ART3D – Parameter Estimation

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 parameter estimation 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 the forward run simulation.
2. Import field observation data.
3. Define additional conditions.
4. Run ART3D in forward run mode to compare with the previous forward run.
5. Run ART3D in inverse mode using several different starting values.

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 ART3D in Inverse Mode

One method of dealing with uncertainty in the input parameters for an ART3D simulation is to calibrate the model to field observed data by varying the input parameters until the output matches field conditions. This can be done manually, but it can be a tedious, difficult process. ART3D has a built in parameter optimization routine. When running in inverse mode, ART3D will try to minimize the difference between observed and calculated concentration values at any number of user-defined observation points by systematically perturbing input parameters within user-defined bounds. In this section, we will add observation points to the forward run simulation, note the error, and then use ART3D to optimize the parameter values.

3.1 Retrieving the data from the Forward Run

We will start with the same simulation we used in the forward run simulation.

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 *Save As* command from the *File* menu and save the project in the tutfiles\art3d directory as **paramest.gpr**.

3.2 Creating an Observation Coverage

The first step in setting up the parameter estimation run is to enter the observation well data. The observed data must be entered in an observation coverage in the *Map* module. To create an observation coverage:

1. In the *Project Explorer* right-click on the empty space and then, from the pop-up menu, select the *New* | *Conceptual Model* Command.
2. In the dialog that comes up, change the *Name:* to "**ART3D**" and select **ART3D** from the *Model:* drop down list.
3. Select the *Define species…* Button.
4. Select the *New* button four times to create four species.
5. 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.
6. Select the *OK* button twice.
7. Right-click on the **ART3D** conceptual model and select the *New Coverage* command from the pop-up menu.
8. Change the *Coverage name* to **Observation**.
9. In the list of *Observation Points*, turn ON the following species that we want to observe: **PCE**, **TCE**, **DCE**, and **VC**.
10. Click *OK* to exit the dialog.

3.3 Entering the Observation Data

Next, we will enter the observation point data using the Observation Coverage dialog. We will create four points in the observation coverage and enter the field data for each point. The field data will correspond to the values observed after 40 years of transport.

1. Right-click on the **Observation** coverage in the *Project Explorer* and select *Attribute Table...*

Creating the Observation Points

1. Click on the *Add Point* button at the bottom of the dialog repeatedly to create a total of four points.
2. Turn on *Show point coordinates* and enter the coordinates for the four observation points according to the following table:

Name	x	y	z
new_point_1	15	75	15

new_point_2	30	75	15
new_point_3	60	75	15
new_point_4	120	75	15

3. In the *All* row, *Type* column, select the **Obs pt.** option.

Entering the Observed Concentrations

Finally, we will enter the observed concentrations. For each observed species, we will enter an observed xy series and a standard deviation. Since the model will have only one time step we will enter the observed value at time zero. The standard deviation defines the estimated error associated with the observation. This value is important because during the parameter estimation process, each observation is given a weight equal to one divided by the square of the standard deviation.

1. For *new_point 1*, select the ... button in the *Obs. PCE* column

2. Enter **14600** for the *Time* and **16.8** for the *Obs. PCE* and hit *OK*.

3. Enter the standard deviation as **1.7** for *new_point_1* in the *Obs. PCE std. dev* column.

4. Repeat the previous three steps with the remaining points and their values according to the following table.

Name	Time (d)	PCE - Observed value	Standard deviation
new_point_1	14600	16.8	1.7
new_point_2	14600	12.6	1.7
new_point_3	14600	4.7	1.7
new_point_4	14600	0.8	1.7

5. Repeat this process for the other species, by selecting the appropriate species column and entering the observed data and standard deviations as shown in the following tables:

Name	Time (d)	TCE - Observed value	Standard deviation
new_point_1	14600	20.4	1.8
new_point_2	14600	9.8	1.8
new_point_3	14600	5.1	1.8
new_point_4	14600	0.3	1.8

Name	Time (d)	DCE - Observed value	Standard deviation
new_point_1	14600	2.2	0.5
new_point_2	14600	3.7	0.5
new_point_3	14600	2.9	0.5
new_point_4	14600	0.5	0.5

Name	Time (d)	VC - Observed value	Standard deviation
new_point_1	14600	0.4	0.13

new_point_2	14600	0.8	0.13
new_point_3	14600	0.9	0.13
new_point_4	14600	0.4	0.13

6. When all the data have been entered, select the *OK* button.

Setting the Number of Time steps

Since the observed values were measured at the end of 40 years, we will just use one time step of length 40 years.

1. In the *Project Explorer* click on the *3D Grid Data* folder .
2. Select the *ART3D* | *Output Control* command.
3. Change the *Number of output time steps* to **1**.
4. Select *OK* to close the dialog.

3.4 Selecting the Observation Coverage

We must first connect the observation coverage to the ART3D model

1. Select ART3D | General Options… command.
2. Select the toggle for **Observation** in the Observation coverage to use spreadsheet.
3. Select OK to close the dialog.

3.5 Comparing the Field Data to the Calculated Data

Now we will run a forward simulation again, this time with the observation points, and when we read in the solution, the calibration targets will show how closely the results from the forward run match the field observed values.

