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

by Mary C. Hill and Claire R. Tiedeman

Computer Instructions for the Exercises, using the US Geological Survey computer programs

MODFLOW-2005 and MODPATH;

UCODE_2005, Residual_Analysis, Model_Linearity, Corfac_Plus, and Model_Linearity_Adv; and

MFI2005, GW_Chart, and ModelViewer

This document first describes the software set up, and then describes how to conduct the computer runs required by some of the exercises of Hill and Tiedeman (2007) using MODFLOW-2005 (Harbaugh, 2005) and MODPATH (Pollock, 1994) to simulate the system involved, and UCODE_2005 (Poeter and others, 2005) to perform sensitivity analysis and estimate parameter values. The input files are constructed using MFI2005 (Harbaugh, 2007, written commun.), which is a basic graphical interface that supports MODFLOW-2005 and UCODE_2005. This document provides instructions for the exercises in which input files for these programs are prepared, the programs are executed, and directions for locating where the information shown in the book is presented in the model output files. For other aspects of the exercises and for all references cited in this document, readers are referred to Hill and Tiedeman (2007).

Refer to Hill and Tiedeman (2007, p. 21-24) for description and illustration of the flow system and management problem involved in these exercises. There it says that MODFLOW-2000 and its ADV Package (Anderman and Hill, 2001) are used to simulate the flow system for calibration and prediction condition; here, we use MODFLOW-2005 and MODPATH.

The documentation for all programs used is included in the “documentation” directory of the directories distributed for class.

The setup of the files distributed for doing the exercises is described in the remainder of this section.

The executables needed to perform the exercises are in the bin and the exer directories (see section “File Setup”. You could also do one of the following: (1) Copy the executables to a directory listed in the PATH environment variable (type “path” at the DOS prompt to display the value of PATH); or (2) Place the files in a different directory and modify the PATH variable on your computer to add the directory to the PATH. To keep the class files self-contained and to avoid changing the PATH on computers used temporarily for class, we just place them in the directory students use to perform the exercises.

File setup

The directories used in the exercises are listed in Table 1.

Table 1. The directories used in the exercises.

Directory	Contents
First level	
bin-plotting\	See table below under "Software setup"
documentation\	This document. MODFLOW-MODPATH\ UCODE-2005\ OPR-PPR\ MMA\
Exercises-UCODE_2005\	answers\ exer\ initial\
Second level	
answers\	Final files for most exercises. This is what exer\ would contain if all the exercises were conducted as described in these instructions. Subdirectories ex5.1a\ ex5.1b\ ex8
bin\	Most of the executables needed to run the exercises.
exer\	The mfi2005 executable and selected files needed to run most exercises. All files and folders that you create when doing the exercises.
initial\	Files needed to conduct exercises that can not be created easily or at all by MFI2005. Subdirectories ex3.2.i\ ex5.1a.i\ ex5.1b.i\ ex8.i\ ex9.4i\
Third level	
ex3.2i\ ex5.1a.i\ ex5.1b.i\ ex8.i\ ex9.4.i\	Files that contain data needed for exercises 3.2, 5.1a, 5.1b, 8, and 9.4. Distributed in directory initial\.
ex5.1a\ ex5.1b\ ex8\	Final files for exercises 5.1a, 5.1b and all parts of exercise 8. Distributed in directory answers\..

Software setup

The executables for the software needed to do the exercises.

Table 2. The executables distributed for the exercises.

Software program	Executable file	Comment
The following are in the bin\ directory		
MODFLOW-2005	mf2005.exe	Ground-water flow model
UCODE_2005	ucode_2005.exe ***get new version	Inverse modeling and sensitivity analysis
Model_Linearity	model_linearity.exe	Calculates the modified Beale's measure of model linearity
Model_Linearity_Adv	model_linearity_adv.exe	Calculates the total, intrinsic, and combined measures of model linearity
Corfac_Plus	Corfac_Plus.exe	Calculates correction factors used to adjust confidence and prediction intervals in some circumstances. See Poeter and others (2007, p. 204) and references cited therein.
Residual_Analysis	residual_analysis.exe	Calculates statistics for residual analysis
Linear_Uncertainty	linear_uncertainty	Calculates linear intervals on predictions
MODPATH	Mpathr4_3.exe	Post-processor for MODFLOW that calculates advective transport paths
PathLineRead	Pathlineread.exe	Used to convert MODPATH output to more convenient form.
	Mf2k.exe	***remove if not needed
The following are in the exer directory		
MFI2005	00-mfi2005.exe	Simple preprocessor for MODFLOW-2005
The following are in the bin\bin-plotting\ directory		
GW_Chart	GW_Chart\gw_chart.exe	Graphs output from UCODE_2005
ModelViewer	ModelViewer\modelviewer.exe	Visualizes results from MODFLOW-2005

To make it easier to access the main programs used most in class, create shortcuts on the Windows desktop for (1) the MFI2005 executable in *exer* (named *00-mfi2005.exe* there so it can be listed first alphabetically to make it easier to find), (2) the gw_chart.exe executable in bin-plotting\GW_Chart, and (3) the ModelViewer.exe executable in bin-plotting\ModelViewer. 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, these programs can be started by double-clicking on the shortcut icon.

In addition to the MFI2005 executable, the exer\ directory includes the following files.

Table 3. Files included in the exer\ directory in addition to the MFI2005 executable.

Exercise	Batch or input file	Comment
Exercises 6.2 and 7.3 do analyses for the regression completed in exercise 5.2c		
6.2e	ex6.2e-residual_analysis.bat	Analyzes model fit to observations.
7.3	ex7.3-model_linearity.bat	Calculates modified Beale's measure of model linearity.
	ex7.3-corfac_plus.bat	Defines that confidence intervals (instead of prediction intervals) are to be calculated.
	ex7.3_ucode.corfac	Input file needed by Corfac_Plus when it is run using ex7.3-corfac_plus.bat.
	ex7.3-model_linearity_adv.bat	Calculates total and intrinsic measures of model linearity.
Exercise 9.11 does the analyses indicated for the regression completed in exercise 9.7.		
9.11	ex9.11-model_linearity.bat	Calculates modified Beale's measure of model linearity.
	ex9.11-corfac_plus.bat	Input file needed by Corfac_Plus when it is run using ex9.11-corfac_plus.bat
	ex9.11_ucode.corfac	Input file needed by Corfac_Plus when it is run using ex9.11-corfac_plus.bat.
	ex9.11-model_linearity_adv.bat	Calculates total and intrinsic measures of model linearity.

MFI2005: Toubleshooting problems getting going

When using MFI2005, the user initiates a MODFLOW-2005 run by using the "Run MF2005" item on the FILE menu. When you select "Run MF2005", MFI2005 tries to invoke a batch file named MFI2005RUN.BAT; this file is in the *exer* directory. If, when you select "Run MF2005", a black window appears and immediately disappears, it means that the operating system cannot find MFI2005RUN.BAT. This will occur if MFI2005RUN.BAT is neither in a directory listed in the PATH, nor in the directory where the MODFLOW data set resides. If this happens, copy MFI2005RUN.BAT into a suitable directory. Similarly, when MFI2005RUN.BAT is executed, it invokes mf2005.exe, which must be in a directory in PATH or in the current directory.

Similarly, when usingMFI2005, the user initiates a UCODE_2005 run by using the "Run UCODE" item on the FILE menu. When you select "Run UCODE", MFI2005 tries to invoke a batch file named MFIUCODERUN.BAT; this file is in the *exer* directory. If, when you select "Run UCODE", a black window appears and immediately disappears, it means that the operating system cannot find MFIUCODERUN.BAT. This will occur if MFIUCODERUN.BAT is neither in a directory listed in the PATH, nor in the directory where the MODFLOW data set resides. If this happens, copy MFIUCODERUN.BAT into a suitable directory. Similarly, when MFIUCODERUN.BAT is executed, it invokes UCODE_2005.exe, which needs to be in a directory in PATH or in the current directory.

The paths of the MODFLOW-2005 and UCODE_2005 executables are defined in the files MFI2005RUN.BAT and MFIUCODERUN.BAT.

GW_Chart and ModelViewer

GW_Chart (Winston, 2000)is a plotting program for output from MODFLOW-2005, and UCODE_2005, and other programs.

ModelViewer (Hsieh and Winston, 2002) enables three-dimensional visualization of spatially variable model input and output; both programs can be downloaded from the book website.

Software versions

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

Exercise 3.1: Steady-state model setup using parameters

This exercise corresponds to exercise 3.1 in Hill and Tiedeman (p. 36).

Objective: Prepare all input for the steady-state simulation used in the exercises and run the simulation. Use the preprocessing program MFI2005 to prepare the input files. Use parameters to define system properties and the parameter values listed in Table 4. These values will be the starting values when nonlinear regression is performed.

Table 4: Parameter names and starting values for properties of the steady-state flow-system for which parameters are estimated in the exercises.
[m/s, meters per second; cm/yr, centimeters per year. This is the same as Table 3.1 of Hill and Tiedeman, 2007, p. 38)]

Flow-system property	Parameter name	Starting value
Horizontal hydraulic conductivity of layer 1, in m/s	HK_1	3.0×10^{-4}
Hydraulic conductivity of the riverbed, in m/s	K_RB	1.2×10^{-3}
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}
Recharge in recharge zone 1, in cm/yr	RCH_1	63.072
Recharge in recharge zone 2, in cm/yr	RCH_2	31.536

Getting started

- Start MFI2005 by double clicking the executable in the *exer* directory.
- Enter *ex3.1.nam* when prompted for the name file. This creates a new MODFLOW-2005 dataset named *ex3.1* in directory *exer*.
- Specify 18 rows, 18 columns, 2 model layers, and free format.

Discretization (DIS) input

The Discretization (DIS) input is described by Harbaugh (2005, p. 4-3 to 4-5, 8-11)**.**

- Click on the “DIS” menu item. In the “DIS Menu” dialog box, click on the buttons below “Check” and enter the following data.
  - Set model time and length units to seconds and meters, respectively.
  - Set DELR = DELC = 1000 m.
  - In LAYCBD, specify that a confining bed below layer 1 is to be simulated.
  - 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).
  - The default in MFI2005 is to simulate one steady-state stress period which is what is needed here. Thus, no change is needed for the “Stress Periods” button.
  - Click “Close”

- BAS input (Harbaugh, 2005, Ch. 4 and p. 8-10 to 8-11): Click on the "BAS" menu item. Do the following for layers 1 and 2.
  - Specify IBOUND=1 for all cells, which means that all cells are active. Though a real number is in the box, the program uses it as an integer.
  - Set initial head = 200 m.
  - Check to be sure all are specified for both layers.
  - Click "Close"

Exercise 3.1a: Parameters that define list data:

List data and using parameters to define list data are discussed by Harbaugh (2005, p. 8-1 to 8-3). For this problem, the River and General-Head Boundary Packages use list data. In the MODFLOW-2005 documentation, these are classified as stress packages; however, generally they define Cauchy boundary conditions for the system.
In the River Package a parameter is defined to calculate the riverbed conductance. In the General-Head Boundary Package no parameters are defined.

River(RIV) Package input

The River Package is described by Harbaugh (2005, 6-6 to 6-12 and p. 8-34 to 8-36)**,** and is used here to represent the river.

