

EFFECTIVE GROUNDWATER MODEL CALIBRATION: With Analysis Of Data, Sensitivities, Predictions, and Uncertainty

By Mary C. Hill and Claire R. Tiedeman

Computer Instructions for the Exercises, using four U.S. Geological Survey computer programs: MODFLOW-2000 and its Observation, Sensitivity, and Parameter-Estimation Processes; MFI2K; GW_Chart; and ModelViewer

This document contains instructions for using the USGS public-domain, open-source software MODFLOW-2000 and related programs to do the exercises that involve model simulations.

File setup

The following directory structure contains the files needed to do the exercises using the Observation, Sensitivity, and Parameter-Estimation Processes of MODFLOW-2000:

Directory	Contents
First level	
MF2K\	Subdirectories bin\ exer\ initial\ answers\
Second level	
bin\	See table below under “Software setup”
exer\	Executables and batch file MFI2KRUN.BAT. Subdirectory steady\ All files and folders that you create when doing the exercises.
initial\	Subdirectories ex5.1b.i\ ex8.1a.i\ ex8.1b.i\ ex8.1e.i\
answers\	Final files for all exercises. This is what exer would look like if all the exercises were conducted as described in the instructions for using MFI2K. Subdirectories ex5.1b\ ex8.1a\ ex8.1b\ ex8.1e\ steady\
steady\	Files needed by exercises 8.1a, 8.1b, and 8.1e.
Third level	
ex5.1b.i\ ex8.1a.i\ ex8.1b.i\ ex8.1e.i\	Files in directory initial\ that contain data needed to begin exercises 5.1b, 8.1a, 8.1b, and 8.1e.
ex5.1b\ ex8.1a\ ex8.1b\ ex8.1e\	Final files for exercises 5.1b, 8.1a, 8.1b, and 8.1e. Distributed in directory answers\.
steady\	This directory has been copied from the second level into exer\ and answers\

Software setup

The executables for the software needed to do the exercises using the Observation, Sensitivity, and Parameter-Estimation Processes of MODFLOW-2000 are in the \bin directory, including:

Program	Executable file	Comment
MODFLOW-2000	mf2k.exe	Ground-water flow model
MFI2K	mfi2k.exe	Simple preprocessor for MODFLOW-2000
BEALE-2000	beale2k.exe	Calculates measures of model nonlinearity
RESAN-2000	resan2k.exe	Calculates statistics for residual analyses
YCINT-2000	ycint2k.exe	Calculates linear intervals on predictions

Suggested setup for using this software:

Some of the executables in the \bin\ directory need to be executed in the \MF2K\exer\ directory which is used by students. These executables have already been copied to this directory. You could also do one of the following: (1) Copy all files in the \bin\ directory to a directory listed in the PATH environment variable (type "path" at the DOS prompt to display the value of PATH); or (2) If you know how to modify the PATH variable on your computer, you could add the \bin\ directory to the PATH.

Create shortcuts on the Windows desktop for mfi2k.exe and gw_chart.exe. To do this, in Windows' File Explorer, right click and drag each of these two programs from Explorer to the desktop and select "Create Shortcuts Here". From then on, either of these programs can be started by double-clicking on the shortcut icon.

With MFI2K the user initiates a MODFLOW-2000 run by using the "Run MF2K" item on the FILE menu. When you select "Run MF2K", MFI2K tries to invoke a batch file named MFI2KRUN.BAT; this file is in the \bin\ directory and the \MF2K\exer\ directory. If, when you select "Run MF2K", a black window appears and immediately disappears, it means that the operating system cannot find MFI2KRUN.BAT. This will occur if MFI2KRUN.BAT is neither in a directory listed in the PATH, nor in the directory where the MODFLOW data set resides. If this happens, copy MFI2KRUN.BAT into a suitable directory. Similarly, when MFI2KRUN.BAT is executed, it invokes mf2k.exe, which must be in a directory in PATH or in the current directory.

GW_Chart is a plotting program for output from MODFLOW-2000, and ModelViewer enables three-dimensional visualization of spatially variable model input and output; both programs can be downloaded from the book website.

It is advantageous to use the executables distributed in the \bin directory, because these versions of the programs are consistent with the exercise instructions in this document, and with the results presented in the book. The latest versions of the programs can be downloaded at <http://water.usgs.gov/nrp/gwsoftware/modflow.html>.

Exercise 3.1. Steady-State Parameter Definition

In this exercise, all input for the steady-state simulation will be prepared, using parameters to define the ground-water system. The preprocessing program MFI2K (<http://water.usgs.gov/nrp/gwsoftware/MFI2K/MFI2K.html>) will be used to simplify preparation of input files. The parameter values listed in Table 3.1 of Hill and Tiedeman (repeated below as Table 1) should be used in the input files. These will be the starting values when nonlinear regression is performed.

Table 1: Parameter Name and Starting Value for Properties of the Steady-State Flow-System for Which Parameters Are Estimated in Subsequent Exercises.

Flow-system property	Parameter name	Starting value
Horizontal hydraulic conductivity of layer 1, in m/s	HK_1	3.0×10^{-4}
Vertical hydraulic conductivity of confining bed, in m/s	VK_CB	1.0×10^{-7}
Horizontal hydraulic conductivity of layer 2 in columns 1 and 2, in m/s	HK_2	4.0×10^{-5}
Hydraulic conductivity of the riverbed, in m/s	K_RB	1.2×10^{-3}
Recharge in recharge zone 1, in cm/yr	RCH_1	63.072
Recharge in recharge zone 2, in cm/yr	RCH_2	31.536

1. **Start MFI2K in directory *exer* and create a new MODFLOW-2000 dataset named *ex3.1*** by entering *ex3.1.nam* when prompted for the name file. Refer to pp. 21-24 in Hill and Tiedeman for description and illustration of the flow system. Specify 18 rows and columns, 2 model layers, and free format.
2. **DIS input** (Harbaugh and others, 2000, p. 45-46): Click on the “DIS” menu item, and then in the “DIS Menu” dialog box, click on the buttons below “Check” and enter the following data: Set model time and length units (seconds and meters). Set DELR = DELC = 1000 m. Specify that a confining bed below layer 1 is to be simulated (LAYCBD). For the top elevation of layer 1, use 100 m. Bottom elevations of layer 1, the confining bed, and layer 2 can be determined from Fig. 2.1 in Hill and Tiedeman (p. 22). Note that the default is to simulate one steady-state stress period.
3. **BAS input** (Harbaugh and others, 2000, p. 50-51): Click on the “BAS” menu item, and specify IBOUND=1 for all cells, which means that all cells are active. Set initial head = 200 m. Be sure to specify IBOUND and initial head values for both layers 1 and 2.
4. **RIV input** (Harbaugh and others, 2000, p. 65-66):
 - Click on the “STRESS” menu item, then click on the RIV button. Click on “New” and define one parameter named K_RB, which will represent hydraulic conductivity of the riverbed. The initial value is given in Table 1 above. Close this window.

