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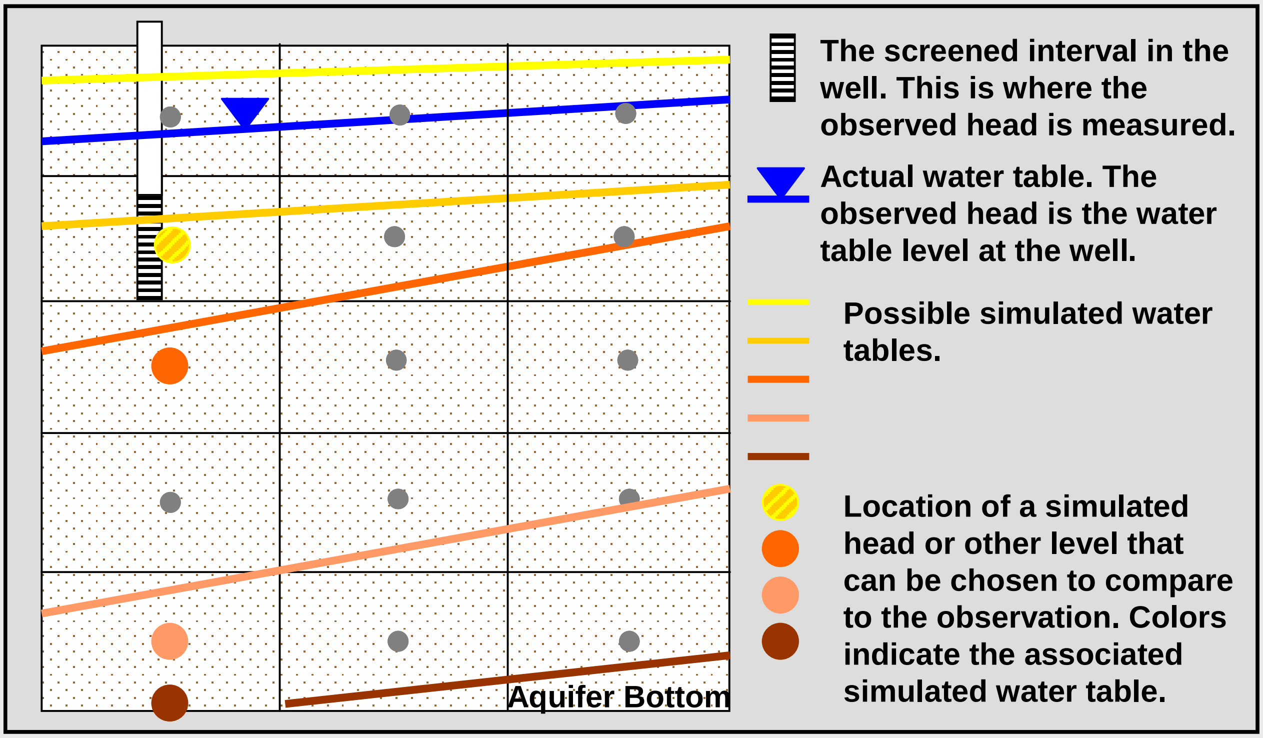
International Ground Water Modeling Center

SIM_ADJUST -- A Computer Code that Adjusts Simulated Equivalents for Observations or Predictions

Constructed using the JUPITER API

JUPITER: **J**oint **U**niversal **P**arameter **I**den**T**ification and **E**valuation of **R**eliability

API: **A**pplication **P**rogramming **I**nterface



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SIM_ADJUST -- A Computer Code that Adjusts Simulated Equivalents for Observations or Predictions

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PREFACE

SIM_ADJUST surmounts an obstacle that is sometimes encountered when using a universal analysis computer code such as UCODE_2005 (Poeter and others, 2005), PEST (Doherty, 2004), and OSTRICH (Matott, 2005; Fredrick and others, 2007). These codes read simulated values that are compared to observations or used as predictions. The simulated values often are read from a list in a file that is produced by a process model (for example, MODFLOW, Harbaugh and others, 2000; Harbaugh, 2005) that represents a system of interest. At times simulated values needed by the universal code are missing or assigned default values because the process model could not produce a useful solution. The computer code described in this report, SIM_ADJUST, is designed to read simulated equivalents from a file produced by a process model that contains space- or tab-delimited columns of data. The columns of data need to include a column of simulated values and a column of related observation or prediction names.

SIM_ADJUST identifies observations or predictions that have been omitted or assigned a default value by the process model, and provides alternate simulated values or defaults. A sequence of alternatives also can be defined to accommodate situations in which earlier alternatives also are not produced by the process model.