- Click on the "STRESS" menu item, then click on the RIV button. See that this menu allows rivers to be defined using parameters on the left and without parameters on the right. We will be defining the river using a parameter.
- Click on "New" and define one parameter named K_RB, which will represent hydraulic conductivity of the riverbed. The initial value of 1.2×10^{-3} is given in Table 4. Close this window.
- To 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 "Internal editing".
  - Specify that the river reach is in layer 1, rows 1-18, and column 1.
  - Stage in the river is 100 m, and the elevation of the riverbed bottom is 90 m.
  - The RIV Package requires riverbed conductance (K×L×W/M) as input, which is calculated in MODFLOW-2005 as the product of the parameter and Condfact. Here, the parameter is defined as the hydraulic conductivity of the confining unit, which is K in the equation, so that Condfact = (L×W/M) = 1000 m for each river cell. Lesser values would be entered if, for example, the stream gages were located such that only part of a cell was to be included in the measured reach, the width or length of stream in each cell varied, to include an independently determined variation of K along the length of the stream, or to support additive parameters used, for example, to represent linear variation of streambed hydraulic conductivity between values at each end of a reach.
- Click the OK.

- Now you are back in the “List Parameter Data” window. Click “OK”.
- Finally, in the “List Data” window, click the “Activate for this stress period” button to activate K_RB for stress period 1. Click “OK”.

General-Head Boundary (GHB) input

General-Head Boundary (GHB) Package is described by Harbaugh (2005, p. 6-4 to 6-5, 8-49 to 8-51), and is used here to represent flow from the highlands bordering the area on the side opposite the river.

- In the Stress Dialog box, click on GHB. Under “Non parameter data”, click Package, and “Internal editing”.

  - Define 36 GHB cells in rows 1-18 of column 18, in both layers 1 and 2.

  - The external head (Bhead) is 350 m.

  - The hydraulic conductance between the cell and the external source/sink is $1.0{\times}10^{-7}$ m^2/s (you can enter “1e-7”).

- Click “OK” or “Close” in all the windows.
- Save the dataset (Under the “File” menu).
- Execute MODFLOW-2005 from the FILE menu. The output files will be produced in directory exer\. Because a flow package (here it will be LPF) has not been activated, an error message is printed in the DOS window. 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 = 1.0E-7.
- Click on the black window where MODFLOW was running and press the space bar before retuning to the MFI window.

Exercise 3.1b: Multiplier and Zone Arrays

Two multiplication arrays and one zone array are needed to define the parameters of this problem. They are all defined here, and are then referred to when the parameters are defined in subsequent exercises.

Multiplier arrays

Multiplier arrays are described by Harbaugh (2005, p.4-6, 8-3 to 8-7, 8-10, and 8-15 to 8-16). Here we use one multiplication array that is a constant value for all cells to convert recharge calculated using the recharge parameters, which are in centimeters per year, to the units of the model, which are meters and seconds. The second multiplication array represents the spacial distribution of the hydraulic conductivity of the lower model layer.

- 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 is used to convert recharge parameter values provided in cm/yr to the model units of m/s.

- 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 “OK”.
- Click “Package” and “Internal editing”.
- Using the 18 by 18 array, approximate a linear variation from 1.0 to 9.0 by taking nine steps. Do this by placing the values 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. Click “OK”.
- Set multiplier = 1.0 in the “Define Multiplier Arrays” dialog box. Click “OK”.

Zone array

Zone arrays are discussed by Harbaugh (2005, p.4-6, 8-4, 8-10, 8016). Here, a zone array is needed to represent the two areas of recharge defined for this problem by Hill and Tiedeman (2007, p. 22).

- Click on the “Zone-Mult” menu item and choose “Zone Arrays”.
- Click “ADD” to define a zone array named “RCH_ZONE”. Click “Package”, then “Internal editing” and define a zone array that has a value of 1 in columns 1-9 and a value of 2 in columns 10-18. Click “OK”, set multiplier = 1.0, and click “OK”.

Note: If you run MODFLOW-2005 at this point, an error message is produced because not all needed files have been produced. However, the MODFLOW_2005 output file can be checked to be sure the files produced so far are being read correctly.

Exercise 3.1c: Parameters that define properties for the top of the system

Properties that can be defined over the top of the system include, for example, areal recharge and evapotranspiration. This problem has areal recharge, which is simulated using the Recharge Package of MODFLOW-2005 (Harbaugh, p. 6-3 to 6-4 and 8-37 to 8-39):

- 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. Use the parameter value from Table 4 above, 63.072 cm/yr.
- 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 by typing in the array names. Set Z1 to 1 to indicate that the parameter applies to zone number 1 in the zone array. Click “OK”.
- Click “New” again, and follow the same steps to define parameter RCH_2. Use the value from Table 1 above, 31.536 cm/yr. For this parameter, set Z1 to 2. Click “OK”.
- 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.

Exercise 3.d: Parameters that define flow properties within the system

MFI2005 supports two of the three internal flow packages available with MODFLOW-2005: Block-Centered Flow (BCF) and Layer-Property Flow (LPF). It does not support Hydrogeologic Unit Flow (HUF). Here, use LPF, which is discussed by Harbaugh (2005, p. chapter 5 and 8-28 to 8-31).

- In MFI2005, click the “Internal Flow” menu item and choose LPF.
- Click “LAYTYP”, to specify model layer flags. Set LAYVKA to “Hor. To Vert. Ani.” for both layers; this makes it so parameters are used to calculate horizontal to vertical anisotropy for each model layer instead of vertical hydraulic conductivity. Keep the default values for the other items (LAYTYP=confined, LAYAVG=Harmonic, horizontal anisotropy=1.0), and click “OK”.
- Question: Both layers are being simulated as confined. Why would one want to do that in a system with a free surface top boundary?!
- Click “Hydraulic” to enter parameter data. On the left under “Parameter Data” there is a list of three types of parameters that can be defined for the LPF Package. HK refers to hydraulic conductivity along rows, VANI stands for vertical anisotropy of model layers, and VKCB stands for vertical hydraulic conductivity of implicit confining beds. VANI would be replaced by VK if the other option for LAYVKA had been chosen in the previous step. Parameters can not be defined for horizontal anisotropy in the interface MFI2005, though they can be defined in MODFLOW-2005. See exercise 3.1h for more on vertical anaisotropy.
- Make sure “HK” is chosen. Click “New” and see the “Array Parameter Definition” dialog box.
- Follow steps similar to the RCH definition to define parameter HK_1 to control hydraulic conductivity (HK) of layer 1. Use the parameter value in Table 4 above, 3.0×10^{-4} m/s.
- Enter a “1” for “Layer”. This parameter has no associated multiplier or zone arrays; the default “ALL” listed under “Zone Array” means that the parameter value applies to all cells in layer 1. Click “OK”
- Follow similar steps to define HK_2 to control HK of layer 2, using the parameter value from Table 1 of 4.0×10^{-5} m/s and multiplier array HK_2_MULT. You can check the name of the multiplier array by clicking the box labeled “Edit Multiplier Arrays”. Click “OK”.
- Change the parameter type to VKCB. Follow the steps for defining HK_1 to define a VKCB parameter called VK_CB; use the parameter value in Table 4 above, 1.0×10^{-7} m/s.
- Finally, define VKA (which here refers to horizontal to vertical anisotropy) using non-parameter input, and specify a constant value of 1.0 for both layers.
- Click “OK”. Click “CLOSE”.

Exercise 3.1e: Solver

Solvers are needed to calculate heads for all cells of the finite-difference grid based on the entered information.

Instructions:

- In MFI2005, choose the "Solver" option. Four solvers are available through MFI2005: PCG2, SIP, DE4, and LMG (LMG is freely available to USGS users only). Any solver can be selected for this problem. The completed set of files distributed in class in the directory "answers" uses the PCG2 solver.
- If PCG2 is selected, change the value of RCLOSE to match HCLOSE. The value needed for HCLOSE and RCLOSE depend on the units used, as discussed by Hill (1990, p. 12-13). Here, the use of seconds for time means that the smaller value of RCLOSE is needed.
- If LMG is selected, BCLOSE may need to be changed. If the global budget error reported in the MODFLOW output file *ex3.1.lst* is larger than 0.01 (1 percent), reduce the value of BCLOSE by a factor of 2 or more. If the global budget error is 0.00, it may be possible to increase BCLOSE to obtain a faster solution, though for this small test case the short execution time is not a problem. (LMG is freely available to USGS users only).

Exercise 3.1f: Output Control

Output Control is described by Harbaugh (2005, p. 3-8, 8-17 to 8-21).

- Click the "OUTPUT" Menu item, and then click "Output file names and formats". This automatically results in some results, such as heads, being saved to default file names and formats. Change the Head Print format to 4, which will provide two digits to the right of the decimal point instead of one.
- Use 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 time step.
- Click "Times for Printing Budget" and select option to print budgets every time step.
- Click "OK" and close the "Output Control Data" dialog box.
- 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-2005's Ground-Water Flow Process (OBS is not listed).

Exercise 3.1g: Final check and first execution

- Click on the "OPTIONS" menu item and choose "Check Complete" to verify that the data entry for all packages is complete.
- Save the dataset.

- Execute MODFLOW-2005 from the FILE menu. The output files will be produced in directory exer\.
- In your ex3.1.lst file, the heads in layer 1, column 1 (beneath the steam) should be 100.23. for all rows. The head in column 18 should all be 190.83m for all rows. Why are the heads the same for all rows in both model layers? Check the global budget at the end of the List file to be sure the percent discrepancy is less than 1.00.
- If different heads are listed, make sure that vertical anisotropy is applied to both model layers, that the right parameter values are entered, and that the recharge and head-dependent boundary conditions have been activated for the stress period. If problems persist, check the other model inputs.

Exercise 3.1h (Optional): Define horizontal and vertical anisotropy parameters

MODFLOW-2005 supports definition of parameters governing horizontal and vertical anisotropy; this exercise considers definition of parameters for vertical anisotropy. The vertical anisotropy or vertical hydraulic conductivity for each model layer can be defined as parameters with parameter type VANI or VK in the Layer-Property Flow Package (Harbaugh, 2005, p. chapter 5 and 8-28 to 8-31). These parameter types affect simulation of the vertical flow of water between the model layers, and are most important when there is no intervening confining unit.

Instructions:

- In MFI2005, use the Save As option on the FILE menu to save the current dataset (ex3.1) as a new dataset called ex3.1h and use the ex3.1h dataset for this exercise.
- Set CHANI = 0 for both layers in LPF input.
- Define horizontal anisotropy of layers 1 and 2 as parameter HANI_1&2 in LPF input. Set the horizontal anisotropy to 1.0 to produce output consistent with the previous results. (This part of the exercise can not be done with MFI2005. Either skip this or complete the exercise by modifying the files directly.)
- Define the vertical anisotropy of layer 1 as parameter VANI_1 in LPF input, and define the vertical anisotropy of layer 2 as parameter VANI_2. No multiplication or zone arrays are needed for these parameter definitions because in this exercise vertical anisotropy is constant throughout layers 1 and 2. Set vertical anisotropy to 1.0 to produce output consistent with the previous results.
- Execute MODFLOW-2005:
- Run MODFLOW-2005, and compare the output file *ex3.1e.lst* to the output file *ex3.1.lst* from exercise 1.
- 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.

Exercise 3.1i (Optional): Define additive parameters for interpolation methods.

MODFLOW-2005 allows model inputs to be calculated as the sum of contributions from more than one parameter (Harbaugh, 2005, p. 8-2, 8-5 to 8-7). 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. One deficiency of the present version of MODFLOW-2005 is that the interpolation can not be accomplished using log-transformed parameter values and the exponential taken of the resulting distribution, as often is needed for kriging. However, this capabilitiy is expected in the near future. In this exercise, you will apply additive parmeters to represent the linear variation in the hydraulic conductivity of layer 2 of the test case.

