a DLL file (named as RXNS_1.DLL). Use the following *DOS* command to rename the DLL as RXNS.DLL

```
RENAM RXNS_1.DLL RXNS.DLL
```

5.5 Testing and Debugging a New Reaction Package

After creating a new reaction package, it is always a good practice to test its response in a batch mode (i.e. how the reactions would behave in a batch reactor). For this purpose, we have developed a utility called BATCHRXN. This debugging tool can read the reaction information in a RXNS.DLL file and simulate its behavior in a batch mode.

To use BATCHRXN, it is recommended that the user define all the kinetic reaction parameters within the rxns subroutine (i.e. using method-#1). This is because the BATCHRXN code will not read information from RT3D input

files, including the RCT file. Therefore, a new reaction module should always be developed in a format similar to Method-#1 (or #2) and later, if required, the kinetic parameters can be moved into a RCT file to run RT3D simulations.

In addition to testing the new reaction module using BATHCHRXN, it is also a good practice to test the transport problem using RT3D in single-species tracer mode. Once a reaction package is tested using BATCHRXN, the DLL can be used with RT3D to run a full-fledged RT3D simulation.

5.5.1 Running BATCHRXN

Whenever BATCHRXN is executed, the code searches for a RXNS.DLL file in the local subdirectory. Thus, you should copy the RXNS.DLL file to the GMS directory (this is where the BATCHRXN.EXE and RT3D.EXE files are stored by default). While developing a new reaction module, always keep the source code (rxns*.f) in a local project directory, and rename and copy the DLL as RXNS.DLL into the GMS directory.

After you have copied the RXNS.DLL file into the GMS directory, open a DOS window and run the BATCHRXN code from your project subdirectory. The code will query for several input data. The queries and the appropriate responses for this example problem are given below:

```
Input-> ncomp, no_of_timesteps, delt
Format-> INTEGER, INTERGER, REAL
4 100 10.
Input-> Initial Values of y(i)
ncomp lines - One REAL entry per line
100.      *Initial PCE concentration in this case*
0.0       *Initial TCE concentration in this case*
0.0       *Initial DCE concentration in this case*
0.0       *Initial VC concentration in this case*
Do you want to change default atol & rtol: y/n
Default values are:- atol=1.0e-10 & rtol=1.0e-9
n
Input-> ncrxndata (number of reaction parameters)
Format-> INTEGER
0
```

You can also store these responses in a data file (say, batch.in) and use the command "batchrxn < batch.in" to automatically answer all the BATCHRXN queries. Here is an example batch.in file:

```
4 1000 1.
100.
0.
0.
0.
y
1.0e-11 1.0e-10
1.0e-11 1.0e-10
1.0e-11 1.0e-10
1.0e-11 1.0e-10
0
```

Note in the second case-atol and rtol values are not initialized as default values, instead are set explicitly by the user.

5.5.2 Viewing the Results

After reading the input, BATCHRXN will execute and create an output file called batchrxn.out. The output file will contain a set of white-space separated ASCII data in column format (written using the Format statement 21E15.5). For our example problem, five columns are output: Time, specie-1 (PCE), specie-2 (TCE), specie-3 (DCE), and specie-4 (VC). Use any spreadsheet software such as *Excel* to plot and analyze this output data. The BATCHRXN output results for the example problem are shown in Figure 5.1.

Figure 5.1. Sample Output from the BATCHRXN Code for the Sample Problem.

The results of a BATCHRXN run should be used to:

1. Debug errors in reaction expressions.
2. Check whether the reaction expressions and parameter values are reasonable (if available, microcosm or batch reactor data may be used to verify this).
3. Select appropriate values for numerical parameters atol (absolute tolerance) and rtol (relative tolerance).

The parameters atol and rtol are used by the differential equations solver to control convergence error while solving the reaction model. The differential equation solver will attempt to control a vector $e = e(i)$, which defines estimated local error (or convergence level) in a variable $y(i)$, according to the inequality: $\max\text{-norm of } [e(i)/\text{ewt}(i)]$ is less than or equal to 1.0, where $\text{ewt} =$

(ewt(i)) is a vector of positive error weights and is computed using the formula: $\text{ewt}(i) = \text{rtol}(i) * \text{abs}(y(i)) + \text{atol}(i)$.