- Now you will specify the cells of the river reach and data associated with them. Click “Modify” in the lower left corner of the “List Data” window. In the window that comes up, click “Send for external editing”. The following window should appear:

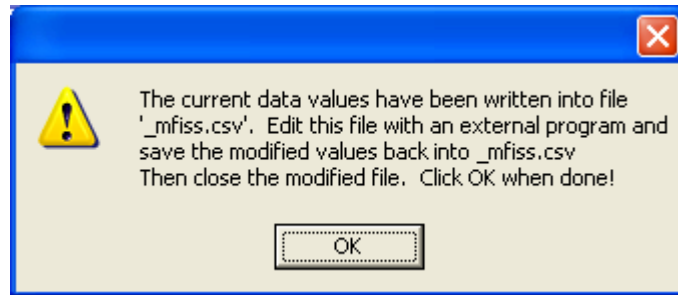


Figure 1.

- **Leave this window open** until you have completed editing the “_mfiss.csv” file.
 - Edit the “_mfiss.csv” file with an external program such as Excel, Notepad, Emacs, or other program to define the list values. Specify that the river reach is in layer 1, column 1, rows 1-18. Stage in the river is 100 m, and the elevation of the riverbed bottom is 90 m. The RIV Package requires riverbed conductance ($K \cdot L \cdot W / M$) as input, which is calculated in MODFLOW-2000 as the product of the parameter and Condfact. Accordingly, $\text{Condfact} = (L \cdot W / M) = 1000 \text{ m}$ for each river cell.
 - When you finish editing “_mfiss.csv”, it needs to be saved in CSV (“comma-separated value”)format. Excel or another spreadsheet program generally can conveniently be used to edit CSV files. When using Excel, the most convenient way to save “_mfiss.csv” in CSV format is to click the X at the upper right corner of the document window (smaller window within the Excel program window). Excel will ask “Do you want to save the changes...” Click “Yes”. Excel will ask “_mfiss.csv may contain features...Do you want to keep the workbook in this format?” Click “Yes”.
 - **Now** click the OK button on the window that looks like Figure 1. MFI2K will now read in the revised “_mfiss.csv” file
 - Click “OK”.
 - Finally, in the “List Data” window, activate K_RB for stress period 1, and then click “OK”.
5. **GHB input (Harbaugh and others, 2000, p. 76-77):**
- In the Stress Dialog box, click on GHB. Under “Non parameter data”, click Package, and “Send for external editing”. Follow the same steps related to the “_mfiss.csv” file as shown above for the RIV package. Define 36 GHB cells in rows 1-18 of column 18, in both layers 1 and 2. The boundary head is 350 m, and hydraulic conductance between the cell and the external source/sink is $1.0E-7 \text{ m}^2/\text{s}$.
 - Click “OK” or “Close” in all the windows.

6. **Execute MODFLOW-2000.** Save the dataset (Under the “File” menu) and execute MODFLOW-2000 from the FILE menu. The output files will be produced in directory *exer*. Because a flow package (e.g. LPF) has not been activated, the calculated heads and budget are meaningless. However, the list file (*ex3.lst*) should show 18 river reaches with stage = 100, conductance = 1.2, and bottom elevation = 90. There also should be 36 GHB cells listed with stage = 350 and conductance = 0.1E-6.
7. **Multiplier arrays** (Harbaugh and others, 2000, p. 47): Click on the “Zone-Mult” menu item and choose “Multiplier Arrays”. Click on “ADD” to define a multiplier array named “RCH_CONV” and set it to the constant 3.170979E-10; this will be used to convert recharge parameter values provided in cm/year to the model units of meters/sec. Click “ADD” again to define a multiplier array named “HK_2_MULT”, which is used to simulate the variability of hydraulic conductivity of layer 2. Click “Package” and “Send for external editing,” and the window in Figure 1 above should appear. Keep this window open, and open the “_mfiss.csv” file externally. In this 18 x 18 array, values should equal 1.0 in all rows of columns 1 and 2, 2.0 in all rows of columns 3 and 4, 3.0 in columns 5 and 6, and so on, ending with values of 9.0 in columns 17 and 18. Close the “_mfiss.csv” file, and set multiplier = 1.0 in the “Define Multiplier Arrays” dialog box, then click “OK”.
8. **Zone array** (Harbaugh and others, 2000, p. 49): Click on the “Zone-Mult” menu item and choose “Zone Arrays”. Click on “ADD” to define a zone array named “RCH_ZONE”. Click “Package” and edit the “_mfiss.csv” file so that the zone array has a value of 1 in columns 1-9 and a value of 2 in columns 10-18. Set multiplier = 1.0 and click “OK”. This array defines recharge zones.
9. **RCH input** (Harbaugh and others, 2000, p. 67-68): Click the “STRESS” menu item and click on the RCH button. Under “Parameter Data”, click “New” and the “Array Parameter Definition” dialog box appears. Define parameter name RCH_1, which controls recharge in recharge zone 1, and specify the parameter value from Table 1 above. In the first line of the table in this dialog box, specify that zone array RCH_ZONE and multiplier array RCH_CONV apply to this parameter, and set Z1 to 1 to indicate that the parameter applies to zone number 1 in the zone array. Click OK, then Click “New” again, and follow the same steps to define parameter RCH_2. For this parameter, set Z1 to 2. When done with the RCH_2 definition, specify that recharge applies to the top model layer, and activate both parameters for stress period 1, click “OK”, and close the STRESS Dialog box.
10. **LPF input** (Harbaugh and others, 2000, p. 59-62). Click the “Internal Flow” menu item and choose LPF.
 - Click “LAYTYP”, to specify model layer flags. Set LAYVKA so that VKA represents horizontal to vertical anisotropy for both layers. Keep the default values for the other items, and click “OK”.
 - Click “Hydraulic” to enter parameter data. Make sure “HK” is chosen, and click “New”. Follow steps similar to the RCH definition to define parameter HK_1 to control hydraulic conductivity (HK) of layer 1 (see table 1 above for parameter values). Although this parameter has no associated multiplier or zone arrays, in the

first line of the table of the “Array Parameter Definition” dialog box, a “1” must be entered for “Layer”; the default “ALL” listed under “Zone Array” means that the parameter value applies to all cells in layer 1. Click “OK”