The performance of SIM_ADJUST has been tested in a variety of applications. Future applications, however, might reveal errors that were not detected in the test simulations. Users are requested to notify the originating office of any errors found in the report or the computer program. Updates might occasionally be made to both the report and to SIM_ADJUST. Users can check for updates on the Internet at URL

http://www.mines.edu/igwmc/freeware/sim_adjust/sim_adjust.html

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Figure 2. Universal codes usually execute batch files, as indicated. To use Sim_Adjust, include it in the batch file. Then, instead of using simulated equivalents from the output of the process model (here, *process._ext)*, the universal code uses output from Sim_Adjust (here, *fn.*_output-sim_adjust)... 4

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SIM_ADJUST -- A Computer Code that Adjusts Simulated Equivalents for Observations or Predictions

By Eileen P. Poeter[1] and Mary C. Hill[2],

ABSTRACT

This report documents the SIM_ADJUST computer code. SIM_ADJUST surmounts an obstacle that is sometimes encountered when using universal model analysis computer codes such as UCODE_2005 (Poeter and others, 2005), PEST (Doherty, 2004), and OSTRICH (Matott, 2005; Fredrick and others (2007). These codes often read simulated equivalents from a list in a file produced by a process model such as MODFLOW that represents a system of interest. At times values needed by the universal code are missing or assigned default values because the process model could not produce a useful solution.

SIM_ADJUST can be used to (1) read a file that lists expected observation or prediction names and possible alternatives for the simulated values; (2) read a file produced by a process model that contains space or tab delimited columns, including a column of simulated values and a column of related observation or prediction names; (3) identify observations or predictions that have been omitted or assigned a default value by the process model; and (4) produce an adjusted file that contains a column of simulated values and a column of associated observation or prediction names. The user may provide alternatives that are constant values or that are alternative simulated values. The user may also provide a sequence of alternatives. For example, the heads from a series of cells may be specified to ensure that a meaningful value is available to compare with an observation located in a cell that may become dry.

SIM_ADJUST is constructed using modules from the JUPITER API, and is intended for use on any computer operating system. SIM_ADJUST consists of algorithms programmed in Fortran90, which efficiently performs numerical calculations.

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Chapter 1: Overview of SIM_ADJUST

Introduction

The SIM_ADJUST code described in this report is a JUPITER Application Program (Banta and others, 2006) designed to surmount an obstacle that is sometimes encountered when using a universal analysis computer code such as UCODE_2005 (Poeter and others, 2005), PEST (Doherty, 2004), and OSTRICH (Matott, 2005; Fredrick and others, 2007). These codes read simulated equivalents from a list in a file produced by a process model such as MODFLOW (Harbaugh and others, 2000 or Harbaugh, 2005) that represents a system of interest. At times values needed by the universal code are missing or assigned default values because the process model could not produce a useful solution. This occurs, for example, in ground-water models when dry cells result in the inability to produce simulated heads in some places. SIM_ADJUST identifies observations or predictions for which simulated values have been omitted or assigned a default value by the process model, and defines alternate simulated values or defaults. The user may provide a constant replacement value, or may indicate that an alternative simulated equivalent from the process model should be used (for example, for a head observation in a dry cell, the head from an underlying cell may be specified). The user may also provide a sequence of alternatives. Indeed, a long chain of alternative values can be specified. For example, the heads from a series of cells may be specified to provide a value for an observation in a cell that may become dry, and may be underlain by a series of dry cells.

Extracting simulated equivalents from the primary output listing file of a code like MODFLOW is often time consuming and cumbersome, so it is preferable to extract them from a file that lists the needed simulated values in a column. Such files are created by codes with mature capabilities for observations and(or) predictions, such as MODFLOW-2000 and MODFLOW-2005. For example, MODFLOW-2000 produces a file named with a prefix supplied by the user as the OUTNAM variable of the Observation Process followed by "._os" (Hill and others, 2000). For MODFLOW-2005, the file name is specified in the name file. If a cell is dry, MODFLOW-2000 omits the observation completely from the file; while MODFLOW-2005 lists a default value in place of the simulated value. The lack of a simulated value, or an arbitrary default value, results in the observation being unusable for calculating residuals, performing sensitivity analysis, or estimating parameters. In some cases, an alternate simulated value could be used, and these are the circumstances for which the SIM_ADJUST program is designed. For example, if a cell in one model layer goes dry and an observation is located there, it may be reasonable to compare the observed value with the head simulated in a neighboring or underlying cell. The result is that the observation can continue being included in the analysis.