We recommend the following rule of thumb to set atol and rtol values. If m is the number of significant digits required in the solution component $y(i)$, set $\text{RTOL}(i) = 10^{-(m+1)}$ and set $\text{ATOL}(i)$ to a small value at which the absolute value of $y(i)$ is essentially insignificant.

Note: since transport is not solved while executing batchrxn, all the retardation factors in the array $\text{reta}()$ are automatically set to 1.0 with the DLL. However, if the same DLL is used with *RT3D*, appropriate species retardation factors will be transferred through the $\text{reta}()$ array.

5.6 Setting up the RT3D Simulation

At this stage, we are ready to run a *RT3D* simulation using the newly developed reaction package. To do this, will define the transport model and enter the input data using the *GMS* interface. Once the model is built, we will save it to a set of *RT3D* input files and launch *RT3D*. When the user-defined reaction package option is selected, *RT3D* automatically launches the *RXNS.DLL* subroutine to solve the reaction terms.

5.7 Launching GMS

Before launching *GMS*, you should have installed *GMS*. If you have not yet installed *GMS*, please do so before continuing.

To launch the PC version of *GMS*:

Select the *GMS* shortcut from the Programs in the Start menu (Windows 95, Windows NT 4.0), or double-click on the *GMS* icon in the *GMS* program group (Windows 3.1).

To launch the *Unix* version of *GMS*:

1. Bring up an xterm window.
2. Change to the directory containing the *GMS* executable.
3. Type *gms* at the command line.

5.8 Required Modules/Interfaces

This tutorial utilizes the following components of the *GMS* interface:

- The 3D Grid module
- The MODFLOW interface
- The RT3D interface

You can confirm whether each of these components has been enabled on your copy of *GMS* by selecting the *Register* command from the *File* menu. If you have licensed and enabled each of the listed items on your version of *GMS*, you can proceed to complete the tutorial in normal mode. If not, you will need to obtain an updated password or hardware lock before continuing.

5.9 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. Switch to the 3D Grid Module
2. Select the *Read Simulation* command in the *MODFLOW* menu.
3. In the *Open* dialog, locate and open the file entitled *gms/tutorial/rt3d/flowmod/flowmod1.mfs*.

At this point, you should see a grid appear.

5.10 Building the Transport Model

Now that the flow model is established, the next step is to perform the *RT3D* simulation. For this part of the simulation, we will select the user-defined reaction option, define and initialize appropriate species and reaction parameters, and assign concentrations to the well.

5.10.1 The BTN Package

The first step is to modify the data in the *Basic Transport Package*. First, we will select the user-defined reaction module option and name appropriate species and initialize their concentrations.

1. Select the *Basic Transport Package* command from the *MT3D/RT3D* menu.

2. Select the *New* button.
3. In the *Model* section, select the *RT3D* option.
4. Select the *Packages* button.
5. Select the *Advection Package*, the *Source/Sink Mixing Package*, the *Dispersion Package*, and the *Chemical Reaction Package*.
6. For the reaction type, select the *User-Defined Reaction* option.
7. Select the *OK* button to exit the *Packages* dialog.

Defining the Species

For a pre-defined reaction package, the appropriate list of species would be automatically loaded by *GMS*. However, for user-defined reactions, we must explicitly define the species.

1. Select the *Define species* button
2. If a name file appropriate to the user-defined reaction package is available, we can click on the *Import* button to initialize all species names in a single step (see Section 5.15). Since it is not available (we are using this new module for the first time), we have to define the species manually. To begin this process, click on the *New* button
3. Type the name of the species as: *PCE*
4. Leave the *mobile* option checked (this is the default)
5. Click on *New* again
6. Type the name of the species as: *TCE*
7. Click on *New* again
8. Type the name of the species as: *DCE*
9. Click on *New* again
10. Type the name of the species as: *VC*
11. Press *Enter*

Notice that the *Starting Concentration* section of the dialog now lists all the four species associated with our new reaction module. 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.

Defining the Layer Parameters

Next, we will define the layer parameters. The aquifer is a uniform horizontal aquifer with a top elevation of 10 m, a thickness of 10 m, and a porosity of 0.3.

