GMS TUTORIALS

ART3D – Basic

ART3D is a 3-dimensional analytical reactive transport model. It considers retardation, advection, dispersion, and the reactions of multiple species. It also allows for complex reaction sequences including sequential, convergent and divergent reactions. Because ART3D finds an analytical solution, it can quickly find exact solutions at any point in the model domain without using interpolation. The solution is based on an analytical strategy published in Clement T.P. 2001, *Water Resources Research*, vol 37, p. 157-163.

This tutorial illustrates the use of GMS to build and solve an ART3D model. The example presented here is a simple hypothetical reactive transport problem involving the reductive dechlorination of chlorinated ethenes. The model can be solved using three different modes: 1) normal forward mode, 2) stochastic mode, 3) automated parameter estimation mode. This tutorial will focus on a normal forward run.

1.1 Outline

This is what you will do:

1. Create a 3D grid.
2. Define conditions.
3. Run ART3D in forward run mode.
4. Set up an animation.

1.2 Required Modules/Interfaces

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

- Grid

- Map
- MODFLOW
- RT3D and ART3D

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

2 Description of Problem

The problem presented here includes a hypothetical aquifer contaminated with perchloroethene (PCE) and trichloroethene (TCE). The site layout is shown in Figure 1. The ground water flow direction is from left to right and there are four monitoring wells with observed contaminant concentrations. We will use ART3D to track the movement of the PCE and TCE through the aquifer due to advection, dispersion and retardation and will simulate their degradation to daughter products dichloroethene (DCE) and vinyl chloride (VC). The model will be subjected to a stochastic analysis and then will be calibrated to match the field data.

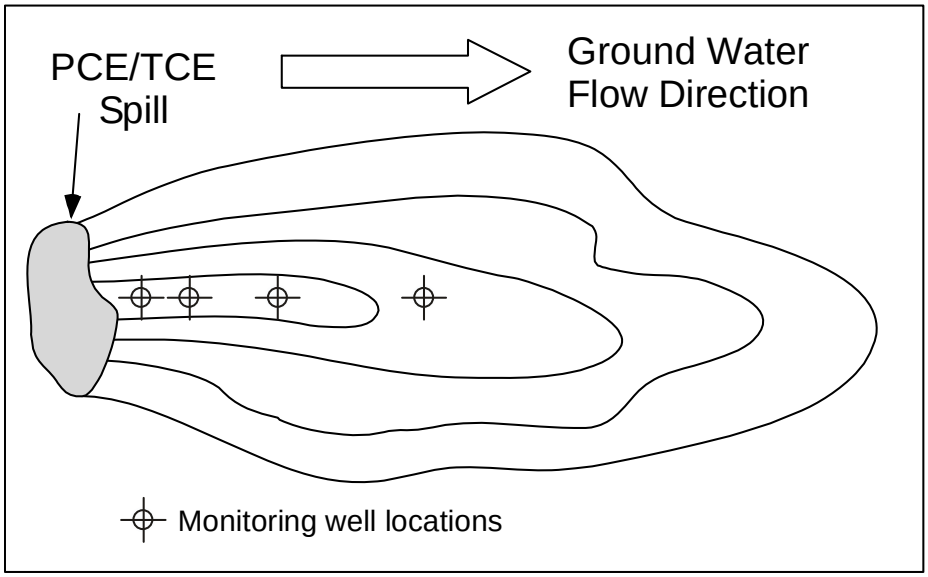

Figure 1. Conceptual Representation of Problem.

3 Getting Started

If you have not yet done so, launch GMS. If you have already been using GMS, you may wish to select the *New* command from the *File* menu to ensure the program settings are restored to the default state.

4 Running a Forward Simulation

First, we will set up the ART3D model and run a simple forward simulation using our best estimate of the input concentrations, decay constants, and aquifer properties. We will do a 40-year simulation with concentration output at the end of each year.

4.1 Units

First we'll define the units we will use.

1. From the *Edit* menu, select the *Units* command.
2. In the *Units* dialog, make sure the *Length* units are set to **m**, the *Time* units to **d** and the *Concentration* units to **mg/l**.
3. Select *OK* to close the *Units* dialog.

4.2 Creating a Grid

Although ART3D is an analytical model and does not require a numerical grid, GMS requires a mesh-centered grid for displaying the model results. Also, the location of the grid defines the location of the contaminant source. The source is always assumed to be at the top of the left (x=0) edge of the 3D grid and the groundwater is assumed to flow from left to right.

To create a grid:

1. In the *Project Explorer* right-click on the empty space and then, from the pop-up menu, select the *New | 3D Grid* command.
2. In the *X dimension* section, enter **300** for the length and **50** for the number of cells.
3. In the *Y dimension* section, enter **150** for the length and **30** for the number of cells.
4. In the *Z dimension* section, enter **15** for the length and **10** for the number of cells.
5. In the *Orientation/Type* combo box, choose *ART3D* to create a mesh-centered grid.
6. Select the *OK* button.

At this point, you should see a grid.