The goal is to maintain the same hydraulic-conductivity distribution in layer 2, but to allow the variation to be more flexible. Here, we will maintain the assumption that hydraulic conductivity varies in a step-wise linear fashion in layer 2, but we will allow the parameter values to represent the increase in hydraulic conductivity within the layer. Setting up the parameters in this manner facilitates imposing different values of hydraulic conductivity at the two ends of the layer, and would allow estimating these values by regression. If the estimated parameter values differed from the startig values, the increase in hydraulic conductivity might be other than a nine-fold increas and(or) the value under the stream might be different.

<u>Instructions</u>:

In MFI2005, use the Save As option on the FILE menu to save the current dataset as a new dataset called ex3.1i and use the ex3.1i dataset for this exercise.

Replace the definition of parameter HK_2 with new parameters HK_2a and HK_2b. Both new parameters will extend throughout layer 2. Make one parameter value equal the hydraulic conductivity in grid columns 1 and 2 (the value for HK_2 in Table 4 is 4.0×10^{-5} m/s); make the other equal the hydraulic conductivity in grid columns 17 and 18 (this will be 9 times the first value, or 36.0×10^{-5}). Use multiplier array names MULTa and MULTb. The arrays need to be defined such that HK_2a × MULTa(i,j) + HK_2b × MULTb(i,j) equals the hydraulic conductivity that occurred at cell i,j before.

- Execute MODFLOW-2005
- Compare the output file ex3.1h.lst to the output file ex3.1.lst from exercise 1.
- 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

This exercise corresponds to exercise 3.2 in Hill and Tiedeman (2007, p. 38).

Defining observations for the test case with MODFLOW-2005 requires one input file for the hydraulic-head observations and one for the flow observations. Observed hydraulic heads for the steady-state model are in table 3-2 of Hill and Tiedeman (2007, p. 51).

The MODFLOW-2005 input instructions for observations are described in OBS.PDF, which is provided in the documentation directory districtured with these exercises.

- In MFI2005, under the "File" menu item, save the *ex3.1* dataset as dataset *ex3.2* and use the *ex3.2* dataset in this exercise.

Exercise 3.2a: Hydraulic-head observations.

- In MFI2005, click Observations. Select the "Single Time Head" option on the Observations Dialog window.
- Review the 12 columns for which data need to be provided to define head observations. Columns 1 through 9 contain data used to construct the MODFLOW head observation input file. Columns 1, 7 and 10 through 12 are used to define observation in the UCODE_2005 input files. Does it make sense that the data provided in columns 2 though 6 and 8 and 9 are not needed by UCODE_2005? Does it make sense that the data listed in columns 10 through 12 are not needed by MODFLOW? Why would the data in columns 1 and 7 be used by both codes?
- Enter data for the 10 steady-state head-observations listed in Table 3.2 of Tiedeman and Hill (2007, p. 39). This can be accomplished in any of three ways. In all cases, the observation wells are assumed to be located at the centers of model cells, so ROFF and COFF equal 0.0. Here you can use any one of the methods. In practice the chosen method will depend on what software is available to assist in constructing the head observation file.

    (1) Type the data in directly from Table 3.2.

    (2) Use the file head-data.txt in the initial/ex3.2i directory. If you have a text editor such as Textpad that allows single columns of data to be copied, the copied columns can be inserted into the MFI2005 window by placing the cursor in the top box to be copied into and typing ctrl-v.

    (3) Use the already constructed head observation file ex3.2.obh in the initial/ex3.2i directory. To accomplish this, enter a fake data point in the "Single-Tine Head Observations" window, specify output file ex3.2._os, and click "OK" and then "Close". Save the files and close MFI2005. In the exer directory, replace the file ex3.2.obh with the file from the initial/ex3.2i directory. Restart MFI2005. Clock "Observations" and "Single-Time Head Observations" to check that the observations are being read.

- Close the Observations Dialog window and save the MFI2005 files.

Exercise 3.2b: Define flow observations

The flow observations are defined as head-dependent flows represented using the River Package, as described in OBS.PDF. For the steady-state simulation, one flow observation, a gain to the river of 4.4 m^3/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%.

A gain to the river is a loss to the ground-water system. The MODFLOW convention is that flows out of the ground-water system are negative. Thus, the observation needs to be entered as a negative value; that is, -4.4 m^3/s.

- In MFI2005, click Observations. Select the “RIV observations” option on the Observations Dialog window.
- Click “ADD Cell Group” and then “EDIT Observation Times”. Name the observation “flow01.ss” and enter the observed value (-4.4) and coefficient of variation used for the statistic value (0.10). Assign a plot symbol of 2. Click “OK”.
- Click “EDIT Cell Locations”. The cell group will include all 18 cell locations defined for the river in exercise 1. FACTOR = 1.0 for all cells in the cell group. These values can be obtained from the file *ex3.2.riv* of the *exer* directory using a text editor that allows single columns of numbers to be copied, as described above in input option (2) for heads.
- For the output file, enter ex3.2._os.
- Close all dialog boxes and save the files.

Exercise 3.2c: Check head and flow observations and their simulated equivalents

- Execute MODFLOW-2005.
- In ex3.2.lst, examine the listing of the observation input and the table of observed and simulated heads and flows. Check simulated values against those in figure 3.2 of Hill and Tiedeman (p. 39). The flow observation and its simulated equivalent are printed with more significant digits in *ex3.2._os*. This will be important when using UCODE_2005.
- Address the question posed for this exercise in Hill and Tiedeman (2007, p. 39).
- Use ModelViewer to visualize the hydraulic-conductivity distribution and the simulated heads over the model domain.

ModelViewer Instructions (also see the instruction file in the bin-plotting directory and your notebooks):

- To start: Execute ModelViewer. Under the File menu item, select New; then in the Model Selection dialog box, select Modflow 2000 (which works for MODFLOW-2005). Click “OK”. In the Modflow 2000 Data files dialog box, specify the name file by browsing to directory *exer*, and selecting ex3.2.nam. Click “OK”.
- In the Data Selection dialog box, keep the defaults.

- When the model domain appears, under the Show menu item, select "Solid" and "Color Bar".. Hydraulic heads are shown. Under the Toolbox menu item, select Geometry and set z to 10 to specify 10x vertical exaggeration. Click on a corner of the figure and move around to see the head distribution throughout the volume.
- To visualize hydraulic conductivity, under the Toolbox menu item select Data, and choose K along rows. Under the Toolbox menu item, select Solid, and then select Blocky.
- To show the location of the boundary conditions simulated using the River and General-Head Boundary Packages, under the Show menu select Model Features.

Additional ModelViewer capabilities and options are described in the online help system.

Exercise 3.2d: Calculate weights on hydraulic-head and flow observations

MODFLOW allows observations to be specified, but to define weights the capabiities of UCODE_2005 are needed. MFI2005 has already used the information entered about observations to produce the files needed by UCODE_2005. Look at the file *ex3.2_ucode.obs*. This is a typical UCODE_2005 input block. Here, STATFLAG is used to identify whether the STATISTIC provided to calculate the weight is a variance or coefficient of variation. Other options are described by Poeter and others (2005, p. 83).

Follow the instructions for exercise 3.2d from Hill and Tiedeman (2007, p. 39-40). Check your calculations against the weights printed in Figure 3.2. The weights also are listed in the UCODE_2005 main output file produced in exercise 3.3 in a table entitled "FIT OF SIMULATED EQUIVALENTS TO OBSERVATIONS".

Exercise 3.3: Evaluate model fit using the starting parameter values

If the evaluation from exercise 3.2 indicates that all observations, equivalent simulated values, and defined parameters are specified correctly, the model fit resulting from the starting parameter values can be evaluated. This exercise corresponds to exercise 3.3 in Hill and Tiedeman (p. 40). Do the first part of the exercise as described in the book. In addition to using figure 3.2, locate the information in file *ex3.2.lst*.

Exercise 3.3a: Produce the Parameter Value File

In the exercises above, the parameter values were defined in the package input files. There are many circumstances in which it is useful to have one file that can be used to alter any of the parameter values. This is provided by MODFLOW-2005 through the Parameter-Value File described by Harbaugh (2005, p. 4-6, 8-10, 8-23 to 8-24). Here we use MFI2005 to produce that file.

<u>Instructions</u>:

- In MFI2005, save the ex3.2 dataset as dataset ex3.3 and use the ex3.3 dataset in this rest of this exercise.
- In MFI2005, choose the “Parameter Values” option. Click the button on the top left and choose to have all defined parameters included in the PVAL file.
- The parameter values from the package input files are listed in the third column, which is labeled “GWF File Value”. This column can not be modified in this window, which is indicated by the shading.
- The values in the second column, which is labeled “PVAL File Value (B)”, are set to the values of the third column, but can be changed. The other columns define values used by UCODE_2005, and default values derived from the package parameter values have automatically been entered by MFI2005. Keep the default values for now.
- Click OK and save the files.
- Execute MODFLOW-2005. Check to see that the same results are obtained as in exercise 3.2. If not, click “Parameter Values” and check to be sure the parameter values are the same as the values in the package files.
- Use the parameter values ability of MFI2005 to do the final part of exercise 3.3 described by Hill and Tiedeman (2007, p. 40).
- When done, return all parameter values to their starting values, which are equivalent to the values from the packages listed in the third column of the parameter values dialog box.

Exercise 4.1: Sensitivity analysis for the initial model

These instructions apply to the parts of exercise 4.1 in Hill and Tiedeman (p. 60-66) for which computer runs are needed.

Exercise 4.1a: Calculate sensitivities for the steady-state flow system using UCODE_2005

Here the sensitivites are calculated with UCODE_2005 by perturbing the parameter values, one at a time, and the sensitivities are used to calculate model evaluation statistics. This mode is listed as “Sensitivity Analysis” mode in the UCODE_2005 documetation (Poeter and others, 2005, table 3, p. 30).

- In MFI2005, save the ex3.3 dataset as dataset *ex4.1* and use the *ex4.1* dataset in this exercise.
- In MFI2005, click “UCODE” to get the menu used to select UCODE_2005 capabilities. At the very top left is a window with the Verbose option, which controls the level of input repetition and error and warning messages produced by UCODE_2005. Below on the left, the UCODE_2005 modes are listed. Output options are listed further to the right but still under the “UCODE”Conrol_Data” banner. Further to the right are the options used to control nonlinear regression. At he bottom is the input used to control prior information, which is used to represent knowledge about the parameter values that is not represented in the observations used in the regression.
- Click “Sensitivities-Central”. Click OK and then “File” and “Save”.
- Use a text editor to look at the files with _ucode in their filename. These are:

  - *ex4.1_ucode.in*, the main UCODE input file;

  - *ex4.1_ucode.obs*, the Observation_Data input block;

  - *ex4.1_ucode.par*, the Parameter_Data input block;

  - *ex4.1_ucode.tpl*, a template file used to construct the MODFLOW-2005 input file *ucode.pvl*, and

  - *ex4.1_ucode.inst*, instructions for reading simulated equivalents from the MODFLOW-2005 *ex4.1._os* file.
- Use the UCODE_2005 documentation to answer the following questions.

  - In the main input file, *ex4.1_ucode.in*, what do the pairs of statements starting with BEGIN and END define? (See chapter 5). What are keywords?

  - What are the three options for organizing data within the input blocks?

  - In the first input block, called “Options”, what does the “3” mean? What other options are there?

  - In the UCODE_Control_Data input block, what keywords control what is called the mode in Table 3 of the UCODE_2005 documentation (p. 30)?

- In the Model_Command_Lines input block, what is the command used to run MODFLOW-2005? Here, MODFLOW-2005 is run directly, but often it is run through a batch file. Batch files would, for example, allow a sequence of models to be executed, such as MODFLOW-2005 and MODPATH or MT3DMS.