- When back in the “LPF Hydraulic Data” dialog box, keep “HK” selected and click “New”. Follow similar steps to define HK_2 to control HK of layer 2, using multiplier array HK_2_MULT, which allows HK to increase with distance away from the river.
- When back in the “LPF Hydraulic Data” dialog box, change the parameter type to VKCB. Follow the steps for defining HK_1 to define a VKCB parameter called VK_CB to control vertical hydraulic conductivity of the confining bed; use the parameter value in Table 1 above.
- Finally, define VKA (horizontal to vertical anisotropy) using non-parameter input, and specify a constant value of 1.0 for both layers.
- Click “OK” on the “LPF Hydraulic Data” dialog box and close the LPF Menu.

11. **Solver Menu:** Use default PCG with all default values. (Harbaugh and others, 82-83)

12. **Output Control** (Harbaugh and others, 2000, 52-55) Click the “OUTPUT” Menu item, and then click “Output file names and formats” to enable saving of heads. Change “Head Print Format” to 4. Use the default file name for a binary output file to which heads are to be saved, and click “OK”. Click “Times for Saving Head” and select option to save heads every stress period. Click “OK” and close the “Output Control Data” dialog box. (Harbaugh and others, 2000, 52-55)

13. Click on the “OPTIONS” menu item and choose “Show Files”. Note that the LIST output file is *EX3.1.LST*. Also note on the main screen what packages are being activated, and that they are all from MODFLOW-2000’s Ground-Water Flow Process (OBS, SEN, and PES are not listed).

14. Click on the “OPTIONS” menu item and choose “Check Complete” to verify that the data entry for all packages is complete.

15. Save the dataset and **run MODFLOW-2000** from the FILE menu. The output files will be produced in directory *exer*.

16. Compare the simulated heads and budget in *ex3.1.lst* to those in *ex3.1.lst* in the MF2K/*answers* directory to check that your model is set up correctly.

OPTIONAL Exercise 3.1a. Define horizontal and vertical anisotropy parameters

MODFLOW-2000 supports definition of parameters governing horizontal and vertical anisotropy. In the model setup thus far, such parameters were not defined. Here, these parameters will be defined in such a way that the simulated values are identical to those in Exercise 3.1.

In the LPF package, the horizontal anisotropy of each model layer can be defined as parameter type HANI, and the vertical anisotropy or vertical hydraulic conductivity for each model layer can be defined as parameter type VANI or VK (Harbaugh and others,

2000, p. 61). Parameter types VANI and VK affect simulation of the vertical flow of water between the model layers, and are most important when there is no intervening confining unit.

- In MFI2K, use the Save As option on the FILE menu to save the current dataset (*ex3.1*) as a new dataset called *ex3.1a* and use the *ex3.1a* dataset for this exercise.
- **Set CHANI = 0 for both layers** under the LAYTYP option for LPF input (under the “Internal Flow” menu item).
- Under the Hydraulic option for LPF input, note that there is now a parameter type called HANI. **Define a new HANI parameter** named HANI_1&2 that represents the horizontal anisotropy of layers 1 and 2. Do so by setting Layer to 1 and 2 in two different lines of the Array Parameter Definition dialogue box. Set the value of HANI_1&2 to 1.0 to produce output consistent with the previous results.
- **Define parameter VANI_1** to represent the vertical anisotropy of layer 1, and **define parameter VANI_2** to represent the vertical anisotropy of layer 2. There are no multiplication or zone arrays needed for these parameter definitions because in this exercise vertical anisotropy is constant throughout layers 1 and 2. Set VANI_1 and VANI_2 to 1.0 to produce output consistent with the previous results.
- **Run MODFLOW-2000**, and compare the output file *ex3.1a.lst* to the output file *ex3.1.lst*.
- Make sure that the simulated hydraulic heads and global volumetric rate budgets are identical. If they are not identical, check your definition of parameters HANI_1&2, VANI_1, and VANI_2.

OPTIONAL Exercise 3.1b. Define additive parameters for interpolation and stochastic methods

MODFLOW-2000 allows model inputs to be calculated as the sum of contributions from more than one parameter (Harbaugh and others, 2000, p. 16-19). This is important when hydraulic conductivity, recharge, and other quantities vary gradually over an area or volume, and are not well represented using zones of constant value. Although this capability is used to represent a simple linear variation in this exercise, it can be used to represent complex interpolation such as kriging, and can be used to add stochastic components to large-scale trends. In this exercise, you will apply this approach to the hydraulic conductivity of layer 2 of the steady-state model.

The goal is to maintain the same hydraulic-conductivity distribution in layer 2, but to allow the variation to be somewhat flexible. Here, we will maintain the assumption that hydraulic conductivity varies in a step-wise linear fashion in layer 2, but we will use two parameters to represent the nine-fold increase in hydraulic conductivity within the layer. One parameter represents the hydraulic conductivity beneath the river and the other

represents the hydraulic conductivity adjacent to the hillside. This definition would allow independently estimating these two parameter values by regression.

- In MFI2K, open dataset ex3.1 and use the Save As option on the FILE menu to save it as a new dataset called ex3.1b.
- **Replace the definition of parameter HK_2 with new parameters HK_2a and HK_2b** (this requires first deleting parameter HK_2, because a parameter name cannot be modified in MFI2K). Both new parameters will extend throughout layer 2. Make one parameter value equal the hydraulic conductivity in model columns 1 and 2; make the other equal the hydraulic conductivity in columns 17 and 18 (this will be 9 times the first value). Use multiplier array names MULTa and MULTb. The arrays need to be defined such that $HK_2a \times MULTa(i,j) + HK_2b \times MULTb(i,j)$ equals the hydraulic conductivity of cell i,j in the model setup for Exercise 3.1.
- **Run MODFLOW-2000**, and compare the output file *ex3.1b.lst* to the output file *ex3.1.lst*.
- Make sure that the simulated hydraulic heads and global volumetric rate budgets are identical. If they are not identical, check your definition of parameters HK_2a and HK_2b and of multiplier arrays MULTa and MULTb.