4.3 Initializing the ART3D Simulation

Now that the grid has been created, we will initialize the ART3D simulation

1. Select the *ART3D* | *New Simulation* command.

2. Select the *User-defined* option and hit *OK*.

4.4 Defining the Species

In this example problem, we are interested in the plumes of four chemical species: PCE, TCE, DCE and VC. Each of these species must be created in the *Define Species* dialog.

1. Select the *ART3D* | *Define Species* command.

2. Select the *New* button four times to create four species.

3. Name each of the species by clicking on each line of the list and typing the names, **PCE**, **TCE**, **DCE** and **VC**. You can use the *Tab* key to move between the edit fields in the spreadsheet control.

4. Select the *OK* button.

4.5 General Options

Next, we will define the type of simulation to run and define the dimensions of the source.

1. Select the *ART3D* | *General Options* command.

2. Make sure that the *Normal forward run* option is selected on the left half of the dialog.

3. Next define the source dimensions by entering **15** in the *ys* text box and **6** in the *zs* text box. This will create a source 15 meters wide and 6 meters deep at the left end of the grid. Note the source will be 15 m wide centered in the y direction at the left edge (x=0) of the grid and will be 6 m deep starting at the top of the grid in the z direction.

4. Select *OK* to leave the *General Options* dialog.

4.6 Output Control

The *Output Control* dialog is used to set the time intervals at which the model data are output. Note that since ART3D is an analytical model, the time steps do not represent traditional time steps required by numerical models for temporal discretization. ART3D can explicitly compute concentrations at any point in time. The time steps are selected purely for convenience in visualizing the model results.

1. Select the *ART3D* | *Output Control* command.

2. Set the *Total simulation time* to **14600** days (40 years).

3. Set the *Number of output time steps* to **20**. This will cause ART3D to create output datasets every two years over the 40 year simulation.

4. Select *OK* to close the *Output Control* dialog.

4.7 Entering the Effective Yield Matrix

ART3D requires a reaction coefficient matrix which is a combination of the yield values, decay fraction and the first order decay coefficients as shown below.

$$\begin{bmatrix} -k_1 & 0 & 0 & 0 \\ f_{1,2}y_{1,2}k_1 & -k_2 & 0 & 0 \\ 0 & f_{2,3}y_{2,3}k_2 & -k_3 & 0 \\ 0 & 0 & f_{3,4}y_{3,4}k_3 & -k_4 \end{bmatrix}$$

Here, k_i is the first order decay constant for species *i* and $y_{i,j}$ is the stoichiometric yield coefficient of species *i* producing species *j*, and f_{ij} is the decay fraction that describes mass fraction of a parent compound c_i decaying into a daughter product c_j. The product f*y is called the effective yield coefficient. The value of yield coefficient can be computed from the ratio of the molecular weights of the reactants and products. Since one mole of PCE yields one mole of TCE, one mole of TCE yields one mole of DCE, etc, the effective yield coefficients are the ratios of the molecular weights of the reactants and products. Thus, $y_{1,2}$ = 0.79, $y_{2,3}$ = 0.74, and $y_{3,4}$ = 0.64. The value of all the decay fractions for this simple sequential degradation example is 1.0. When running ART3D using the GMS interface, the user need only enter the effective yield values in matrix form, and GMS will calculate the entries for the reaction coefficient matrix with the appropriate *k* values.

1. Select the ART3D | Yield Coefficients command.

The *Effective Yield Coefficients* dialog is a matrix with the reactants listed across the top as column headings and with the products listed along the left side as row headings. The diagonals have been dimmed since no specie will react to form itself.

2. Enter **0.79** for the *effective yield coefficient* for the reaction PCE → TCE (first column, second row).

3. Enter **0.74** for the *effective yield coefficient* for the reaction TCE → DCE (second column, third row).

4. Enter **0.64** for the *effective yield coefficient* for the reaction DCE → VC (third column, fourth row).

5. Select *OK* to close the dialog.

4.8 Entering the Parameters

In the final step, we will enter the flow and transport parameters. These parameters include the retardation factor, the groundwater flow velocity (seepage velocity), dispersion coefficients, decay constants, and initial concentrations at the source.

1. Select the *ART3D* | *Parameters* command.

2. Fill in the *Parameters* dialog using the values shown in the table below. The alpha terms represent the dispersion coefficients, the K terms represent the decay constants, and the Co terms represent the concentrations of the species at the source.

Parameter	Value
Retard	1.1
Velocity (m/d)	0.027
AlphaX (m)	16.8
AlphaY/AlphaX	0.2
AlphaZ/AlphaX	0.01
PCE K (1/d)	0.000355
TCE K (1/d)	0.000534
DCE K (1/d)	0.000445
VC K (1/d)	0.00092
PCE Co (mg/l)	50.0
TCE Co (mg/l)	25.0
DCE Co (mg/l)	0.0
VC Co (mg/l)	0.0

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

4.9 Saving and Running the ART3D Simulation

Now that all the model data have been entered, we will save the simulation and run RT3D.