- The data for the Parameter_Data input block and the Observation_Data input block are read from files *ex4.1_ucode.par* and *ex4.1_ucode.obs*, respectively. Look in *ex4.1_ucode.par* and find the parameter values you specified using the MFI2005 Parameter Values option. Look in *ex4.1_ucode.obs* and find the observed values.

- The last two input blocks in *ex4.1_ucode.in* define how UCODE_2005 interacts with the process model (here, MODFLOW-2005) input and output files.

- Identify the name of the MODFLOW-2005 input file and look at the template file. How big are the fields into which UCODE_2005 can substitute numbers? Why might this be important?

- Identify the name of the MODFLOW-2005 output file and look at the instructions used to read it.

- The input blocks in the UCODE_2005 main input file need to be listed in the order in which they are presented in Table 4 of the documentation (p. 43), though all input blocks need not be present. List which input blocks are not included in this UCODE_2005 main input file.

- Most keywords in the UCODE_2005 input files have default values that are used if the keyword does not appear. Thus, UCODE_2005 input files can be very short in many circumstances. Here, it is easier for an interface such as MFI2005 to always include the same set of keywords. Go through the UCODE_Control_Data input block and determine which keywords could have been omitted because the defaults are specified.

- Execute UCODE_2005 by clicking “File” and then “Run UCODE”.
- 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 the parameter entries in *ex4.1.pvl*. In *ex4.1.pvl*, the columns after the first two are not read by MODFLOW-2005; they are used by MFI2005.
- Using GW_Chart (make sure you specify “UCODE_2005”, plot the dimensionless scaled sensitivities (listed in file *ex4.1-ucode._sd*), composite scaled sensitivities (*ex4.1-ucode._sc*), and leverage statistics and (*ex4.1-ucode._so*). Inspect the parameter correlation coefficients (*ex4.1-ucode._pcc*).

Exercises 4.1b, c, d, and e

Please see Hill and Tiedeman (2007, p. 60-63).

Table 5. The statistics used in these exercises and filename extensions of the files where they are listed are as follows. The file name prefix is always ex4.1.

Exercise	Statistic name	Filename extension[1]
4.1b	dimensionless and composite scaled sensitivities	_sd _sc
4.1c	parameter correlation coefficients	_pcc: values larger than or equal to 0.95 _mc: the entire parameter correlation matrix
4.1d	one-percent scaled sensitivities	_s1: values related to individual observations:
4.1e	leverage	_so

[1] Files with scaled sensitivities and leverage have extensions that start with _s. Files that contain matrices have extensions that start with _m.

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

Read the description of this exercise in Hill and Tiedeman (2007, p. 80-81). This document provides instructions for obtaining results such as those shown in Figure 5.4 and Tables 5.1 to 5.3 using UCODE_2005. MFI2005 does not support the Derived_Parameters input block of UCODE_2005 needed to combine the parameters or the Observation_Groups input block that can be used to make omission of selecgted observations easier. As a result, we will be working with many files produced previously by MFI2005, and some that will need to be modified in a text editor. The runs will be accomplished using batch files executed outside of MFI2005.

Exercise 5.1a: Assess relation of objective-function surfaces to parameter correlation coefficients

- Copy the directory initial\.ex5.1a.i to exer\ex5.1a. In this directory, most of the files to be inspected, changed, or run have names beginning with “00-“ so that they are listed at the top of the directory when the “name” header bar is clicked in the Windows file manager. The instructions below refer to the ex5.1a directory unless specified.
- There are two main UCODE_2005 input files: 00-ex5.1_ucode.in and 00-ex5.1_ucode.noflow.in. Inspect the UCODE_Control_Data input block and find the keyword used to determine what this run will do. Consider the instructions on Page 55 to 56 of the UCODE_2005 input instructions (Poeter and others, 2005).
- In the Parameter_Data in put block, identify keywords LowerConstraint, UpperConstraint, and SOSincrement, which are discussed by Poeter and others (2007, p. 70 and 72). How many runs will be executed to create the data set for Figure 5.4a or b?
- Inspect the Observation_Groups input block in either of the main input files and note the keyword “UseFlag”. The Observation _Data input block identifies files 00-EX5.1_ucode.head.obs and 00-EX5.1_ucode.flow.obs where the observation data are listed.
- Produce data needed for the graphs of Figures 5.4a and b by executing the batch files in this directory. For Figure 5.4c, the file 00-ex5.1_ucode.flow.obs change the coefficient of variation used for the flow observation.

Exercise 5.1b: Examine the performance of the modified Gauss-Newton method

- Copy the directory initial\.ex5.1b.i to exer\ex5.1b.
- To perform the first set of four regression runs listed on page 83 of the text book for the model with observations only, modify 00-ex5.1_ucode.noflow.in and run UCODE_2005 by double-clicking the batch file 00-ex5.1_ucoderun.noflow.bat. The runs require changing MaxChange and the parameter values. MaxChange is in the Reg_GN_Controls input block (the third input block from the top).

Exercise 5.2

- Plot the sets of parameter values calculated by the regression on the full contour plots provided with the course notes. Small versions of the plots are shown in Figure 5.4a and 5.4b on p. 82 of Hill and Tiedeman. The parameter values for KMult and RchMult are in the Parameter_Data input block (the fifth input block from the top). The parameter values from each iteration needed in the exercise will be printed in file ex5.1_ucode._pa and file ex5.1_ucode._summary (the last is new and is not mentioned in the UCODE_2005 documentation.
- Model fit to the observations as the regression proceeds is measured using the weighted least-squares objective function values listed in ex5.1_ucode._ss. Plot these values using GW_CHART. Start GW_Chart. Choose UCODE_2005. From the "File" menu item, choose "Open file" and navigate to the desired directory. Close GW_CHART before proceeding; MFI2005 sometimes can not proceed correctly when GW_Chart is open.
- You are next asked to repeat runs 1 through 4 above with the river observation weighted using a coefficient of variation of 10 percent and then 1 percent. Use the 00-ex5.1_ucode.in and 00-ex5.1_ucoderun.bat files. The coefficient of variation is already 10 percent. To make it 1 percent, change the value in the file 00-ex5.1_ucode.flow.obs.

Exercise 5.2: Nonlinear regression

These instructions apply to the parts of exercise 5.2 in Hill and Tiedeman (p. 87) for which computer runs are needed.

- In MFI2005, save the *ex4.1* dataset as dataset *ex5.2* and use the *ex5.2* dataset in this exercise.

Exercise 5.2a: Define range of reasonable parameter values

- In MFI2005, click “Parameter Values” MFI has inserted values for “LowerValue” and “UpperValue” that are higher and lower than the starting value by two orders of magnitude. These are non-constraining values used to identify unreasonable parameter estimates, which can be useful indicators of model error (see Hill and Tiedeman, 2007, p.140-142). Do the values specified make sense for these parameters? Change values as needed to reflect the ranges you think would be apply to typical field sites. To approximate the results discussed in exercise 7.1g, use the following values. These imply that a range defined by multiplying and dividing by a factor or 0.4 for the hydraulic conductivity parameters forms a reasonable range. Comment on this assumption.

Parameter name	Lower reasonable value	Upper reasonable value
HK_1	1.20E-04	7.50E-04
HK_2	1.60E-05	1.00E-04
VK_CB	4.00E-08	2.50E-07
K_RB	6.00E-04	3.00E-03
RCH_1	32	126
RCH_2	16	63

- Make all the parameters Adjustable (check in box) and do not log transform any parameters (uncheck the Log Trans box).

Exercise 5.2b: First attempts at estimating parameters by nonlinear regression

- In mfi2005, click “UCODE”. Activate “Optimize”. See that MAX-ITER=10, MaxChange=2.0, TolPar=0.01, and TrustRegion=“No”. These are the regression related variables that are changed most often.
- Click “Parameter Values” and place constraints on the four hydraulic-conductivity parameter values so that negative values for these parameters are not allowed. Do this by turning on “Constrain” and assigning lower constraints equal to the starting value times 0.01. For this problem the upper constraints are less critical; use the starting value times 100. Negative values could also be avoided by log-transforming the parameter values; this is considered later.
- Save files and perform nonlinear regression by executing UCODE. Look at the iteration information in the file ex5.2_ucode.#uout. In iteration 1, the regression tries to assign parameter K_RB a negative value, and in iteration 2, the regression tries to

assign parameter HK_2 a negative value. This indicates that the solution is performing poorly.

- Use GW_CHART to look at ex5.2_ucode._pa (click “yes” when asked to divide the values by their initial values). Note that in file ex5.2_ucode._pa, the values of the K parameters are positive. This results from constraining the parameter values and permits successive parameter estimation iterations. Look at any other files you wish, and then close GW_Chart.
- In ex5.2_ucode._pasub, the parameter values are in a format that can be used in the Parameter_Values input block of UCODE_2005. If desired, parameter estimation could be restarted from any intermediate iteration by copying the parameter values from ex5.2_ucode._pasub into a Parameter_Values input block.
- Save file ex5.2_ucode.#uout as ex5.2_ucode.#uout-nolog.
- To prevent the regression from calculating negative values for parameters K_RB and HK_2 and to hopefully obtain a better posed regression problem, the log transform of these parameters can be estimated instead of the native value. To specify that the log transform is to be estimated, in MFI2005 click “Parameter Values” and click to obtain check marks in the “LogTrans.” boxes for the four hydraulic-conductivity parameters. Remove the constraints on the parameter values by removing the check under “Constrian”.
- Execute UCODE_2005 to again perform parameter estimation.
- Save file *ex5.2_ucode.#uout* as *ex5.2_ucode.#uout-log*. If constraints were not removed as suggested, this run regression converges with the value of parameter HK_2 on its constraint. Without constraints the run does not converge.
- Results are in a table at the bottom of *ex5.2_ucode.#uout.log*. Use gw_chart to examine *ex5.2_ucode._pa* and *ex5.2_ucode._ss*. Performance is similar to that shown in Table 5.4; differences are caused by differences in the accuracy of the sensitivities and in differences in the regression routines.
- Do the Problem on p. 88-89 of Hill and Tiedeman.

Exercise 5.2c: Assign prior information on parameters.

- Save *ex5.2* as *ex5.2c* and use *ex5.2c* for this exercise
- In “Parameter Values”, remove all checks under “logTrans” so that native parameter values are estimated. Click OK.
- To define prior information on parameters, click UCODE.
- For K_RB, the prior equation name (PriorName on the menu) is “K_RB_PR”. Use the starting values of the parameters as the prior estimates (1.2×10^{-3}). The equation is the parameter identifier, K_RB.
- For VK_CB, the prior equation name is “VK_CB_PR”. Use the starting value (1.0×10^{-7}). The equation is the parameter identifiers, VK_CB.

- Use a coefficient of variation of 0.3 to define the weights of both parameters. Specify a plot symbol of 3. General instructions for constructing prior information equations in UCODE_2005 are provided by (Poeter and others (2005, p. 93-97).
- Execute UCODE_2005. If it does not converge with TrustRegion=no, try one of the other options. Differences occur depending on whether the constraints on th parameter values are defined in the "Parameter Values" menu of MFI2005.
- Do the Problem on p. 91 of Hill and Tiedeman.
- Use ModelViewer to visualize the hydraulic heads and hydraulic conductivities (see instructions in Exercise 3.2b).

Exercise 6.1

Exercise 6.1a, c, and d

See Hill and Tiedeman (2007, p. 114). The values are located in file ex5.2c.#uout toward the bottom. You can search for "CALCULATED ERROR VARIANCE".

Exercise 6.2

Exercise 6.2a, b, and d

The graphs mentioned can be produced with GW_Chart and files produced in exercise 5.2c.