Exercise 3.2. Observations for the Steady-State Problem

Defining observations for the steady-state model with MODFLOW-2000 requires one input file that applies to all observations, one input file for the hydraulic-head observations, and one input file for the flow observations. Observed hydraulic heads for the steady-state model are in Table 3.2 of Hill and Tiedeman (p. 38).

3.2a - Define hydraulic-head observations.

- In MFI2K, under the “File” menu item, save the *ex3.1* dataset as dataset *ex3.2* and use the *ex3.2* dataset in this exercise.
- **File that applies to all observations** (OBS input, Hill and others, 2000, p. 27-30): Activate the Observation Process by clicking the “Observations” menu item, which opens the Observations Dialog window. Click “All Observations” and select the ISCAL5 option that specifies that both dimensionless and one-percent scaled sensitivities are to be printed. These will be used in later exercises.
- **Head observations file** (HOB input, Hill and others, 2000, p. 31-40): Enter data for the 10 steady-state head-observations listed in Table 3.2 of Tiedeman and Hill (p. 38), using the “Single Time Head” option on the Observations Dialog window. All observation wells are assumed to be located at the centers of model cells, so ROFF and COFF equal 0.0.
- Keep the Observations Dialog window open.

3.2b - Define the flow observation

The flow observation is defined as a head-dependent flow represented using the River Package (Hill and others, 2000, p. 41-46; 55-58). For the steady-state simulation, one flow observation, a gain to the river of $4.4 \text{ m}^3/\text{s}$, is available for the 18,000-ft reach of the river simulated in the model. The coefficient of variation for the observation is 10%. Note that a gain to the river is a loss to the ground-water system, so the observation should be entered as a negative value.

- **River observations file** (RVOB input, Hill and others, 2000, p. 55-58). On the Observations Dialog window, click “RIV Observations”. Click “ADD Cell Group” and then “EDIT Observation Times”. Name the observation “flow01.ss” and enter the observed value (called “HOBS” here) and coefficient of variation used for the statistic value. Assign a plot symbol of 2. Click “OK” and then “EDIT Cell Locations”. Define the flow observation using one cell group, which will include all 18 cell locations defined for the river in Exercise 3.1. Set FACTOR = 1.0 for all cells in the cell group. Close all dialog boxes.
- **Run MODFLOW-2000.** Examine the table of observed and simulated heads and flows that is near the end of *ex3.2.lst*. Verify that the observed head and flow information was entered correctly by comparing with Figure 3.2 of Hill and Tiedeman (p. 39). The *ex3.2._os* file lists simulated and observed values with more precision than in the LIST file.

- **Use ModelViewer** to visualize the hydraulic conductivity distribution and the simulated heads over the model domain.
To get started: Under the File menu item, select New; then in the Model Selection dialog box, select Modflow 2000; and then in the Modflow 2000 Data files dialog box, browse to directory *exer*, and specify *ex3.2.nam* as the name file. Keep the defaults in the Data Selection dialog box. When the model domain appears, under the Show menu item, select Solid, and under the Toolbox menu item, select Geometry and set z to 10 to specify 10x vertical exaggeration. Hydraulic heads are shown.
To visualize hydraulic conductivity, select Data under the Toolbox menu item, and choose K along rows. Under the Toolbox menu item, select Solid, and then select Blocky.
Additional ModelViewer capabilities and options are described in the online help system.

Exercise 3.3. Evaluate Model Fit Using Starting Parameter Values

Instructions for attempting to achieve a better model fit:

- In MFI2K, save the *ex3.2* dataset as dataset *ex3.3* and use the *ex3.3* dataset in this rest of this exercise. You will use the MODFLOW-2000 mode “Forward with Observations and Parameter-Value Substitution.”
- **Prepare a Sensitivity-Process input file (SEN file)** (Hill and others, 2000, p. 72-75) by clicking the Sensitivity menu item in MFI2K. Select the option “Do not calculate sensitivity and turn off PES.” With this option, values for parameters listed in the SEN file will override the values assigned in the individual package files, but sensitivities will not be calculated. Parameter values can then easily be changed in the SEN file rather than in the individual package files. To put the parameter values that you entered for the individual packages into the SEN file, click “Select Parameters to be included in the SEN file”, and then check “Include” for all parameters. Do not change any other options for the SEN file.
- **Run MODFLOW-2000** to demonstrate that the same results are obtained as in Exercise 3.2.
- Follow the instructions in the third bullet under “Problem” on page 40 of Hill and Tiedeman. To change parameter values in the “Sensitivity Dialog,” replace values in the column “SEN File Value (B)”.
- **Return all parameter values to their starting values** (listed in Table 1 above).

Exercise 4.1.: Sensitivity Analysis for the Steady-State Model with Starting Parameter Values

4.1a. Calculate sensitivities for the steady-state flow system

To calculate sensitivities in MODFLOW-2000, the Sensitivity Process must be activated by specifying a file name with file type SEN in the name file (MFI2K does this automatically if you access the Sensitivity Dialog, as was done in Exercise 3.3). In this exercise, you will calculate (1) the sensitivities related to the quantities defined as observations and (2) parameter correlation coefficients, by executing MODFLOW-2000 in the mode “Sensitivity Analysis to Evaluate Potential for Parameter Estimation.” This mode is listed as “Sensitivity Analysis” mode in Hill and others (2000, table 3, p. 12). Although parameters are not yet being estimated, this mode requires that the Parameter-Estimation Process also be activated, in order to calculate initial parameter correlations, discussed in exercise 4.1c.

- In MFI2K, save the *ex3.3* dataset as dataset *ex4.1*.
- **For the SEN file** (Hill and others, 2000, p. 72-75), **specify that sensitivities related to all six defined parameters are calculated.** Do this in the “Sensitivity Dialog” box. Set ISENALL=0 (“Use ISENS flags to determine if sensitivity will be calculated”) and for all parameters, set ISENS=1 (checked) and LN=0 (unchecked). Ensure that all parameter values are those listed in Table 1 above.
- **Activate the Parameter-Estimation Process input file (PES file)** (Hill and others, 2000, p. 78-84) by clicking the “Par. Est.” menu item. Use the default value of MAX-ITER=0 so that parameter estimation is not performed, but parameter correlations are calculated. Default values supplied by MFI2K also can be used for all other input variables.
- **Specify that both GLOBAL and LIST output files be produced.** In MFI2K, this is done from the OPTIONS menu; select GLOBAL/LIST. Name the global output file *ex4.1.glo* and the list output file *ex4.1.lst*. Sensitivity and regression information of most interest and information about the parameterization will be printed in *ex4.1.glo*, while the forward and sensitivity solutions will be printed in *ex4.1.lst*.
- **Run MODFLOW-2000** and make sure that the simulated hydraulic heads and global volumetric rate budgets in *ex4.1.lst* are the same as those in *ex3.3.lst*. If the hydraulic heads and volumetric rates in the two files are not the same, check your parameter entries in the SEN file.
- The composite, dimensionless, and one-percent scaled sensitivities are listed in the GLOBAL output file *ex4.1.glo* and in output files *ex4.1._sc*, *ex4.1._sd*, and *ex4.1._sl*, respectively. **Plot the composite and dimensionless sensitivities in GW_CHART** by selecting “Open File” from the “File” menu item, navigating to the *exer* directory, and selecting *ex4.1._sc* or *ex4.1._sd*. Parameter correlation

coefficients are located near the bottom of *ex4.1.glo* in the table “CORRELATION MATRIX FOR THE PARAMETERS”.