1. Select the *File* | *Save* command.
2. Select the *ART3D* | *Run ART3D* command.
3. When the line "*Simulation completed successfully"* appears, make sure the "*Read solution on exit*" toggle is checked and close the dialog by selecting *Close*.
4. Click on any of the data sets in the *Project Explorer*. The plume contours will be displayed in addition to the calibration targets for each observation point. Click on each of the species and watch the calibration targets change. An analysis of these calibration targets shows that the output does not match the field observed data very closely.

3.6 Setting up the Inverse Simulation

Now that the observation values have been entered, we will run several inverse runs and attempt to calibrate the model to match field data.

5. First, save the project under a new name by choosing the *Save As* command from the *File* menu. Enter **paramest2.gpr** for the name of the project.

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

7. Change the simulation type to *Parameter estimation mode* and leave the stopping tolerances at their default values.

8. Select the *OK* button.

9. Select the *ART3D | Parameters* command.

10. Uncheck the following parameters in the *Solve* column:

- **AlphaY/AlphaX**
- **AlphaZ/AlphaX**
- **PCE_Co**
- **TCE_Co**
- **DCE_Co**
- **VC_Co**

11. This should leave the **Retard, Velocity, AlphaX** and the four decay constants as the parameters that will be optimized.

12. Fill in the starting values and upper and lower bounds for each of the parameters to be optimized according to the following table:

Parameter	Start value	Min Value	Max Value
Retardation	1.46	1	1.5
Velocity	0.027	0.003	0.03
Alphax	8.53	6.1	18.3
PCE_k	0.00044	0.00035	0.0007
TCE_k	0.00022	0.00015	0.00054
DCE_k	0.00056	0.00044	0.00061
VC_k	0.00076	0.0007	0.00094

1. Select *OK* to close the dialog

3.7 Running in Inverse Mode

Now we will run in inverse mode to optimize the parameter values.

1. Select the *File | Save* command.

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

This will open up a progress dialog for the Run. The spreadsheet in the middle will show the values for each parameter and the observation error as the iterations run. The error at the observation points will also be displayed in the plot at the top of the dialog. When the line *Simulation completed successfully* appears, the simulation has finished. The final error should be 21.9875.

The same window shows the reason the optimization stopped. *False Convergence* means that a local minimum was reached without the error dropping below the *Absolute Convergence Tolerance* entered in the *General Options* dialog. This does not necessarily mean that the solution found does not correspond to the global minimum. In many cases, the optimal solution will be found without satisfying the absolution convergence tolerance. We can attempt to reduce this error by changing the upper and lower bounds and/or the starting values. This optimization routine, like others, is very dependent on the chosen starting point value, so we will repeat this process several more times to see if we can improve the results. But first we will read in the computed solution.

3. Make sure the "*Read solution on exit*" check box is selected and then select the *Close* button.

3.8 Viewing the Optimized Solution

After the optimized parameter values are returned, ART3D automatically runs one more time with the optimized values. This optimized solution will be read in now.

1. The solution should have been automatically read in when the previous dialog was closed.

2. Expand the *paramest2 (ART3D)* item  in the *Project Explorer*.

3. Click on any of the datasets in the *Project Explorer* to see the calibration targets. Note that some of the targets show that the computed values are quite close to the observed values.

4. To see the final optimized values, select the *ART3D | Parameters* command.

5. Select the *Import Parameters* button. This changes the start values to the optimized values. At this point it is often useful to check and see if any of the optimized parameter values correspond to the upper or lower limit for the parameter. Leave the dialog open for the next step.

3.9 Trying Other Starting Points

Like all optimization routines, optimization is very sensitive to the starting point provided by the user. In order to ensure a good calibration, we will run the inverse simulation two more times with other starting point values and compare the error values to determine the best fit.

1. Enter the following data into the *Parameters* dialog.

Parameter	Start Value
Retardation	1.18
Velocity	0.03
Alphax	14.4
PCE_k	0.00064
TCE_k	0.00022
DCE_k	0.00053
VC_k	0.00078

2. Select *OK*.

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

4. Rename the file "**paramest3.gpr**" and select *save*.

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

6. When the simulation finishes, hit the *Close* button.

This time, the final error is 26.2962, not as good as the previous simulation. Now we will try a third set of starting values.

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

2. Select the *Import Parameters* button to view the final optimized parameter values.

3. Enter the following values in the *Parameters* dialog:

Parameter	Start Value
Retardation	1.2
Velocity	0.015
AlphaX	12.2
PCE_k	0.000525
TCE_k	0.000345
DCE_k	0.000526
VC_k	0.00082

4. Save the project as "**paramest4.gpr**" and run the simulation again.

In this third case, the final error is 21.4409. The best calibration occurred with the third set of starting values, although all four inverse runs yielded similar parameter values. You may wish to try other starting values and try to get a closer fit to the observed data. Changing the standard deviations assigned to the observation points may also change the results.

4 Conclusion

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

1. ART3D can be run in parameter estimation mode.

2. You can compare the results of an ART3D run to field data by using observation points.

3. You must have observation data to run ART3D in parameter estimation mode.