For Figure 6.7a with unweighted residuals on the horizontal axis, use *ex5.2c_ucode._ws*.

For Figure 6.7b, use file *ex5.2c_ucode._ww*.

For Figure 6.7c, use *ex5.2c_ucode._os.*

For Figure 6.11, use file *ex5.2c_ucode._nm*.

Exercise 6.2e: Determine acceptable deviations from independent normal weighted residuals

Figures 6.13 and 6.14 are plotted using output files from the program RESIDUAL_ANALYSIS, which is not supported by MFI2005.

- In most circumstances, the input needed for the RESIDUAL_ANALYSIS program is produced by UCODE_2005 upon completion of a successful regression run. This requires that DataExchange=yes in the UCODE_Control_Data input block by designation or default. For this exercise, RESIDUAL_ANALYSIS needs to be executed in the directory with your output files from exercise 5.2c, and specify *ex5.2c* on the command line. This can be accomplished using the batch file *ex6.2e-residual_analysis.bat* located in the *exer* directory. Double click on this file.
- The output files from RESIDUAL_ANALYSIS are *ex5.2c_ucode.#resan*, which contains all the generated random numbers and other information, *ex5.2c_ucode._rd*, which contains the independent random numbers, and *ex5.2c_ucode._rg*, which

contains the correlated random numbers. The latter two files can be used to make normal probability plots such as those shown in figures 6-14 using GW_Chart .

- The other files produced by RESIDUAL_ANALYSIS are *ex5.2c_ucode._rb* and *ex5.2c_ucode._rc* ,which contain values of the influence statistics DFBETAS and Cook's D, respectively. These statistics are the subject of exercise 7.1c.
- Do the Problem on p. 123 of Hill and Tiedeman.

Exercise 7.1: Parameter Statistics

Exercise 7.1a and b

The composite scaled sensitivities and leverage statistics needed for these exercise are in files *ex5.2c_ucode._sc* and *ex5.2c_ucode._so*, respectively.

Exercise 7.1c

The DFBETAS and Cook's D statistics needed for this exercise were calculated as part of exercise 6.2e and are in files *ex5.2c_ucode._rb* and *ex5.2c_ucode._rc*.

Exercise 7.1e: Evaluate the uniqueness of the parameter estimates using parameter correlation coefficients

Part 1

This exercise requires that the flow observation be removed. With MFI2005 this can be accomplished as follows.

- Click "Options"
- Click "Deactivate"
- Click "RVOB"
- Click "OK"
- When an observation is deactivated the _os filename is removed for all remaining observations. To reestablish it for the other observations, click "Observations", then "Sngl. Time Heads". Define the output file as "ex7.1e._os".
- Run UCODE

Proceed with the exercise questions listed in Hill and Tiedeman (2007, p. 150-151).

Part 2

Part 2 of this exercise starts on page 151. To start the regression from different initial values, do the following.

- Close MFI2005, then re-execute the program and open dataset *ex5.2c*. Save the *ex5.2c* dataset as dataset *ex7.1e2* and use the *ex7.1e2* dataset for this part of exercise 7.1e.
- Click "Parameter Values" and change the starting parameter values to the values in set 1 of table 7-7 (p. 151), perform nonlinear regression. For the first set of parameter values, the regression does not converge with TrustRegion=no, but it does with TrustRegion=dogleg. Rename the file *ex7.1e2_ucode.#out* to *ex7.1e2_ucode.#out.1*.

Then, change the values to those in set 2 of table 7-4, perform nonlinear regression and rename the *#uout* from this run to *.1e2_ucode.#out.2*.

- Do the Problem at the top of p. 151 of Hill and Tiedeman.

Exercise 7.1f

The parameter standard deviations, linear confidence intervals, and coefficients of variation are listed in the main output file ex5.2c_ucode.#uout and the data-exchange file ex5.2c_ucode._pc.

Exercise 7.1g

GW_Chart can use the parameter estimates, reasonable range upper and lower values, and confidence interval upper and lower limits listed in the ex5.2c_ucode._pc file. The resulting graph will be similar to the graph shown by Hill and Tiedeman (2007, p. 153, fig. 7.7) if the following values are used for the reasonable ranges.

Parameter name	Lower reasonable limit	Starting value	Upper reasonable limit
HK_1	1.2×10^{-4}	3.0×10^{-4}	7.5×10^{-4}
HK_2	1.6×10^{-5}	4.0×10^{-5}	1.0×10^{-4}
VK_CB	4.0×10^{-8}	1.0×10^{-6}	2.5×10^{-7}
K_RB	6.0×10^{-4}	1.2×10^{-3}	3.0×10^{-3}
RCH_1	32	63.072	126
RCH_2	16	31.536	63

In GW_CHART, accept the option of dividing by the parameter values to produce a graph similar to figure 7.7, except that the values are the fraction of the estimated value instead of the percent. That is, the values in figure 7.7 are multiplied by 100 while those plotted by GW_CHART are not.

Exercise 7.2

This exercise has no computer runs.

Exercise 7.3: Test for Linearity

- To begin, with MFI2005, copy model ex5.2c to ex7.3.

To test linearity, sets of model parameters are generated, as discussed by Hill and Tiedeman (2007, p.143, eq. 7.11). For the hydraulic conductivity parameters to remain positive in the generated parameter sets, it is necessary in this problem (indeed, it is often necessary) to log-transform them. When such a change is made, it is also necessary to repeat the regression using the changed status of the parameters so that the variance-covariance matrix of the parameters of eq. 7.11 is correct. Another complication in this problem is that some of the parameters that are to be log-transformed have prior information. This requires a change in the prior information equation used, and a change in the statistic using Hill and Tiedeman (2007, p. 130, eq. 7.6), however UCODE_2005 now automatically makes these cahnges for you. The needed runs are accomplished through the following steps.

- Click Parameter Values. Click to get checks in the LogTrans column for the four hydraulic-conductivity parameters (HK_1, HK_1, VK_CB, K_RB). The starting parameter values do not need to be modified; execution time would be saved by substituting in the previously estimated values, but that is not important for the model considered here. Click OK.
- The following is now done for you by UCODE_2005. The prior information equations are changed to "log10(K_RB)" and "log10(VK_CB)". Based on, equation 7.6 of Hill and Tiedeman (2007, p. 130), standard deviations on the log-transformed values equivalent to the coefficients of variation on the native values are determined to be 0.123 for both log-transformed K_RB and VK_CB. Check the weights for th prior information on the parameters to show that the weights are consistent with this standard deviation.
- "Optimize" should still be selected on the upper left side of the window. Click OK.
- Save the files and run UCODE to repeat the regression with the changed status of the parameters.
- Click UCODE. Click to select "Linearity" on the upper left side of the window. Click OK.
- Save the files and run UCODE to produce the sets of parameter values and do the forward runs needed to evaluate model linearity, as described by Hill and Tiedeman (2007, p.142-144). The main output file has the filename extension #umodlin.
- Produce modified Beale's measure and other indications of model linearity by executing the computer program MODEL_LINEARITY using the batch file *ex7.3-model_linearity.bat*. The results found in Figure 7.9 of Hill and Tiedeman (2007, p. 156) can be found a little up from the bottom of the file *ex7.2_ucode.#modlin*. Change the name of this file to *ex7.2_ucode.#modlin.cv-.3*.

Before changing the statistic for the prior information, it is easier to proceed to ex7.3b to calculate the total and intrinsic model nonlinearity for this weighting of the prior information. This requires the following steps.

- Execute CORFAC_PLUS using the batch file *ex7.3-corfac_plus.bat*. For this problem, the main purpose of this run is to provide a list of quantities for which uncertainty intervals are to be calculated. While we are only interested in the total and intrinsic model nonlinearity in this exercise, we will also end up with the combined intrinsic model nonlinearity which will indicate how well linear intervals are likely to perform for these quantities. Here, the quantities are defined as the six parameter estimates. The input file *ex7.3_ucode.corfac* is constructed using the input instructions of Poeter and others (2005, p. 203-210). There is no need to look at the output from this run.
- In MFI2005, click UCODE and choose LinearityAdv to be "Conf" to indicate that confidence intervals are to be calculated. This is used for a nonlinearity measure important to intervals calculated for predictions; which are not being calculated here. Click OK and run UCODE. The main output file has the filename extension #umodlinadv_conf.

- Execute MODEL_LINEARITY_ADV using the batch file *ex7.3-model_linearity_adv.bat.* The total and intrinsic model nonlinearity are listed about half-way through the output file *ex7.3_ucode.#modlinadv*. Rename this file to *ex7.3_ucode.#modlinadv.cv-.3*

Now the sequence of runs is repeated using different values of the statistics for the prior information.

- The coefficient of variation of 0.3 used for the prior information reflects greater confidence in the parameter values than one might reasonably expect in practice. Repeat the analysis using a coefficient of variation of 1.0, which UCODE_2005 uses to produce a standard deviation of 0.31 for the log-transformed parameter values. The measures calculated are slightly different than those shown in the book because a slightly different statistic was used to weight the prior information.

Briefly, the sequence of runs is as follows.

1. With the Optimize option in the UCODE menu, run UCODE_2005 through MFI2005.
2. With the Linearity option in the UCODE menu, run UCODE_2005 through MFI2005.
3. Execute *ex7.3-model_linearity.bat* to get the modified Beale's measure in *ex7.3_ucode.#modlin*. Change the name of this file to *ex7.3_ucode.#modlin.cv-1.0*.
4. Execute *ex7.3_ucode.corfac*
5. With the ModelLinearity Adv=Conf option in the UCODE menu, run UCODE_2005 through MFI2005
6. Execute *ex7.3-model_linearity_adv.bat* to get measures of total and intrinsic model nonlinearity in *ex7.3_ucode.#modlinadv_conf*. Rename this file to *ex7.3_ucode.#modlinadv_conf.cv-1.0*.

- Address the last part of exercise 7.3a on page 156 of Hill and Tiedeman (2007).
- Address the last part of exercise 7.3b on page 157 of Hill and Tiedeman (2007).

Exercise 8

Many of the statistics for analysis of predictions are not yet supported by GW_Chart. Therefore, you will be shown where the data are located but in class we will just use the figures in the book to show you what the associated graphs look like.

Exercises 8.1 and 8.2

Exercises 8.1 and 8.2 involve predictions, which are not yet supported by MFI2005. For these exercises, the necessary input files have already been constructed, and you will mainly be executing batch files and examining the results. The file structure for these exercises is under folder *initial/ex8.i/*, as follows:

Directory	Contents
First level	
ex8\	mf-mp-runs\ ucode-opr-ppr-runs\
Second level	
mf-mp-runs\	data-ss\ data-preds\ data-new-obs\ data-grid-sensitivities\
ucode-opr-ppr-runs\	ex8.1a\ ex8.1b\ ex8.1b-obs-pred\ ex8.1c\ ex8.1c-predgroups\ ex8.1d\ ex8.1e\ ex8.1f\ ex8.1f+grid\ ex8.2a\ ex8.2b\ files-ss\ files-preds\ files-new-obs\
Third level	
data-ss\ data-preds\ data-new-obs\ data-grid-sensitivities\	Files for running MODFLOW-2005 and MODPATH
ex8.1a\ ex8.1b\ ex8.1b-obs-pred\ ex8.1c\ ex8.1c-predgroups\ ex8.1d\ ex8.1e\ ex8.1f\ ex8.1f+grid\ ex8.2a\ ex8.2b	Batch files and input files for exercises 8.1a to 8.1f, 8.2a, and ex8.2b
files-ss\ files-preds\ files-new-obs\	Batch files and input files used by the runs conducted in folders ex8.1a* and ex8.2a

In exercises 8.1 and 8.2 for this class, advective transport is simulated using MODPATH, rather than the Advective Transport Observation Package of MODFLOW-2000, which was used to produce the output for prediction analyses presented in exercises 8.1 and 8.2 of Hill and Tiedeman (2007). ADV will no longer be supported; MODPATH is being modified to include selected capabilities previously available only in ADV.