4.1d. Use contour maps of one-percent sensitivities for the steady-state flow system

For all active cells, MODFLOW-2000 calculates one-percent sensitivities of hydraulic head at each finite-difference cell in the grid to each parameter, because the sensitivity-equation method is used (Hill and others, 2000, p.67-71). These values can be printed, saved, and contoured, as for hydraulic heads. In MODFLOW-2000, the sensitivities printed and saved as entire arrays are not scaled if the parameter value equals 0.0 or if PID=CH. In this exercise MODFLOW-2000 will be run in the mode “Parameter Sensitivity with Observations” (Hill and others, 2000, p. 12).

Instructions for producing data files for the sensitivity contour maps:

- In MFI2K, save the *ex4.1* dataset as dataset *ex4.1d*.
- **Deactivate the Parameter Estimation (PES) Process** using the OPTIONS menu.
- To print hydraulic-head sensitivities calculated for the parameter values, **use the Sensitivity Dialog to specify a sensitivity print file** as *ex4.1d.sco* (Hill and others, 2000, p. 72-75).
- Save files and **run MODFLOW-2000**.
- The one-percent sensitivity arrays for all parameters are in *ex4.1d.sco*.

Exercise 5.1. Modified Gauss-Newton Method and Application to a Two-Parameter Problem

5.1.b. Examine the performance of the modified Gauss-Newton method

MODFLOW-2000 does not permit parameters from different flow process packages to be lumped together, so the lumped hydraulic-conductivity parameter includes only HK_1, HK_2, and VK_CB. The redefined three-parameter problem has the lumped hydraulic-conductivity parameter (K_MULT), the lumped recharge parameter (RCH_MULT), and K_RB. To produce a regression problem that is a function of only two parameters, the value of parameter K_RB is specified. Because the simulated equivalents of the head and flow observations are much less sensitive to K_RB than to most other model parameters, the resulting objective-function surfaces produced with this parameter setup are virtually identical to those produced by UCODE_2005 (for which it is possible to lump HK_1, HK_2, VK_CB, and K_RB together). Thus, for the situation with only head observations, the lumped recharge and hydraulic-conductivity parameters are essentially completely correlated.

- The two-parameter model has been set up for you, and is in directory *initial/ex5.1b.i/*. Copy all files from this directory to *exer*, and open dataset *ex5.1b* in MFI2K.
- **To include only the hydraulic-head observations, omit the flow observation from the regression.** Click on the “OPTIONS” menu item and choose “Deactivate”, then click on RVOB.
- **To perform the four regression runs listed on p. 83 of Hill and Tiedeman, modify the starting parameter values for KMult and RchMult using the “Sensitivity” menu item, and modify MAX-CHANGE using the “Par. Est.” menu item.** Then run MODFLOW-2000, and observe the behavior of the value of the weighted least-squares objective function summarized in *ex5.1b._ss*, and the changing parameter values from each iteration, which are listed in *ex5.1b._pa*. Plot the values in each of these files using GW_CHART.
- **Repeat these runs with the flow observation included.** In MFI2K, it is not possible to re-activate a process or set of observations that have been deactivated. To do so, exit MFI2K. Open the *ex5.1b.nam* file in a text editor and add an entry for the river observations file. Its file type is ‘RVOB’ and the name of the file is *ex5.1b.orv*. Then, re-open dataset *ex5.1b* in MFI2K, and you should see RVOB listed under ACTIVE OPTIONS on the main MFI2K window.
- **First repeat runs 1 through 4 above with the river observation weighted using a coefficient of variation (c.v.) of 10 percent.** This c.v. is already entered in the *ex5.1b.orv* file. Plot the values in *ex5.1b._ss* and *ex5.1b._pa* using GW_CHART.

- **Next, repeat runs 1 through 4 above with the river observation weighted using a c.v. of 1 percent.** To change this value, click on the “Observations” menu item, then on “RIV Observations”, then on “EDIT Observation Times”. Change the STATISTIC to 0.01.

Exercise 5.2. Estimate the Parameters of the Steady-State Model

5.2a. Define a range of reasonable values for each parameter

- In MFI2K, save the *ex4.1* dataset as dataset *ex5.2*.
- **In the SEN file, specify upper and lower reasonable values** (BU and BL) for each parameter on the basis of your experience regarding likely variability in hydraulic conductivity and recharge parameters. Make sure ISENS is set to 1 (checked) and LN is set to 0 (unchecked) for each parameter.