1. Select the *HTOP* button.
2. Select the *Constant -> Grid* button.
3. Enter a value of 10 and select *OK*.
4. Select the *OK* button to exit the *HTOP* dialog.
5. Select the *Thickness* button.
6. Select the *Constant -> Grid* button.
7. Enter a value of 10 and select *OK*.
8. Select the *OK* button to exit the *HTOP* dialog.
9. Select the *Porosity* button.
10. Select the *Constant -> Grid* button.
11. Enter a value of 0.3 and select *OK*.
12. Select the *OK* button to exit the *Porosity* dialog.

Setting up the 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 (three years).

1. Select the *Stress Periods* button.
2. Select the *Initialize* button.
3. Enter 1 for the *No. of stress periods*, 730 for the *Length*, 10 for the *No. of time steps*, leave the *Transport step size* at 0.0, and select *OK*.
4. Select *OK* at the prompt.
5. Select the *OK* button to exit the *Stress Periods* dialog.

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).

1. Select the *Output Control* button.
2. Select the *Print at specified times* button.
3. Select the *Times* button.
4. Select the *Initialize Values* button.
5. Enter 73.0 for the *Initial time step size*.
6. Enter 73.0 for the *Maximum delta time step*.
7. Enter 730.0 for the *Maximum simulation time*.
8. Select the *OK* button to exit the *Variable Time Steps* dialog.
9. Select the *OK* button to exit the *Output Control* dialog.

This completes the input for the Basic Transport package.

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

5.10.2 The Advection Package

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

1. Select the *Advection Package* command from the *MT3D/RT3D* menu.
2. Select the *Upstream finite-difference* option.
3. Select the *OK* button to exit the dialog.

5.10.3 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 assumed equal to the longitudinal dispersivity.

1. Select the *Dispersion Package* command in the *MT3D/RT3D* menu.
2. Select the *Longitudinal Dispersivity* button.
3. Select the *Constant -> Grid* button.

4. Enter a value of 10.0 and select *OK*.
5. Select the *OK* button to exit the *Longitudinal Dispersivity* dialog.
6. Enter a value of 0.3 for the *Ratio of the trans. dispersivity to long. dispersivity* value.
7. Select the *OK* button to exit the *Dispersion Package* dialog.

5.10.4 The Source/Sink Mixing Package

Next, we will initialize the Source/Sink Mixing package and define the concentration at the spill location.

1. Select the *Source/Sink Mixing Package* command in the *MT3D/RT3D* menu.
2. In the *Source/Sink Types* section, select the *Well* option.
3. In the *Initialize* section, select the *Well* option.
4. Select the *OK* button.

We will define the concentrations at the wells by selecting the cells and assigning the concentration directly with the *Point Source/Sink* command. 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 *Select Cell* tool .
2. Select the well at the spill location.
3. Select the *Point Source/Sink* command in the *MT3D/RT3D* menu.
4. In the *Well* section, note appropriate species names are automatically set at this menu based on your earlier definition. Select the *PCE* species and enter a value of 1000.0 for concentration.
5. Select the *OK* button to exit the *Point Source/Sink* dialog.

5.10.5 The Chemical Reaction Package

Next, we will review the data for the Chemical Reaction package.

Select the *Chemical Reaction Package* command in the *MT3D/RT3D* menu.

Note that the reaction parameter box is blank. We will leave it blank in this case because in the DLL we coded all of the reaction constants directly within the reaction subroutine. We will demonstrate how to define them as user-defined variables later in this tutorial.

Select the *OK* button to accept the defaults.

5.11 Running RT3D

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

1. Select the *Save Simulation* command from the *MT3D/RT3D* menu.
2. At the top of the dialog, enter "rtmod1" for the prefix.
3. To the right of the prefix, select the *Update* button.
4. At the top of the dialog, select the *File Browser* button .
5. In the *Save File* dialog, locate and open the directory entitled gms/tutorial/rt3d/userdef/.
6. Select the *Save* button to exit the *Save File* dialog.
7. Select the *OK* button to save the files.

To run *RT3D*:

1. Select the *Run RT3D* command from the *MT3D/RT3D* menu.
2. Select *OK* at the prompt.
3. When the simulation is finished, select the *Yes* button to return to *GMS*.