As distributed in answers, these directories to not include the output files because these can be easily created by double-clicking the batch files. Once executed, the output files can be removed using the 00-clean.bat file located in each directory.

Exercise 8.1. Predict advective transport and perform sensitivity analysis

- In *exer*\, create folder *ex8*\ and copy all folders in *ex8.i*\ into *exer**ex8*\.

8.1a. Predict advective transport

The input files for this exercise, which uses the model as calibrated in Exercise 5.2c, are in folder *ex8.1a*. Most of the files for the MODFLOW-2005 and MODPATH runs are in folder *files-preds*. The MODFLOW-2005 files in this folder have the root name *ex8-preds*, and are based on those used in Exercise 5.2c. The files for Exercise 8.1a have been modified as follows.

The Well Package input file, *ex8-preds.wel*, has been constructed and its name added to the name file *ex8-preds.nam* and *ex8-preds.nam.ucode* using file type WEL. (This was done in MFI2005 using the Stress menu item and clicking on "WEL"). Other changes to the files include (1) the estimated parameter values from *ex5.2c._paropt* have been copied into *ex8-preds.pvl*, and (2) the head and flow observations have been omitted.

For the MODPATH run, the following files have been constructed: the Main input file *ex8-preds.mpath.mai*, the Name file *ex8-preds.mpath.nam*, and the response file *ex8.1a.mpath.rsp*. The first two files reside in folder *files-preds*, and the latter in folder *ex8.1a*. In the MODPATH run, one particle is placed on the upper face of the center of the cell in row 2, column 16, layer 1, in the northeast part of the model (Hill and Tiedeman, fig. 8.7, p. 197). The file *prediction.times* lists the 10 year, 50 year, and 100 year times at which predictions are of interest. This file is read by MODPATH, and in the *pathline* output file, coordinates of the particle at these times are listed in addition to the standard pathline file output, which lists a particle's position for times when it moves from one cell to another.

- Copy the two *folders* "mf-mp-runs" and "ucode-opr-ppr-runs" under ex8.i into the new directory exer\ex8.
- In *ex8\ex8.1a*, execute batch file *01-ex8.1a.bat*, which runs MODFLOW-2005 and MODPATH.
- Use the output in the *pathline* file to answer the Problem in Exercise 8.1a (Hill and Tiedeman, p. 195).

In the pathline file, there are 10 columns, as labeled in the following example.

```
@ [ MODPATH Version 4.00 (V4, Release 3, 7-2003) (TREF=   0.000000E+00 ) ]
    1 1.55000E+04 1.65000E+04 9.99900E-01 9.99950E+01  0.00000E+00  16   2   1      1
    1 1.51565E+04 1.63903E+04 7.87957E-01 8.93978E+01 -3.15000E+08  16   2   1      1
    1 1.51565E+04 1.63903E+04 7.87957E-01 8.93978E+01  3.15000E+08  16   2   1      1
    1 1.50000E+04 1.63422E+04 7.10433E-01 8.55216E+01  4.46763E+08  15   2   1      1
    1      2           3           4           5           6          7    8   9     10
```

The columns contain the following:

Column	Contents	Column	Contents
1	Particle number	6	Time. In seconds. "-" identifies observation time.
2	Distance parallel to rows, measured from outside edge of column 1	7	Column
3	Distance along columns, measured from the outside edge of the last row. (ADV starts from the outside edge of the first row.)	8	Row
4	Vertical location measured in local model layer coordinates. Negative values locate particles within implicit confining layers	9	Layer
5	Vertical location measured from the datum consistent with the Discretization file.	10	Particle number

Plotting the pathline

The pathline can be plotted on the pages provided showing the model grid, or in three dimensions using ModelViewer. The instructions for using ModelViewer are as follows:

(1) Modpath and Modflow files need to be in same directory. To obtain this, copy all files from
Ex8\mf-mp-runs\data-preds
to
Ex8.1a

(2) Start ModelViewer.
File> New
MODFLOW2000
In the next menu, browse to fine
Name file: ex8-preds.nam
Pathline file: pathline

(3) Show: pathlines

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 directories *ex8.1b* and *ex8.1b-pcc*.

In folder *ex8.1b*, batch file *01-ucode-obs-sensitivity-noprior.bat* runs UCODE-2005 in Sensitivity Analysis mode with the prior information on parameters K_RB and VK_CB removed, to calculate the *pcc* with only the calibration observations. The process model is a MODFLOW-2005 run of the steady-state model without pumping; files for this simulation are located in folder *data-ss*. Examine file *01-ucode-obs-sensitivity-noprior.in* and verify that the input is correct for performing a run in Sensitivity Analysis mode with no prior information.

Batch file *02-ucode-prediction.bat* calculates the prediction scaled sensitivities (*pss*) for the advective transport predictions, using UCODE input file *02-ucode-prediction.in*. The process models are the MODFLOW-2005 run of the steady-state model with pumping and the MODPATH run; files for these simulations are located in folder *data-preds*. Examine the UCODE input file *02-ucode-prediction.in* and note that (1) predictions=yes in the UCODE Control_Data block; (2) an extra parameter for the predictive run, the effective porosity of aquifers 1 and 2 (POR_1&2) has been defined in the PARAMETER_DATA_FOR_PREDICTION block; and (3) nine predictions have been defined, corresponding to transport in the x, y, and z directions at 10, 50, and 100 years; and (4) prior information has been defined for the effective porosity parameter. The weights defined for the prior information are discussed under Exercise 8.1c on p. 200 of Hill and Tiedeman.

To obtain parameter correlation coefficients with the calibration observations and the predictions, the predictions need to be defined as observations and included with the calibration observations in a Sensitivity Analysis mode run. In folder *ex8.1b-pcc*, this has been done in input file *01-ucode-obs-pred-sensitivity.in*. Examine the contents of this file.

- In folder *ex8.1b*\, run batch file 01-ucode-obs-sensitivity-noprior.bat to calculate the pcc without prior information on VK_CB and K_RB. The pcc matrix is in the main UCODE output file; pcc > 0.90 are in listed *ex8.1b._pcc*.
- In folder ex8.1b\, run batch file 02-ucode-prediction.bat to calculate the pss. Of the four different pss files produced by UCODE-2005, data-exchange file *_sppr* contains the scaling used to produce Figure 8.8 of Hill and Tiedeman (p. 198).
- In folder *ex8.1bobs-pred*, run batch file *01-ucode-obs-pred-sensitivity.bat* to calculate the pcc with both the calibration observations and the predictions.
- Verify that the output from these runs is similar to that shown in Figure 8.8 and Tables 8.4 and 8.5.

Overview of OPR-PPR input files for Exercises 8.1c, 8.1d, and 8.1f

The *opr* and *ppr* statistics are calculated using the computer software OPR-PPR (Tonkin et al., in press). OPR-PPR is designed to use as input up to seven data-exchange files that are produced as output by UCODE_2005 calibration and prediction simulations. These include files containing general model data (*_dm*, *_dmp*), sensitivities (*_su*, *_spu*, *_supri*, *_suprip*), and weighting (*_wt*, *_wtpri*, *_wtprip*) files. The only additional, user prepared, file that is needed by OPR-PPR is its main input file, which specifies the type of analysis to be conducted and various *opr* and *ppr* calculation options. Input instructions for the OPR-PPR main input file are in the pdf version of the OPR-PPR documentation in your *Documentation+* folder.

The UCODE data-exchange files from the sensitivity analysis and prediction runs of Exercise 8.1b that are used in the OPR-PPR calculations of Exercises 8.1c, 8.1d, and 8.1f are:

ex8.1b._dm	model data file
ex8.1b._dmp	model data file from prediction run
ex8.1b._su	existing observations sensitivity file
ex8.1b._wt	existing observations weight file
ex8.1b._spu	prediction sensitivities file
ex8.1b._suprip	sensitivities file for prior on prediction-only parameters
ex8.1b._wtprip	weights file for prior on prediction-only parameters

Exercises 8.1c, d, f. Using GW_Chart

GW_Chart can now be used to plot the ppr and opr statistics. Navigate to the appropriate directory from GW_Chart. All the ppr and opr values or average values for each parameter or observation (averaged over the predictions) can be plotted.

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

In folder *ex8.1c*, the OPR-PPR main input files for the *ppr* runs of Exercise 8.1c are *ppr-pargroups-no.in* and *ppr-pargroups-yes.in*. Both these files are in folder *ex8.1c* and folder *ex8.1c-predgroups*. In the input files for the latter folder, a prediction group is defined that includes all 9 of the predictions, so the values listed in the *_ppr* output file for individual parameters (*pargroups-no*) are the average *ppr* statistics for all predictions, as shown in Figure 8.9a of Hill and Tiedeman (p. 201).

- Run batch files *01a-PPR-PARGROUPS-NO.BAT* and *01b-PPR-PARGROUPS-YES.BAT* in both folders *ex8.1c* and folder *ex8.1c-predgroups*, to produce the *ppr* statistics for individual and groups of parameters.

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

In folder *ex8.1d*, the OPR-PPR main input file for the *opr* run of Exercise 8.1d is *opromit.in*.

- Run batch file *01-opromit.bat* to produce the *opr* statistics shown in Figure 8.10a of Hill and Tiedeman. The *_OPR_ABSCHG* file contains the values plotted in Figure 8.10b.

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

In folder *ex8.1e*, batch file *01-ucode-obs-newobs-sensitivity.bat* runs UCODE-2005 in Sensitivity Analysis mode with the prior information on parameters K_RB and VK_CB removed, and with the calibration observations and the potential new observations. The process model for simulating the new observations is a MODFLOW-2005 run of the steady-state model with pumping, and with the potential head and flow as observations (in files *ex8.obh* and *ex8.obr*); files for this simulation are located in folder *data-new-obs*. Examine file *01-ucode-obs-newobs-sensitivity.in* and verify that the input is correct for performing this UCODE run.

- In folder *ex8.1e*, run batch file *01-ucode-obs-newobs-sensitivity.bat* to calculate the *pcc* with the potential new observations and the calibration observations. The pcc produced should be similar to those in Table 8.7(c) of Hill and Tiedeman. The pcc matrix is in the main UCODE output file; pcc > 0.90 are listed in *ex8.1e._pcc*.
- To produce the pcc matrix shown in Table 8.7(a) of Hill and Tiedeman, open file *01-ucode-obs-newobs-sensitivity.in* and in the OBSERVATION_GROUPS block, change the USEFLAG for observation ‘newhead’ to ‘no’. To produce the *pcc* matrix shown in Table 8.7(b) of Hill and Tiedeman, change the USEFLAG for observation ‘newhead’ back to ‘yes’, and change the USEFLAG for observation ‘newflow’ to ‘no’.

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

Files for the first part of this analysis are in folder *ex8.1f*.

To produce the *opr* statistics for the two potential new observations, first a UCODE sensitivity analysis run is needed to obtain the sensitivities of the simulated equivalents of the potential new observations, and then OPR-PPR is run for an OPRADD analysis.

For the UCODE-2005 run, with main input file *01-ucode-new-obs.in*, the process model is that in folder *data-new-obs*, described above. This UCODE-2005 run produces the sensitivity file *ex8.1f-new._su*, which is listed in the main OPR-PPR input file for this exercise, *opradd.in*, so it can be read by OPR-PPR when conducting the analysis of adding the potential new observations. Weights on the potential observations are required for the OPRADD analysis; for this example the weights on the potential head and flow are the same as those on the head and flow calibration observations, respectively.