5.2b. First attempts at estimating parameters by nonlinear regression

- Click the “Par. Est.” button to examine variables in the PES file that control the nonlinear regression behavior and output. Set MAX-ITER to 10, MAX-CHANGE to 2.0, and TOL to 0.01.
- **Perform nonlinear regression by running MODFLOW-2000.** Look at the iteration information in the file *ex5.2.glo* and note that in iteration 1, parameter K_RB becomes negative, and in iteration 2, parameter HK_2 becomes negative, indicating physically unreasonable values for these parameters.
- *Optional:* To obtain the composite scaled sensitivities (*css*) for each parameter-estimation iteration shown in Table 5.5 of Hill and Tiedeman (p. 88), change IPRINT to 1 in the PES file and run MODFLOW-2000 again. This causes additional information to be printed for each iteration in the global output file. After examining the *css* in this file, change IPRINT back to 0 and run MODFLOW-2000 again.
- **Use GW_CHART** to look at *ex5.2._b* by choosing “Open file” from the “File” menu item (click “yes” when asked to divide the values by their initial values). Note that in file *ex5.2._b* (and *ex5.2._pa*), the values of these parameters are positive. MODFLOW-2000 makes this change to permit the regression to proceed. Close GW_CHART before proceeding; MODFLOW-2000 will not run if a needed file is open in GW_CHART.
Note that in *ex5.2._b*, the parameter values are in the same format as in file *ex5.2.sen*, and, if desired, parameter estimation could be restarted from any intermediate iteration by copying the parameter values from *ex5.2._b* into *ex5.2.sen*.
- Save file *ex5.2.glo* as *ex5.2b.ln0.glo*.
- To prevent parameters K_RB and HK_2 from becoming negative, the log transform of these parameters can be estimated instead of the native value. MODFLOW-2000 allows for log transformation of hydraulic conductivity, specific storage, and specific yield parameters (Hill and others, 2000, p. 71). **Specify that the log transform is to be estimated** by setting LN=1 for all four hydraulic-conductivity parameters, by checking the appropriate “Log Trans. (LN)” boxes in the Sensitivity dialog box. Execute MODFLOW-2000 to again perform parameter estimation.

- Save file *ex5.2.glo* as *ex5.2b.ln1.glo*.
- Examine the main output files *ex5.2.lst* and *ex5.2b.ln1.glo*, as well as the output files *ex5.2._b*, *ex5.2._pa*, and *ex5.2._ss*. Use GW_CHART to examine the changing parameter values.

5.2c. Assign prior information on parameters.

- Save dataset *ex5.2* as *ex5.2c*.
- **In the SEN file, set LN=0** for all parameters so that native values are estimated.
- **In the PES file, define prior information.** For K_RB, the prior equation name (EQNAM in MFI2K) is “K_RB_PR” and for VK_CB, the prior equation name is “VK_CB_PR”. Use the starting values of the parameters as the prior estimates (PRM in MFI2K) (1.2×10^{-3} for KRB and 1.0×10^{-7} for VK_CB). The “Expression for model equivalent of PRM” is the parameter identifier, K_RB or VK_CB. Use a coefficient of variation of 0.3 for defining the weights of both parameters. Specify a plot symbol of 3. General instructions for constructing prior information equations in the PES file are given in Hill and others (2000, p. 78-84).
- Under the Solver menu item, set MXITER=50, ITER1=100, HCLOSE=0.001, and RCLOSE=0.001. The results from this regression run that are presented in Hill and Tiedeman used these PCG solver parameters. By making this change, the values from the simulations should more closely match those presented in Figures and Tables of Hill and Tiedeman.
- **Run MODFLOW-2000**, and examine the results in *ex5.2c.glo* and in the underscore files.
- **Use ModelViewer** to visualize the hydraulic heads and hydraulic conductivities (see instructions in Exercise 3.2b).

5.2e. Use objective-function surfaces to explore regression performance (Optional).

This exercise can be done using UCODE_2005.

Exercise 6.2. Graphical Analyses of Model Fit and Related Statistics

6.2a. Graph of weighted residuals versus weighted simulated values and the minimum, maximum, and average weighted residuals.

Weighted simulated values are in the first column and weighted residuals are in the second column of output file *ex5.2c._ws*. Create the graph shown in Figure 6.7a by opening this file in GW_CHART. By default, the standard error of the regression is used to scale the vertical axis. Minimum, maximum, and average weighted residuals are listed in the LIST file; the minimum and maximum weighted residuals also are printed in the GLOBAL file in the list of the 5 smallest and 5 largest weighted residuals.

6.2b. Graph of observed versus simulated values

Weighted simulated values are in the first column and weighted observed values are in the second column of output file *ex5.2c._ww*. **Create the graph shown in Figure 6.7b in GW_CHART.**

Simulated values are in the first column and observed values are in the second column of output file *ex5.2c._os*. **Create the graph shown in Figure 6.7c in GW_CHART.**

6.2c. Graphs of weighted residuals against independent variables

Software for posting values at spatial locations can be used to produce Figure 6.9.

6.2d. Normal probability graph

Create the graph shown in Figure 6.11 in GW_CHART by opening file *ex5.2c._nm*.

6.2e. Determine acceptable deviations from independent normal weighted residuals.

- **Use the post-processing program RESAN-2000 to generate the datasets used to produce the graphs in Figures 6.13 and 6.14.** The primary input file to RESAN-2000 is the *_rs* file. A file with the suffix *_rs* is created at the completion of a successful regression run in which OUTNAM in the Observation Process input file is not “none”. A default value in this file specifies that four sets of independent and four sets of correlated random numbers be produced. For this exercise, run RESAN-2000 (*resan2k.exe*) in the *exer* directory, and specify *ex5.2c.nam* as the name file.
- Output files from RESAN-2000 include *ex5.2c.#rs*, which contains all the generated random numbers and other information, *ex5.2c._rd*, which contains the independent random numbers, and *ex5.2c._rg*, which contains the correlated random numbers. GW_CHART can be used to plot the four sets of random or correlated numbers on a single normal probability graph, to graphically analyze the results in a manner similar to that shown in Figure 6.14, by opening either *ex5.2c._rd* or *ex5.2c._rg*. GW_CHART does not support plotting each set in a separate graph; these can be made using, for example, Excel.

Exercise 7.1. Parameter Statistics

7.1a. Evaluate composite scaled sensitivities.

- As in Exercise 4.1, the composite scaled sensitivities in output file *ex5.2c._sc* can be plotted in GW_CHART by opening this file.

7.1b. Evaluate leverage statistics

MODFLOW-2000 and its post-processing programs do not calculate the leverage values. To produce a file with leverage values, UCODE_2005 needs to be used.

7.1c. Evaluate importance using influence statistics

Post processing program RESAN-2000 produces Cook's D and DFBETAS values; the files for this exercise were produced during the run of RESAN-2000 in Exercise 6.2e. Cook's D values are in file *ex5.2c._rc* and DFBETAS values are in file *ex5.2c._rb*. GW_CHART can be used to produce graphs of the Cook's D and DFBETAS values in these output files (and shown in Tables 7.2 and 7.3) by opening the *_rc* or *_rb* file.