5.12 Viewing the Results

To view the results, select the *Data Browser* command from the *Data* menu and import the concentration files to view the results. To verify your results, compare the concentration values with the output from the tutorial entitled: *Sequential Anaerobic Degradation: PCE->TCE->DCE->VC*.

5.13 Developing a Reusable Reaction Package

Defining a new reaction model via a reaction package is a powerful option supported by the *RT3D* code. Once tested and developed, the reaction package (or DLL) can be used in other projects that have different conceptual flow and transport models. DLLs can also be distributed via web pages to other users who might be interested in modeling similar type of reactive transport systems. This section outlines the steps involved in developing a reusable version of reaction package.

In an earlier section, we mentioned that there are three different methods available for coding the reaction subroutine. Method-#1, which is the preferred method for testing and debugging a new reaction package, was discussed in detail in previous sections. Now, let's assume that we have sufficiently tested the reaction package and are ready to distribute the package to other users who might be interested in using it without having to recompile the code. To accomplish this, we have to re-code the reaction package based on either method-#2 or method-#3. We will utilize method-#3 (which is the most advanced method) here for demonstration purposes. As described earlier, method-#3 provides an option to let some or all of the reaction parameters be defined as spatially variable parameters. This method also allows the user to set the values of reaction parameters via the *.RCT input file (i.e., in the *Chemical Reactions Package* dialog in *GMS*).

5.13.1 Editing the Source Code

In this test problem, we have a total of seven reaction parameters. For illustration purposes, we will assume that five of them are constant parameters: K_{pce} , K_{tce} , $Y_{tce,pce}$, $Y_{dce,tce}$, and $Y_{vc,dce}$ (note *NCRXNDATA* = 5), and two of them are spatially variable parameters: K_{dce} and K_{vc} (note *NVRXNDATA* = 2). The following FORTRAN listing for the reaction module (using method-#3) incorporates these changes:

```

      SUBROUTINE rxns(ncomp,nvrxndata,j,i,k,y,dydt,
      $      poros,rhob,reta,rc,nlay,nrow,ncol,vrc)
c ***** Block 1: Comments block *****
c234567890123456789012345678901234567890123456789012345678901234567890123456789012
c ncomp - Total number of components
c nvrxndata - Total number of variable reaction parameters to be input via RCT file
c J, I, K - node location (used if reaction parameters are spatially variable)
c y - Concentration value of all component at the node (array variable y(ncomp))
c dydt - Computed RHS of your differential equation (array variable dydt(ncomp))
c poros - porosity of the node
c reta - Retardation factor (array variable dpreta(mcomp))
c rhob - Bulk density of the node
c rc - Stores spatially constant reaction parameters (up to 100 values)
c nlay, nrow, ncol - Grid size (used only for dimensioning purposes)
c vrc - Array variable that stores spatially variable reaction parameters
c ***** End of Block 1 *****

c *** Block 2: Please do not modify this standard interface block ***
!MS$ATTRIBUTES DLLEXPORT :: rxns
IMPLICIT NONE
INTEGER ncol,nrow,nlay
INTEGER ncomp,nvrxndata,j,i,k
INTEGER First_time
DATA First_time/1/
DOUBLE PRECISION y,dydt,poros,rhob,reta

```

```

      DOUBLE PRECISION rc,vrc
      DIMENSION y(ncomp),dydt(ncomp),rc(50)
      DIMENSION vrc(ncol,nrow,nlay,nvrndata),reta(50)
C ***** End of block 2 *****

C *** Block 3: Declare your problem-specific new variables here ***
C      INTEGER
      DOUBLE PRECISION pce,tce,dce,vc,kpce,ktce,kdce,kvc
      DOUBLE PRECISION ytcepcce,ydcetce,yvcdce
C ***** End of Block 3 *****

C *** Block 4: INITIALIZE YOUR CONSTANTS HERE, IF DESIRED ***
      IF (First_time .EQ. 1) THEN
        kpce = rc(1) !PCE first-order degradation rate (constant)
        ktce = rc(2) !TCE first-order degradation rate (constant)
        kdce is a spatially variable parameter, it is defined in block-5
        kvc is a spatially variable parameter, it is defined in block-5
        ytcepcce = rc(3)
        ydcetce = rc(4)
        yvcdce = rc(5)
        First_time = 0 !reset First_time to skip this block later
      END IF
C ***** End of Block 4 *****

C *** Block 5: Definition of other variable names ***
      pce = y(1)
      tce = y(2)
      dce = y(3)
      vc = y(4)
      kdce = vrc(j,i,k,1)!Spatially variable DCE decay rate
      kvc = vrc(j,i,k,2) ! Spatially variable vc decay rate
C ***** End of Block 5 *****

C *** Block 6: Definition of Differential Equations ***
      dydt(1) = -kpce*pce/reta(1)
      dydt(2) = (-ktce*tce + kpce*pce*ytcepcce)/reta(2)
      dydt(3) = (-kdce*dce + ktce*tce*ydcetce)/reta(3)
      dydt(4) = (-kvc*vc + kdce*dce*yvcdce)/reta(4)
C ***** End of Block 6 *****

      RETURN
      END