This run produces an error message from UCODE_2005 because it tries to calculate a variance-covariance matrix using the two potential observations. Given the six parameters defined, this produces a singular matrix and the program fails trying to take the inverse. All we want are the sensitivities, which are produced. So, while annoying, the error is not problematic for our purposes.

- First run batch file *01-ucode-new-obs.bat*. Then run batch file *01-opradd.bat* to produce the *opr* statistics shown in Figure 8.12 of Hill and Tiedeman.

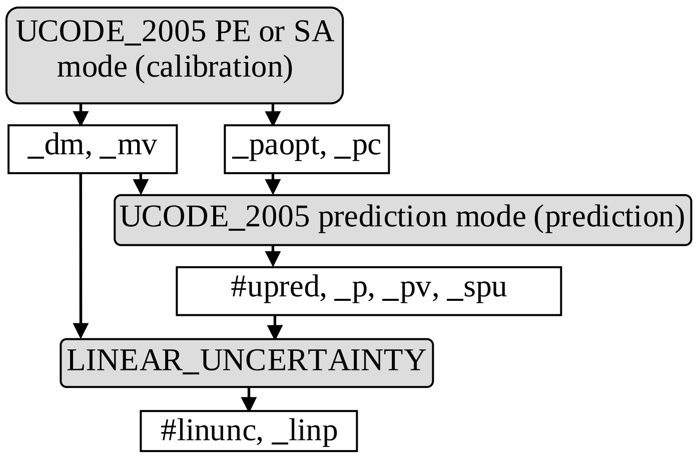
Files for the second part of this analysis are in folder *ex8.1f+grid*. The capability in OPR-PPR of calculating *opr* statistics for a potential new head observation at every node of the model requires a 'grid sensitivity' file containing the sensitivity of head to all model parameters, for every model node. This file can easily be produced using the Sensitivity Process of MODFLOW-2000, but not yet MODFLOW-2005. Obtaining it using UCODE_2005 is tedious. For this exercise, we use a file produced in a MODFLOW-2000 run, under pumping conditions (file *withpumping._grid-sensitivities*). The grid sensitivities file can be produced using any process model, as long as it is formatted so that it can be read by OPR-PPR. This run also requires weights for the potential new observations at every model node; these are the same as those for the calibration observations of head and are specified in file *grid._wt*. These grid sensitivity and grid weights files are listed in the main OPR-PPR input file for this analysis.

- Run batch file *01-opraddnode.bat* to produce the grid of *opr* statistics used to produce Figure 8.13 of Hill and Tiedeman. Values in file opraddnode._OPCNOD are used to produce Figure 8.14.

Exercise 8.2. Prediction Uncertainty Measured Using Inferential Statistics

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

The post processing program LINEAR_UNCERTAINTY is used to calculate linear confidence intervals on predictions. This run requires input from a sensitivity analysis or regression run, and from a prediction run. In folder *ex8.2a*, batch file *01-ucode-obs-sensitivity.bat* produces the sensitivities for the calibration observations, calculated at the optimal parameter values, and batch file *02-ucode-prediction.bat* produces the prediction sensitivities. Consider these batch files in the context of the flow chart for calculating linear intervals presented by Poeter and others (2005, p. 158) and repeated here.



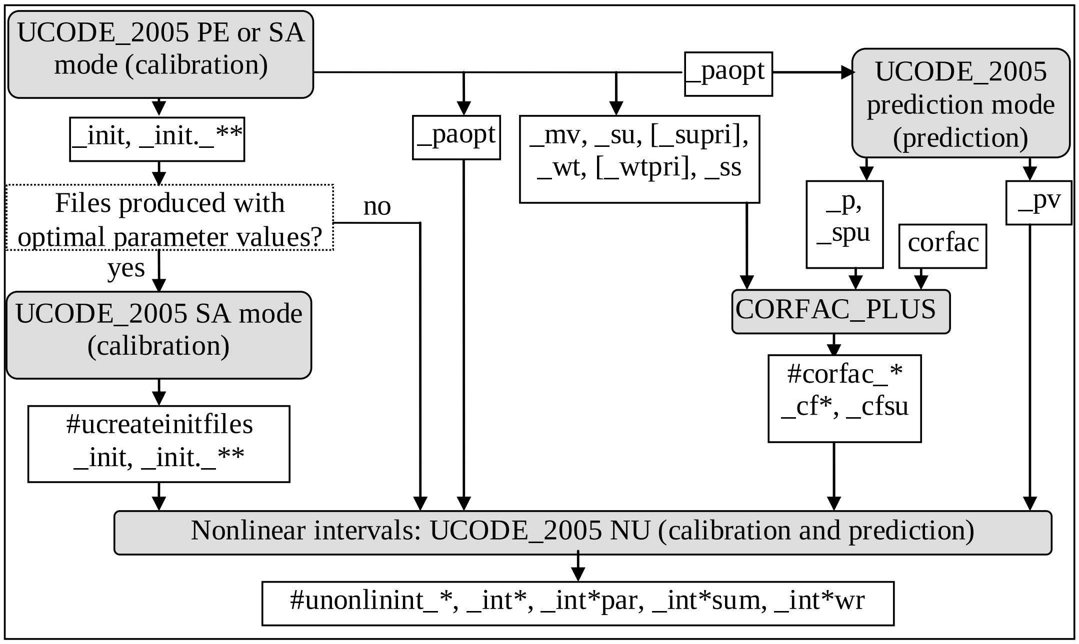
- Run batch files *01-ucode-obs*-sensitivity.bat and 02-ucode-prediction.bat in sequence
- Run batch file 03-linunc.bat to produce the linear confidence intervals. The LINEAR_UNCERTAINTY program has no main input file; all input comes from the data-exchange files produced in the sensitivity analysis and prediction runs. The main output file is *ex8.2a.#linunc*, and the data-exchange file containing the intervals is *ex8.2a._linp*.

The program LINEAR_UNCERTAINTY always calculates confidence and prediction intervals. Find them in the output file ending in _linp.

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

Files for calculating nonlinear confidence intervals are provided in directory initial\ex8.i\ucode-opr-ppr-runs\ex8.2b. These files are constructed usingthe steps listed by Poeter and others (2005, p. 216-218). Look at the following aspects of these files.

- Inspect the batch files that are used to accomplish the runs noted in the following flow chart, which is modified slightly from Poeter and others (2005, p. 193). They are named *01-ucode-sensitivity.bat*, *01-zcreate-init.bat*, *02-ucode-prediction.bat*, *03-corfac.bat*, and *04-ucode-nonlin-uncert.bat*. Consider these batch files in the context of the flow chart for calculating nonlinear intervals presented by Poeter and others (2005, p. 193). A modified version is repeated here.



* is replaced by "conf" when confidence intervals are calculated and "pred" when prediction intervals are calculated. (see Poeter and others, 2005, p. 189-190).

** is replaced as described by dm, mv, su, and, when prior information is defined, supri. See Poeter and others (2005, p. 189-191).

- Inspect the UCODE_2005 main input files to determine how the 04-ucode-nonlin-uncert.bat accounts for the calibration conditions and observations, and predictive conditions and predictions, which are accounted for separately in other input files. In particular, identify the following.
    1. The model command lines in the different files.
    2. The parameter definition in the different files. Note that the porosity parameter is included for all runs, even the sensitivity runs for which is has no affect on the simulated values. Future versions of UCODE_2005 may allow parameters that apply only to predictions to be omitted from the runs to which they do not apply.
    3. The observations and predictions in the different files.
    4. The prior information in the different files (note that it is the same for all runs in this set of files).
    5. The model input files and template files defined for each run.
    6. The model output files and instruction files defined for each run.
- Inspect how the limits calculated are controlled by the input block Reg_GN_NonLinInt, keyword WhichLimits, and the input blocks Prediction_Groups and Prediction_Data.
- Run the batch files *01-ucode-sensitivity.bat*, *01-zcreate-init.bat*, *02-ucode-prediction.bat*, *03-corfac.bat*, and *04-ucode-nonlin-uncert.bat*

- Inspect the output file *ex8.2b._intconf*. Identify the interval limit, the sum-of-squared weighted residuals at the limit, and the objective function goal. Note how the identifier in the first column is negative for the lower limit and positive for the upper limit.
- Inspect the parameter values used to calculate each of the limits are listed in the output file *ex8.2b._intconfpar*.
- Inspect the summary of the regressions for each limit in the output file *ex8.2b._intconfsum*.
- Inspect the weighted residuals calculated using the parameter values for each limit in the output file *ex8.2b._intconfwr*.

Exercise 9.1 and 9.2: Simulate Transient Hydraulic Heads and Perform Preparatory Steps

Prepare input for transient simulation using parameters, and run the simulation in forward mode. The parameter values listed in table 2 should be used in the input files. These will be the starting values when nonlinear regression is performed.

Table 2: Parameter names and starting values for properties of the transient system for which parameters are estimated in the exercises.
[Same as Table 9.2 of Hill and Tiedeman (2007, p. 231)]

Flow-system property	Parameter name	Starting value
Specific Storage of layer 1 (m^{-1})	SS_1	2.65e-5
Specific Storage of layer 2 (m^{-1})	SS_2	4.0E-6
Pumping rate in each model layer 1 and 2 (m^3/s)	Q_1&2	-1.1

<u>Instructions</u>:

- In MFI2005, save the *ex4.1* dataset as dataset *ex9.1* and use the *ex9.1* dataset in this exercise.
- DIS input: Click "Stress Periods". Specify that the simulation will include a total of 5 stress periods. The first stress period will be steady-state, and the others will be transient. Stress-period length, number of time steps, and time-step multiplier are shown in the following table. (Harbaugh, 2005, p. 4-4 to 4-4, 8-11 to 8-14)

Stress period	Stress-period length (seconds)	Number of time steps	Time-step multiplier	SS or TR
1	0	1	1.0	SS
2	87,162	1	1.0	TR
3	261,486	1	1.0	TR
4	522,972	1	1.0	TR
5	23,567,451	9	1.2	TR

- Internal Flow input: LPF. Click "Hydraulic".

  Two SS parameters (see table 2 for parameter values):

  Define parameter SS_1 to control specific storage (SS) of layer 1.

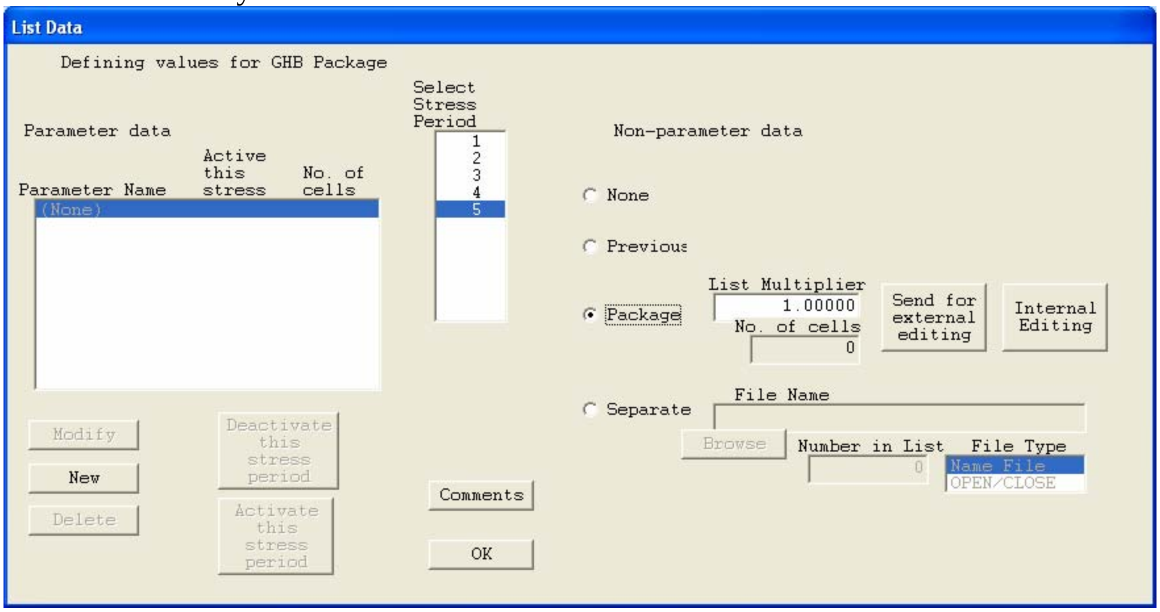
  Define parameter SS_2 to control SS of layer 2.