To calculate the correlation coefficients with the omission of observation *hd07.ss*, follow these steps:

- In MFI2K, save the *ex5.2c* dataset as dataset *ex7.1c.no7ss*.
- **Put the final parameter estimates from regression run ex5.2c into the SEN file** for run *ex7.1c.no7ss*. This can be easily done in a text editor outside of MFI2K. Exit MFI2K and in the text editor, copy the final parameter estimates in file *ex5.2c_b* into the last 6 lines of *ex7.1c.no7ss.sen*.
- **Run MFI2K** and open dataset *ex7.1c.no7ss*. Open the list of head observations under "Single Time Head" in the "Observation Dialog", and omit observation *hd07.ss* by deleting its name in the first column.
- **In the PES file, set MAX-ITER to 0.**
- **Run MODFLOW-2000** and examine the parameter correlation coefficient matrix near the bottom of *ex7.1c.no7ss.glo*.

7.1d - Evaluate parameter correlation coefficients

The matrix of parameter correlation coefficients (calculated with all observations and prior information) and a listing of $pcc > 0.90$ are located near the bottom of *ex5.2c.glo*; these values are not listed in any underscore file.

7.1e - Evaluate the uniqueness of the parameter estimates using correlation coefficients

First, perform a regression run with the flow observation and prior information omitted:

- In MFI2K, save the *ex5.2c* dataset as dataset *ex7.1e.hdsonly*.
- **Omit the flow observation** by clicking on "Deactivate" under the Options menu in MFI2K, and deactivate RVOB.

- **In the PES file, remove the prior information equations** by deleting the EQNAM entry for each equation.
- **Run MODFLOW-2000 to perform regression.** Use output in *ex7.1e.hdonly.glo* to complete the exercise.
- Because the regression did not converge, MODFLOW-2000 does not calculate the *pcc*. They can be obtained by performing a run with MAX-ITER set to 0 in the PES file. This run was done in Exercise 4.1c and the results are shown in Table 4.3.

Next, include the flow observation and prior information, and start the regression from different initial values:

- Close MFI2K, then re-execute the program, open dataset *ex5.2c*, and save it as dataset *ex7.1e.allobs*.
- In the SEN file, change the starting parameter values to the values in set 1 of Table 7.7 (p. 151), perform nonlinear regression, and rename the global output file from this run *ex7.1e.allobs.run1.glo*. Then, change the values to those in set 2 of Table 7.4, perform nonlinear regression and rename the global output file *ex7.1e.allobs.run2.glo*.

7.1f and 7.1g. Linear confidence Intervals and reasonable ranges

Confidence intervals and reasonable ranges can be plotted in GW_CHART by opening file *ex5.2c._pc*.

7.1h. Nonlinear confidence intervals

The nonlinear confidence intervals can be calculated with the UNC Package of MODFLOW-2000 (Christensen and Cooley, 2005). However, the intervals for Exercise 7.1h, shown in Figure 7.8, were calculated by UCODE_2005. To perform these simulations, see the computer instructions for the exercises using UCODE_2005.

Exercise 7.3. Testing for linearity

7.3a. Use the modified Beale's measure

- In MFI2K, open the *ex5.2c* dataset, and save it as dataset *ex7.3a*.
- **Substitute the final calibrated parameter values from file *ex5.2c._b* into the SEN file**, so they are used as the starting parameter values in the run to generate the parameter sets. To do this in MFI2K, you must copy each individual parameter value from *ex5.2c._b* into the entry in the “Sensitivity Dialog” window. Alternatively, you can use a text editor to replace the last 6 lines of the file *ex7.3a.sen* with the last 6 lines of *ex5.2c._b*; in this case, dataset *ex7.3a* must not be open in MFI2K.
- **Set IBEFLG=1 in the PES file, and run MODFLOW-2000** to create *ex7.3a._b1*, which contains the generated parameter sets.

In the attempt to calculate Beale's measure with MODFLOW-2000, all parameter sets are generated and shown in *ex7.3a._b1*. Notice that in this file there are sets of generated parameter values in which HK_2, K_RB, or VK_CB are negative. When physically implausible values of parameters are generated during this step of calculating Beale's measure, the regression needs to be run with these parameters log transformed. Thus, log transform all the hydraulic conductivity parameters in the SEN file. For the weights on the prior for K_RB and VK_CB, MODFLOW-2000 will internally convert the specified statistics on the native values to statistics on the log-transformed values.

- **After log-transforming the appropriate parameters, run MODFLOW-2000.** Check *ex7.3a.glo* to make sure the regression converged. This run will also generate the *ex7.3a._b1* file.
- **Set IBEFLG=2 in the PES file and run MODFLOW-2000** to generate *ex7.3a._b2*.
- **Run BEALE-2000** in directory *exer*, using the name file *ex7.3a.nam*. The output file is *ex7.3a.#be*. The modified Beale's measure is printed near the end of this file. Save this file as *ex7.3a.origwts.#be*.

The statistics used to calculate the weights on prior for K_RB and VK_CB (coefficients of variation of 0.3) probably reflect an unrealistically small level of uncertainty in these hydraulic conductivity parameters. Next, recalculate Beale's measure using a statistic that more accurately reflects the uncertainty of the prior information, as suggested in Guideline 6:

- **For the prior information, increase the STATISTIC in the PES file.** Consider a coefficient of variation of 1.0.
- **Set IBEFLG=1 in the PES file, and execute MODFLOW-2000** to generate *ex7.3a._b1*. Check that the regression run converges.

- **Set IBEFLG=2 in the PES file, and execute MODFLOW-2000** to generate *ex7.3a._b2*.
- **Execute BEALE-2000.** Save this file as *ex7.3a.smallerwts.#be*.

7.3b. Use total and intrinsic model nonlinearity

Total and intrinsic model nonlinearity can be calculated with the UNC Package of MODFLOW-2000 (Christensen and Cooley, 2005). However, for this exercise they were calculated by UCODE_2005. To perform these simulations, see the computer instructions for the exercises using UCODE_2005.

Exercise 8.1. Predict advective transport and perform sensitivity analysis

8.1a. Predict advective transport

The input files for this exercise, which uses the model as calibrated in Exercise 5.2c, are in directory */Exercises/initial.mf/ex8.1a.i*. The root name for all MODFLOW-2000 files used for Exercise 8.1 is *exss*, and the files are based on those used in Exercise 5.2c. The files for Exercise 8.1a have been modified as described below.

The ADV2 Package input file, *exss.adv*, and the Well Package input file, *exss.wel*, have been constructed and the names added to the name file *exss.nam* using file types ADV2 and WEL. With the existence of the OBS file type, the presence of the ADV2 file type activates the advective-transport calculations. Other changes to the files include (1) the estimated parameter values from *ex5.2c._b* have been copied into *exss.sen*, and ISENALL has been set to -1 to perform a forward run with parameter substitution, (2) the head and flow observations have been omitted by modifying file *exss.nam* so that a # (the character used to comment out a line) was added as the first character preceding file types OHD and ORV, and (3) in *exss.dis* the stress period length (PERLEN) has been changed to 200 years (6.3×10^9 seconds), because the ADV2 package requires that PERLEN is at least as long as the latest advective transport observation or prediction.