```

Note that this subroutine is identical to the previous version except that in blocks 4 and 5, the `rc()` and `vrc()` arrays are used to initialize reaction parameters. The values of the parameters will be defined in the *RT3D* input file **.RCT*. In the section below, we will demonstrate how the reaction parameter values can be defined efficiently using the *GMS* interface.

5.13.2 Compiling the Source Code

Now follow the steps detailed in Section 5.4 to compile and create a new *rxns.dll* file. The FORTRAN source code is provided in the following file:

```
gms\tutorial\rt3d\userdef\rxns_2.f
```

Once the source is compiled, rename the DLL as *rxns.dll* and copy it to the *GMS* subdirectory where *RT3D.EXE* is saved. If you wish to preserve the previous version of the *rxns.dll* file, you will need to rename the old version before copying the new version to the *GMS* directory.

5.14 Modifying the Transport Model

We are now ready to use the new module for reactive transport simulations. If you have exited *GMS*, or if you have made any changes to the *RT3D* simulation defined above, you will need to re-import both the *MODFLOW* and *RT3D* simulation.

5.14.1 The Chemical Reaction Package

Next, we will define and initialize the chemical reaction parameters.

Select the *Chemical Reaction Package* command in the *MT3D/RT3D* menu.

Note that the reaction parameter box is blank. In this section, we will define and initialize the reaction parameters.

1. Click on *Define Parameters* button.
2. Once again, if a name file appropriate to the user-defined reaction package, is available, we can click on the *Import* button and initialize all reaction parameter names in a single step (see Section 5.15). Since it is not available in this case, we will define them manually. To begin this process, click on *New* button.
3. Enter the name of reaction parameter as: *Kpce*.
4. Do not select the *Spatially variable* option (it is off by default).
5. Click on *New*.
6. Enter the name of reaction parameter as: *Ktce*
7. Click on *New*.
8. Enter the name of reaction parameter as: *Kdce*
9. Select the *Spatially variable* option.
10. Click on *New*.
11. Enter the name of reaction parameter as: *Kvc*
12. Check the *Spatially variable* option.
13. Click on *New*.
14. Enter the name of reaction parameter as: *Ytce_pce*

15. Click on *New*.
16. Enter the name of reaction parameter as: Ydce_tce
17. Click on *New*.
18. Enter the name of reaction parameter as: Yvc_dce
19. Select the *OK* button.

Now notice in the *Define Parameters* section all the reaction parameters are listed. Next, we will assign values for all these parameters.

1. In the *Reaction Constants* section, click on K_{pce} and set the constant value to 0.005.
2. Click on K_{tce} and set the constant value to 0.003
3. Click on Y_{tce_pce} and set the constant value to 0.792
4. Click on Y_{dce_tce} and set the constant value to 0.738
5. Click on Y_{vc_dce} and set the constant value to 0.644
6. Now, click on K_{dce} (variable).
7. Select the *Variable* button.
8. Click on *Constant to Grid* option and set the value to 0.002
9. Click on K_{vc} (variable)
10. Select the *Variable* button.
11. Click on *Constant to Grid* option and set the value to 0.001
12. Select the *OK* button.