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

2. Locate and open the **\tutfiles\ART3D\art3d** directory.

3. Enter **forward** for the name of the file and select the *Save* button.

4. Select the *ART3D* | *Run ART3D* command.

5. After a few seconds, when the line, "*Simulation completed successfully*" appears in the window, make sure the "*Read solution on exit*" toggle is checked, and then select the *Close* button to exit the model wrapper dialog. The solution will be automatically read into memory.

4.10 Viewing the Results

A new folder, called *forward (ART3D)*, will appear in the Project Explorer at the right of the screen. This folder contains the concentration data sets generated as part of the ART3D solution. Any of the four species can be viewed by clicking on the name of the corresponding data set in the Project Explorer. The current time step can be changed by selecting a time in the *Time Steps* list at the bottom of the *Project Explorer*.

1. Expand the solution *forward (ART3D)* folder to show the four data sets.
2. Click on the "**PCE**" data set.
3. Select the 14600 time step in the *Time Steps Window* below the *Project Explorer*.

4.11 Iso-Surfaces

ART3D solutions are best viewed using either contours or iso-surfaces. First, we will experiment with the iso-surface approach. An iso-surface is a 3D display of a surface corresponding to a threshold concentration value. To set up the display of iso-surfaces, we will turn off the display of the grid cells and turn on the iso-surfaces.

1. Select the *Display* | *General Mode* command. This allows us to view the grid in an oblique direction, rather than only along the I, J, and K axes.
2. Select the *Display Options* macro.
3. Turn off the *Cell Edges* option.
4. Turn on the *Grid Shell* option. This displays a line along the border of the 3D grid.
5. Turn off the *Contours* option.
6. Turn on the *Iso-surfaces* option.
7. Select the *Options* button next to the *Iso-surfaces* option.
8. Change the *Number of iso-surfaces* item to **7**.
9. Select the *Default* button. This creates 7 evenly spaced iso-values between the max and min values for the data set.
10. Turn on the *Iso-surface faces* option
11. Select the *OK* button twice to exit both dialogs.

You should see some nested iso-surfaces corresponding to the selected concentrations. To get a better view of the iso-surfaces:

12. Select the *Oblique View* macro.

13. Select the *Display Options* macro .
14. Change the *Z magnification* value to **3.0**.
15. Select the *OK* button.

To view iso-surfaces for a different data set:

16. Click on the **DCE** item in the *Project Explorer*.

Notice that the iso-surfaces have disappeared. This is because the DCE data set has a smaller range of values than the PCE data set. To change the iso-values:

17. Select the *Data* | *Iso-Surface Options* command.
18. Select the *Default* button. Notice how the values change.
19. Select the *OK* button.

4.12 Contours

Another useful way to view the model results is with contours.

1. Select the *Display* | *Display Options* command.
2. Turn off the *Iso-surfaces* option.
3. Turn on the *Contours* option.
4. Select the *OK* button.

The best way to view contours on a 3D grid is to view one layer at a time. This can be accomplished using the "Ortho Mode".

5. Select the *Display* | *Ortho Mode* command.
6. Click on the up arrow in the *Mini-grid plot* in the *Tool Palette* if necessary to move the display to the top-most layer (number 11).

Another useful contour option is to use the "Color fill contour" feature.

7. Select the *Data* | *Contour Options* command.
8. Select the *Color fill* option from the *Contour method* combo box.
9. Select the *OK* button.

At this point, you may wish to try selecting different species and different time steps from the *Project Explorer* window. Notice how the contours are automatically updated.

4.13 Setting Up an Animation

Finally, we will set up an animation to illustrate how the DCE solution changes over time. To speed up the generation of the film loop, we will switch back to linear contours, but we will associate a color ramp with the contours.

To change the contouring options:

1. Select the *Data* | *Contour Options* command.
2. Select the *Linear* option from the *Contour method* combo box.
3. In the *Line options* section, change the *Line color method* to be **Color Ramp**.
4. Click on the *Color Ramp* button.
5. Turn on the *Legend* option
6. Select the *OK* button twice to exit both dialogs.

To set up the animation:

7. Select the *Display* | *Animate* command.
8. Make sure the *Data set* option is on and click *Next*.
9. Turn on the *Display clock* option.
10. Select the *Finish* button.

You should see some images appear on the screen. These are the frames of the animation which are being generated.

1. After viewing the animation, select the *Stop* ■ button to stop the animation.
2. Select the *Step* ▶| button to move the animation one frame at a time.
3. You may wish to experiment with some of the other playback controls. When you are finished, close the window and return to GMS.

5 Conclusion

This concludes the *ART3D - Basic* tutorial. Here are the things that you should have learned in this tutorial:

1. ART3D is a 3-dimensional analytical reactive transport model.
2. ART3D considers retardation, advection, dispersion, and the reactions of multiple species. It also allows for complex reaction sequences.

3. The ART3D model runs relatively quickly and is useful as a screening tool.

4. You can visualize the result from ART3D as 3D isosurfaces or contours in GMS.

5. You can create animations of 3D isosufaces or contours in GMS from the output produced by ART3D.