MODFLOW-2000 can be run with this set of files to predict the advective transport path.

- Create directory *ex8.1a* in directory *exer* and copy over all files from */initial.mf/ex8.1a.i*.
- Review the input instructions for the ADV2 package (Anderman and Hill, 2001, p. 49-53.), and use these instructions to understand the contents of *exss.adv*. Identify the porosity value used for the simulation, where the particle is being introduced, and the times at which predictions are to be calculated.
- **Run MODFLOW-2000** using the batch file *exss.bat* and look at the output file *exss.lst*. The particle path coordinates are listed in this file as well as in *exss.pth*.

8.1b. Determine the parameters that are important to the predictions using prediction scaled sensitivities and parameter correlation coefficients

The input files for Exercise 8.1b have been constructed and are in directory *ex8.1b.i*. Sensitivities and parameter correlation coefficients will be calculated in two separate runs, one with predictions (*with_pred*) and the other without predictions (*no_pred*), using the “Sensitivity Analysis” mode of MODFLOW-2000 (Hill and others, 2000, Table 3). These runs are explained in the description of Exercise 8.1b in Hill and Tiedeman (p. 196-198). The “Sensitivity Analysis” mode requires that the Sensitivity and

Parameter-Estimation Processes be activated by including the SEN and PES file types in the name file, and that MAX-ITER=0 in the PES file. The prior information has been omitted from the PES file. Examine *exss.nam-no_pred*, *exss.nam-with_pred*, *exss.sen*, and *exss.pes* and verify that the input is correct for performing a run in Sensitivity Analysis mode with no prior information. Note that the 200-year advective travel time has been removed from *exss.adv* because the results from Exercise 8.1a showed that the particle reaches the well prior to 200 years.

Also, note that two stress periods are now defined in *exss.dis*, and that there are data for two stress periods in *exss.wel*, with pumpage in the first stress period and with no pumpage in the second stress period. In the ADV2 package, particle travel times are defined relative to the beginning of the simulation, and thus the first stress period must have the pumpage conditions associated with the advective-transport predictions. Because the head and flow observations are now associated with the second stress period (no pumpage) files *exss.obh* and *exss.orv* have been modified so that IREFSP is 2 for all observations.

- Create directory *ex8.1b* in */Exercises/exer/* and copy over all files from */Exercises/initial.mf/ex8.1b.i*.
- **Run MODFLOW-2000** twice by executing the batch files *with_pred-exss.bat* and *no_pred-exss.bat*, to produce the results with and without the predictions. Note: the parameter correlations without the predictions will slightly differ from those in Table 8.5, but the differences do not affect the conclusions drawn from these *pcc*.

8.1c. Determine the parameters that are important to the predictions using the parameter-prediction statistic

The *ppr* statistic is calculated using the computer software OPR-PPR (Tonkin et al., in press). OPR-PPR is designed to use as input several files that are produced as output by UCODE_2005 calibration and prediction simulations. Because of the ease with which UCODE_2005 output can be used in OPR-PPR, the calibration and prediction simulations needed to produce the OPR-PPR input for this exercise were done using UCODE_2005. Information about performing these simulations and the OPR-PPR runs is provided in the computer instructions for the exercises using UCODE_2005.

OPR-PPR is distributed with post-processing software MF2K2DX that facilitates using OPR-PPR with output from MODFLOW-2000 calibration and prediction runs. MF2K2DX processes information in MODFLOW-2000 output files, and produces the input files needed for OPR-PPR that would be produced by using UCODE_2005. Information about using MF2K2DX is included in the documentation for OPR-PPR (Tonkin et al., in press).

8.1d. Assess the importance of existing observations to the predictions using the observation-prediction (opr) statistic

The *opr* statistic is calculated using the computer software OPR-PPR (Tonkin et al., in press). As discussed under Exercise 8.1c, information for simulations using OPR-PPR are provided in the computer instructions for the exercises using UCODE_2005.

8.1e Assess the likely importance of potential new observations to the predictions using dimensionless and composite scaled sensitivities and parameter correlation coefficients

The potential observed head and flow have been added to files as needed in directory *ex8.1e.i*. The simulated conditions are the same as in Exercise 8.1b, with pumpage occurring during the first steady-state stress period, and no pumpage during the second steady-state stress period. The potential hydraulic-head and flow observations apply in the first stress period and the existing head and flow observations apply in the second period.

- **Create directory *ex8.1e*** in */Exercises/exer/* and copy over all files from */Exercises/initial.mf/ex8.1e.i*.
- Three runs have been set up, in which (1) both potential observations are included, (2) only the flow observation is included, and (3) only the head observation is included. **Run MODFLOW-2000** for each of these cases by executing the batch files *both-potential-obs.exss.bat*, *potential-flow-only.exss.bat*, and *potential-head-only.exss.bat*. The *dss* and *pcc* calculated for the three cases are in files *exss.glo.both-potential-obs*, *exss.glo.potential-flow-only*, and *exss.glo.potential-head-only*.

8.1f Assess the likely importance of potential new observations to the predictions using the observation-prediction (opr) statistic

See discussion under Exercise 8.1c and d.

Exercise 8.2. Predict advective transport and perform sensitivity analysis

8.2a. Calculate linear confidence intervals on the components of advective transport

Calculating confidence intervals on the components of advective transport requires defining effective porosity as a parameter in the ADV2 package, so that the uncertainty in effective porosity is accounted for in the calculation of prediction uncertainty. Effective porosity has been defined as a parameter in the UCODE_2005 simulations to calculate the linear confidence intervals. See the computer instructions for the exercises using UCODE_2005 to perform these simulations.

8.2b. Calculate nonlinear confidence intervals on the components of advective transport

The nonlinear confidence intervals on predictions can be calculated with the UNC Package of MODFLOW-2000 (Christensen and Cooley, 2005). For this exercise, however, the intervals were calculated using UCODE_2005. To perform these simulations, see the computer instructions for the exercises using UCODE_2005.

Exercises in Chapter 9

Computer instructions for the exercises in Chapter 9 are similar to those of previous exercises covering the same topic. Please the instructions for the related exercises.