We have defined five spatially constant reaction parameters and two spatially variable reaction parameters. Therefore, in the *.RCT package file, NCRXNDATA will be set to 5 and NVRXNDATA will be set to 2. During execution, the RT3D code stores and transfers all the constant reaction parameters through a one-dimensional reaction constant array rc(). The parameter values are transferred in the order in which they are originally entered; i.e. K_{pce} is stored in rc(1), K_{tce} is stored in rc(2) and so on. Similarly, all the variable reaction parameters are stored and transferred through a four-dimensional variable reaction constant array vrc().

Note that although two of the reaction parameters can vary spatially, for the sake of keeping this tutorial simple, we have assigned a single value to all cells in both cases. The reaction parameters can be edited on a cell by cell basis using the array editor dialog in the Chemical Reaction package or by selecting a set of cells and selecting the *Cell Attributes* command in the *MT3D/RT3D* menu.

5.14.2 Running RT3D

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

1. Select the *Save Simulation* command from the *MT3D/RT3D* menu.
2. At the top of the dialog, enter "rtmod2" for the prefix.
3. To the right of the prefix, select the *Update* button.
4. At the top of the dialog, select the *File Browser* button .
5. In the *Save File* dialog, locate and open the directory entitled *gms/tutorial/rt3d/userdef*.
6. Select the *Save* button to exit the *Save File* dialog.
7. Select the *OK* button to save the files.

To run *RT3D*:

1. Select the *Run RT3D* command from the *MT3D/RT3D* menu.
2. Select *OK* at the prompt.
3. When the simulation is finished, select the *Yes* button to return to *GMS*.

5.14.3 Viewing the Results

Select the *Data Browser* command from the *Data* menu and import the appropriate concentration files to view the results. The results should be similar to those computed earlier.

5.15 Creating a Name File for GMS import

When a new reaction package is created, the package developer should create a name file. The information regarding species names, species types, species order, reaction parameter names, reaction parameter types, and reaction

parameter sequence are stored in a name file. All of the information needed for a name file is included in the *RT3D* super file created by *GMS*. Thus, the simplest way to create the name file is to set up the first simulation using the steps defined above and then open the *RT3D* super file for the simulation (*.rts) in a text editor. Delete all the cards except the first card, and the cards beginning with *SPC* and *RXNPARAM*. The edited file should look like this:

```
RT3DSUP
SPC "PCE" 1 1
SPC "TCE" 2 1
SPC "DCE" 3 1
SPC "VC" 4 1
RXNPARAM "kdce" 3 1
RXNPARAM "kvc" 4 1
RXNPARAM "kpce" 1 0
RXNPARAM "ktce" 2 0
RXNPARAM "Ytce_pce" 5 0
RXNPARAM "Ydc_tce" 6 0
RXNPARAM "Yvc_dce" 7 0
```

Save this information in a new file, say "specie.nam". This file can be later used for directly importing species and reaction parameter information. Whenever a user-defined reaction package (as a DLL or source code) is distributed to another *GMS* user, a specie name file, appropriate to the reaction package, should be included with it.

5.15.1 Importing Species Names

The specie name file can be used to set-up a new *RT3D* transport problem using a (previously developed) user-defined reaction package. To import the specie names into *GMS*, select *Basic Transport Package*, click on the *Define Species* option, click on the *Import* button, and read the "specie.nam" file. These steps will import appropriate specie names in the correct order.

5.15.2 Importing Reaction Parameter Names

To import reaction parameter names, select *Chemical Reaction Package*, click on *Define Parameters* option, click on *Import* button, and read the "specie.nam" file again. This will import appropriate reaction parameter names in the correct order.

5.16 Special Instructions for UNIX Users

Since development of a DLL requires *Microsoft* or *Digital's visual FORTRAN* compiler specific commands, this option is incompatible with *Unix* platforms. Therefore, *Unix* users should always comment the first line in the block-2 of rxns.f file that begin with a command "!MS\$ATTRIBUTES". Also whenever any changes are made to the *RXNS.F* code, the *RT3D* executable should to be

recreated, using a FORTRAN-90 compiler, by linking RXNS.OBJ with the RT3D.LIB (to use *RT3D*) or with BATCHRXN.LIB (to use BATCHRXN).

5.17 Conclusion

This concludes the *User-Defined Reactions* tutorial. If you wish to exit *GMS* at this time:

1. Select the *Exit* command from the *File* menu.
2. Select the *OK* button at the prompt.