- Stress input: Click "RCH". Activate both RCH parameters for all stress periods.
- Click "RIV". Activate parameter K_RB for all stress periods.
- Click "GHB". Activate all GHB cells for all stress periods.. Non-parameter data can be reused by selecting the "Previous" option.

The General-Head boundary Package is used to represent the boundary condition on the side of the region farthest from the stream. It is not defined using a parameter, and its activation for additional stress periods is different than for other aspects of the system.

Exercise from Chapter 9

For GHB, activate for additional stress periods by clicking on the stress period and clicking on “Previous”. This makes the definition of the input the same as the previous stress period. Start with stress period 2. Here, stress period 5 has been selected and “Previous” is ready to be selected.



- Click “WEL”. Define one parameter called Q_1&2 to control two well cells, in layers 1 and 2, row 9, column 10. See table 2 above for parameter value. Activate the parameter for stress periods 2-5. (Harbaugh, 2005, p. 8-40 to 8-42)
- Click “Parameter Values”. Click button at upper left “Select Parameter Values…” and select the three new parameters.
- Save the dataset and execute MODFLOW-2005 from the File menu. Output files are produced in directory *exer*.
- Evaluate the resulting heads as follows.

The MFI2005 default is to print the final heads of the simulation in the LST output file. A good check when running a transient model that starts with a steady-state stress period is to compare the heads from the initial steady-state stress period with the heads from the model that included only the steady-state stress period. To print the heads from the steady-state stress period, do the following.

- Click “Output”
- Choose “Times for Printing Heads”
- Select list
- List two print times: stress period 1, timestep 1, and stress period 5, timestep 9.
- Rerun MODFLOW-2005.
- Heads will be printed to output file ex9.1.lst.

Compare the steady-state heads with the values in ex4.1.lst.

Evaluate the heads at later time steps by looking at them in the output file or by plotting them using ModelViewer. Presently, only the final heads are saved. Additional heads can be saved using the MFI2005 Output menu mentioned above.

Also look at the global budgets in the output file. Is the system at steady-state at the end of the simulation? That is, is the change in storage small?

Exercise 9.3: Transient Parameter Definition

Define the three parameters listed in Table 9.2 of Hill and Tiedeman (2007, p. 231). Double check that the proper layers and stress periods are used. For example, pumpage applies only to stress periods 2 through 5. Also, under Parameter Values, use the “Select parameters to be in PVAL file” button.

Exercise 9.4: Observations for the Transient Problem

Transient observations are listed in tables 9.3 and 9.4 of Hill and Tiedeman, p. 232-234. They are also provided in files in the initial\ex9.4.i\ directory. Input instructions for observations for MODFLOW-2005 are provided in OBS.PDF. Input instructions for observations for UCODE_2005 are provided in Poeter and others (2005).

- In MFI2005, save the *ex9.1* dataset as dataset *ex9.4* and use the *ex9.4* dataset in this exercise.
- To make use of a partially complete file already prepared, exit MFI2005 and copy the file *ex9.4.hob* from the *exer\initial.mfi2005\ex9.4.i* directory to the *exer* directory, overwriting the existing *ex9.4.hob* file. Restart MFI2005.
- Use the “Multi-Time Head” button to add observations for well 1 (hd01.ss, dd01.1, dd01.283; here we use slightly different observation names than those defined by Hill and Tiedeman, 2007).
  - Set TOMULTH to 86400, which allows the time offset (TOFFSET) from the beginning of the reference stress period (IREFSP) to be in units of days, although the model time unit is seconds.
  - For the header name, use well1 and well2, respectively.
  - When transient data are defined, MODFLOW-2005 allows the regression to use either the measured hydraulic heads or the initial hydraulic head and subsequent drawdowns as observations. Specify that drawdowns are to be calculated by MODFLOW-2005 and used in the objective function (applies to observations following the first for each well). In both cases, HOBS needs to be head; the program will take the difference to produce drawdowns. The statistic for all but the initial value depends on whether heads or drawdowns are used at these times. This is because subtracting subsequent heads from the initial heads results in some types of errors being omitted from the resulting drawdowns. See Hill and Tiedeman (2007, p. 231).
- Use the “RIV Observations” button to add the two gains observed in river flow presented in table 9.4 of Hill and Tiedeman (2007, p. 234).

- Set the time offset multiplier to 86400 so that observation-time offsets can be entered in days.
- Flow is out of the ground-water system. MODFLOW sign conventions require observed river gains to be negative.
- Assign plot symbol as 2.

- Use MFI to run MODFLOW-2005, and examine the tables of simulated and observed heads and flows.

Exercise 9.5: Evaluate Transient Model Fit Using Starting Parameter Values

Address the problem in Hill and Tiedeman (p. 235) using the table of simulated equivalents of the observations, the residuals, and weighted residuals located at the end of the file *ex9.4.lst*.

Exercise 9.6: Sensitivity Analysis for the Initial Model

Producing the results needed to conduct a sensitivity analysis of the initial model can be accomplished by the following steps. Exercises 9.6 b and c (Hill and Tiedeman, 2007, p. 240 and 243) are addressed using results in the *ex9.6._sc* and *ex9.6._pcc* files, respectively.

- Save the *ex9.4* model to *ex9.6*.
- Click UCODE. Click the button next to “Sensitivities - Central”.
- As before, we will begin without prior information to obtain a clear understanding of what information the observations provide on the parameter. Remove the prior information by deleting the PriorNames. Click OK. Click UCODE again to see that, indeed, the prior information has been removed.
- Use MFI to run UCODE.
- Use GW_Chart to look at the results in the files *ex9.6._sc* and *ex9.6._pcc*.

Exercise 9.7: Estimate Parameters for the Transient System by Nonlinear Regression

Regression can be performed by the following steps.

- Save the ex9.6 model to ex9.7.
- Click “Parameter Values” and log-transform the six parameters related the hydraulic conductivity and storage characteristics. Click OK.
- Click UCODE. Click the button next to “Optimize”. Click OK.
- Use MFI to save the files and run UCODE.
- The results presented in Hill and Tiedeman (2007, p. 245 to 246) for this problem were produced by MODFLOW-2000 using sensitivity-equation sensitivities. Here, we are using less accurate forward-difference sensitivities. For this problem, the

method used to solve the regression matters when forward difference sensitivities are used. In the UCODE menu on the right side, the input for the Reg_GN_Controls input block of UCODE_2005 are presented. If the only change made is to change "Trustregion" to "Dogleg", regression converges in eight iterations. If Trustregion=no or HookStep, regression does not converge in 10 iterations; if Generally, the HookStep method is the most robust, but for this problem the DogLeg method performs better.

- The results shown in Hill and Tiedeman (2007, figure 9.12a, p. 245) are listed in two tables located toward the end of file *ex9.7.#uout*. All of the methods achieve nearly the same model fit and estimated parameters, despite two being unable to satisfy a TolPar convergence criterion of 0.01.
- Produce the graph shown in Hill and Tiedeman (2007, figure 9.12b, p. 245) using GW_Chart and file *ex9.7._pa*.

Exercise 9.8: Evaluate Measures of Model Fit

A modified version of the fragment of output shown in the lower part of Figure 9.13 of Hill and Tiedeman (2007, p. 246) occur toward the end of the output file *ex9.7_ucode.#uout*. The new versions provide confidence intervals on the calculated error variance and the standard error of the regression, to make it easier to determine whether the values are significantly different than 1.0. Here, we see that they are not, which is consistent with our knowledge that the model is correct and the weights correctly reflect the observation erros.

```
LEAST-SQUARES OBJ FUNC (OBS. ONLY)----- =  23.992
  NUMBER OF INCLUDED OBSERVATIONS-------- =      35 OF      35
  NUMBER OF PRIOR ESTIMATES-------------- =       0
  NUMBER OF ESTIMATED PARAMETERS--------- =       9

  CALCULATED ERROR VARIANCE (CEV)-------- = 0.92275
  95% CONFIDENCE INTERVAL ON CEV--------- = 0.57232      1.7335
  STANDARD ERROR ----------------------- = 0.96060
  95% CONFIDENCE INTERVAL ON STD ERR----- = 0.75652      1.3166

  CORRELATION COEFFICIENT---------------- = 0.99999
  ITERATIONS----------------------------- =       8


  STATISTICS FOR EVALUATING ALTERNATIVE MODELS:

    No prior used in this parameter estimation
    MAX LIKE OBJ FUNC OBSERVATIONS ONLY (MLOFO)----------- = -13.218
    LN DETERMINANT of Fisher Information Matrix (OBS ONLY) =  118.51

    MODEL EVALUATION MEASURES:

      OBSERVATIONS ONLY (no prior used in this parameter estimation)
      AIC STATISTIC-------------  =  6.7823
      AICc STATISTIC------------  =  15.949
      BIC STATISTIC-------------  =  22.336
      KASHYAP STATISTIC---------  =  77.473
```

Exercise 9.9: Perform Graphical Analyses of Model Fit and Evaluate Related Statistics.

The graphs shown in Figure 9.14 of Hill and Tiedeman (2007, p.247) can be produced using GW_Chart and files (a) *ex9.7_ucode._ws*, (b) *ex9.7_ucode ._ww*, and(c) *ex9.7_ucode ._os*. The graph of Figure 9.17a can be produced using GW_Chart and the file *ex9.7_ucode._nm*.

Exercise 9.10: Evaluate Estimated Parameter Values

Figure 9.18 of Hill andTiedeman (2007, p.251) can be constructed using GW_Chart and the file ex9.7_ucode._sc.

A graph similar to the one shown in Figure 9.19 can be constructed using GW_Chart and file ex9.7_ucode._pc if the reasonable lower and upper limits are defined consistently.

The large parameter correlation coefficients of Table 9.7 are listed in file *ex9.7_ucode._pcc*.

Exercise 9.11: Test for Linearity

Model nonlinearity can be evaluated as for exercise 7.3 using the following sequence of runs. There are no complicating factors such as the need to log-transform parameters (they are already transformed). The sequence of steps, briefly, is as follows.

- Begin by using MFI2005 to copy the *ex9.7* files to *ex9.11*.
- Use MFI2005 and the Optimize option in the UCODE menu.
- Use MFI2005 and the Linearity option in the UCODE menu.
- Execute ex9.11-model_linearity.bat
- Execute ex9.11_ucode.corfac
- Use MFI2005 with the ModelLinearity Adv=Conf in the UCODE menu.
- Execute *ex9.11-model_linearity_adv.bat*

Exercises 9.12: Predictions

Files are not provided for this exercise. Please perform the exercises using results provided in Hill and Tiedeman (2007).