ART3D - Stochastic

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 stochastic run. We will be working with the same problem described in the *ART3D – Basic* tutorial. You should complete the *ART3D – Basic* tutorial, prior to beginning this tutorial.

1.1 Outline

This is what you will do:

1. Open a forward run simulation.
2. Edit ART3D parameters.
3. Run ART3D in stochastic mode.
4. Run a threshold concentration risk analysis for each contaminant.

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 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.

3 Running a Stochastic Simulation

As with any groundwater model, there is typically a significant amount of uncertainty in the input parameters used to build an ART3D simulation. One approach for addressing this type of uncertainty is to perform a stochastic simulation. The ART3D model has built in capabilities for performing simple Monte Carlo style stochastic simulations. In this mode, ART3D will run multiple simulations with randomly chosen parameter values. These parameter values can be purely random or can follow a normal distribution. The output from a stochastic simulation is a number of equally likely solutions. These solutions can be analyzed as a group in a threshold analysis to determine the probability that Maximum Contaminant Levels (MCL) will be exceeded in the aquifer. We will now run a stochastic simulation using the same case study as that used in the forward run.

3.1 Selecting the Stochastic Option

In the *General Options* dialog, we will set ART3D to run in stochastic mode and we will designate the number of simulations to be run.

1. Select the Open button.
2. Locate and open the **tutfiles\ART3D\art3d\sample** directory.
3. Open the file entitled **forward.gpr**.
4. Select the ART3D | General Options command.
5. Select the Stochastic Mode options from the Simulation Type section of the dialog.
6. Set the Number of Simulations to 30.

7. Select the OK button.

3.2 Changing the Output Frequency

For the stochastic run, we will analyze the conditions at the end of 40 years. To minimize the amount of information stored on disk, we will change the output control options to only save the solution at t=40 yrs, rather than at every two years as was the case with the forward run.

1. Select the *ART3D | Output Control…* command.
2. Set the *Number of output time steps* to **1**.
3. Select *OK* to close the *Output Control* dialog.

3.3 Setting up the Parameters Dialog

When running in stochastic mode, we must select the parameters to be varied in each simulation and provide statistical data for these parameters. These data include a mean value, upper and lower bounds, a distribution type, and (in the case of a normal distribution) a standard deviation value. In this simulation, we will randomize the retardation factor, velocity, longitudinal dispersivity and decay constants.

1. Select the *ART3D | Parameters* command.
2. By default all of the parameter values are selected for randomization. Unselect the *Vary* column for the following parameters: *AlphaY/AlphaX*, *AlphaZ/AlphaX*, *PCE Co*, *TCE Co*, *DCE Co*, and *VC Co*. This will dim out the *Max*, *Min*, *Distribution* and *Standard Deviation* columns for each of these parameters.
3. Make sure that the rest of the parameters have *Normal* selected in the *Distribution* column.
4. Fill in the other four columns as shown in the table below. Note that the mean values are not the same as the values used in the forward run in Section **Error! Reference source not found.**.

Parameter	**Mean**	**Min**	**Max**	**St. Dev.**
Retard	1.2	0.9	1.5	0.1
Velocity (m/d)	0.015	0.003	0.03	0.0061
Alpha x (m)	12.2	6.1	18.3	2.44
PCE K (1/d)	0.000525	0.00035	0.0007	0.00008
TCE K (1/d)	0.000345	0.00015	0.00054	0.00008
DCE K (1/d)	0.000526	0.00044	0.00061	0.00003
VC K (1/d)	0.00082	0.0007	0.00094	0.00005

5. Select the *OK* button when you are finished.

3.4 Saving and Running the ART3D Stochastic Simulation

We are now ready to save the simulation and run ART3D in stochastic mode.

1. Select the *File | Save As* command.
2. Enter **stochastic** for the project name and select the *Save* button.
3. Select the *ART3D | Run ART3D* command.

When the simulations begin running, a progress dialog will appear. The spreadsheet at the top of this dialog shows the random values being used in each simulation. The progress bar in the middle estimates the progress through the simulations. The text window at the bottom lists any error messages and indicates when the solution has finished by printing the line “Simulation completed successfully”.

4. When the simulations finish, make sure the “*Read solution on exit*” toggle is checked, and then select the *Close* button.

The output from this stochastic ART3D simulation is 30 separate sets of solution files. GMS reads these in automatically.

A new folder will be added to the Project Explorer called *stochastic*. Inside this folder, there will be another folder for each of the separate solutions. These are titled *stochastic1(ART3D)*, *stochastic2(ART3D)*, etc.

The individual solutions can be viewed by clicking on a folder or on a data set name within a folder.

3.5 Threshold Concentration Risk Analysis

Each of the 30 solutions computed by ART3D in this stochastic run can be analyzed separately or as a group using a threshold concentration risk analysis. Next, we will perform a risk analysis to determine the probability that the contaminant concentrations will exceed the US EPA’s maximum contaminant levels (MCL). These levels are 0.005 mg/l for PCE and TCE and 0.002 mg/l for VC (http://www.epa.gov/safewater/mcl.html). Because there are separate MCL levels for the different isomers of DCE, they will not be considered here.

1. Right-click on the folder containing all 30 of the solutions (the one called *stochastic*) and choose *Risk analysis*.
2. Accept the default options in the first dialog and select the *Next* button.
3. Choose **PCE** as the dataset, ‘>’ as the operator, and **0.005** as the value.
4. Enter **PCE_MCL** for the *Analysis title*.
5. Select *Finish* to begin the analysis. The analysis may take a minute or two.

After the analysis finishes and the dialog disappears, a new data set will appear in the *stochastic* folder called *PCE_MCL*. This data set can be displayed using any of the visualization tools in GMS including contours and iso-surfaces. You may notice that the contours are slightly "irregular." This is because the analysis was performed using only 30 simulations and each cell has a probability that is based on some integer between 0 and 30 divided by 30 (8/30, 12/30, etc.). The contours become smoother when a larger number of stochastic runs are performed.

6. Repeat the previous steps to perform a threshold concentration analysis for TCE (value = **0.005**) and VC (value = **0.002**).

Analysis of these data sets shows that there is a fairly large area in the center of each plume where all of the random simulations resulted in concentrations over the EPA MCL. An even larger area includes the areas with these high concentrations in 50% or more of the simulations.

A stochastic simulation helps keep a modeler from thinking in terms of "one right answer." Instead, it encourages the consideration of a range of possibilities. The stochastic simulation also allows the solution to mirror the uncertainty in the input parameters.

4 Conclusion

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

1. ART3D can be run in stochastic mode.
2. When running in stochastic mode the input parameters to ART3D are allowed to vary.
3. The output from a stochastic run can be used to do a threshold risk analysis in GMS.