With SIM_ADJUST, for example, in a multi-layer model (Figure 1), the user can specify that the observation MW3-B (that is, head in monitoring well 3 with an open interval in layer B) should be compared to the value of the simulated head in layer C if layer B is dry at that location. Further, it can be specified to use the simulated head in layer D if layer C is also dry, and the simulated head in layer E if layer D is dry. Finally, the sequence could end by specifying that if all layers are dry use the elevation of the bottom of the model. Although MW3-B may only physically penetrate layer B at the field site, heads from the underlying layers provide useful information on the magnitude of the difference between the observed head and the simulated value of head (residual). It should be noted that the use of the aquifer bottom elevation as a final resort is arbitrary and will result in zero sensitivity to head at that location if the bottom layer is dry. Sensitivity is the derivative of the simulated value with respect to a parameter (see, for example, the UCODE_2005 documentation by Poeter and others, 2005 or Hill and Tiedeman, 2007). If the simulated value does not change when a parameter value changes, the sensitivity is zero. Consequently, if the cell is dry for a given parameter value and also for a slightly changed parameter value, the same simulated equivalent (aquifer bottom elevation) will be obtained and the sensitivity will be zero.

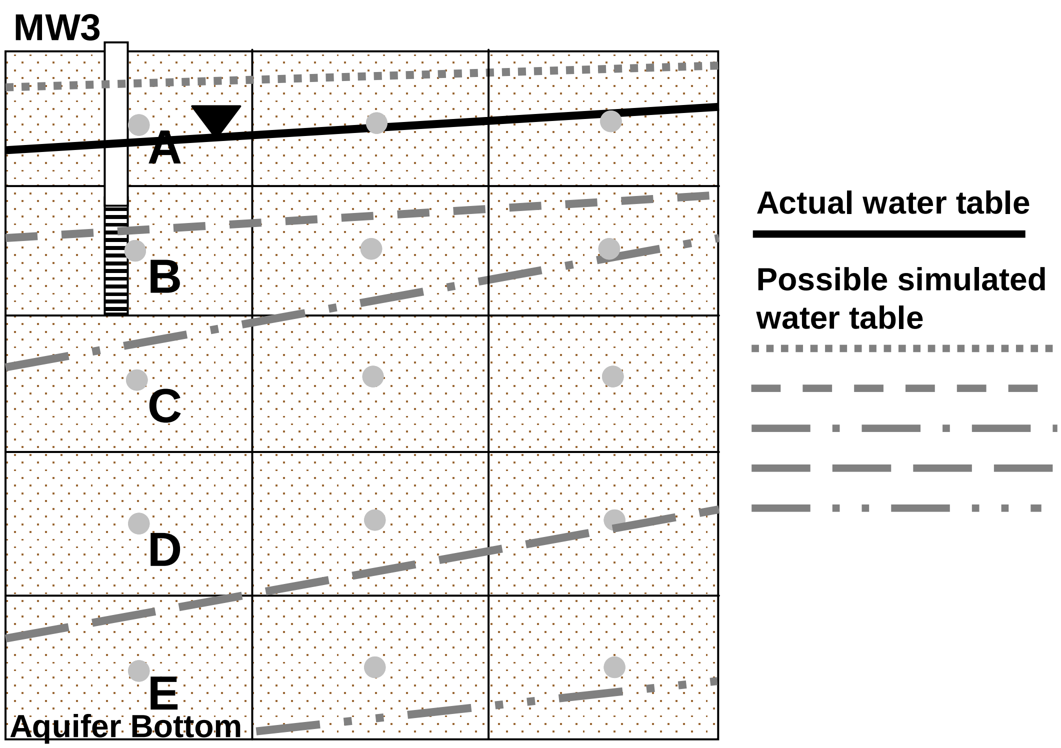

Figure 1. Possible simulated equivalents for a head observation when a free-surface water table forms the upper boundary of the simulated ground-water system. The observed head reflects conditions in the open interval of the well (indicated by the horizontal stripes). If the simulated head at the well location is in model layer A or B, the head in layer B is used. If the simulated water table is low enough that the cell in layer B is dry at the well location, the following sequence can be defined by SIM_ADJUST. First try to compare the observed head to the head simulated in the underlying cell of layer C. If the cell in layer C is dry, use the head in the cell in layer D. If the cell in D is dry, use the head in the cell in layer E. If the cell in layer E is dry, use the elevation of the aquifer bottom.

In order to accomplish this, SIM_ADJUST performs the steps shown in figure 2 and described briefly here.

- Read user input from *input-sim_adjust* to:
  - identify the file produced by the process model,
  - define its structure,
  - set global default values, and

  - o describe the procedure for determining the alternative value for each listed observation or prediction.
- Read the process model output file *process._ext* that contains simulated equivalents of observations or predictions and associated names in space or tab delimited data columns to:
  - o obtain simulated values from the data column specified by the user, and
  - o obtain observation or prediction names from the data column specified by the user.
- Identify observations or predictions that have been omitted or assigned a default value by the process model in the *process._ext* file.
- Define alternate simulated values or defaults.
- Print a file with a complete set of simulated equivalents *fn.*_output-sim_adjust (using the alternative simulated equivalents as appropriate). This file has a column of simulated values and a column of observation or prediction names.

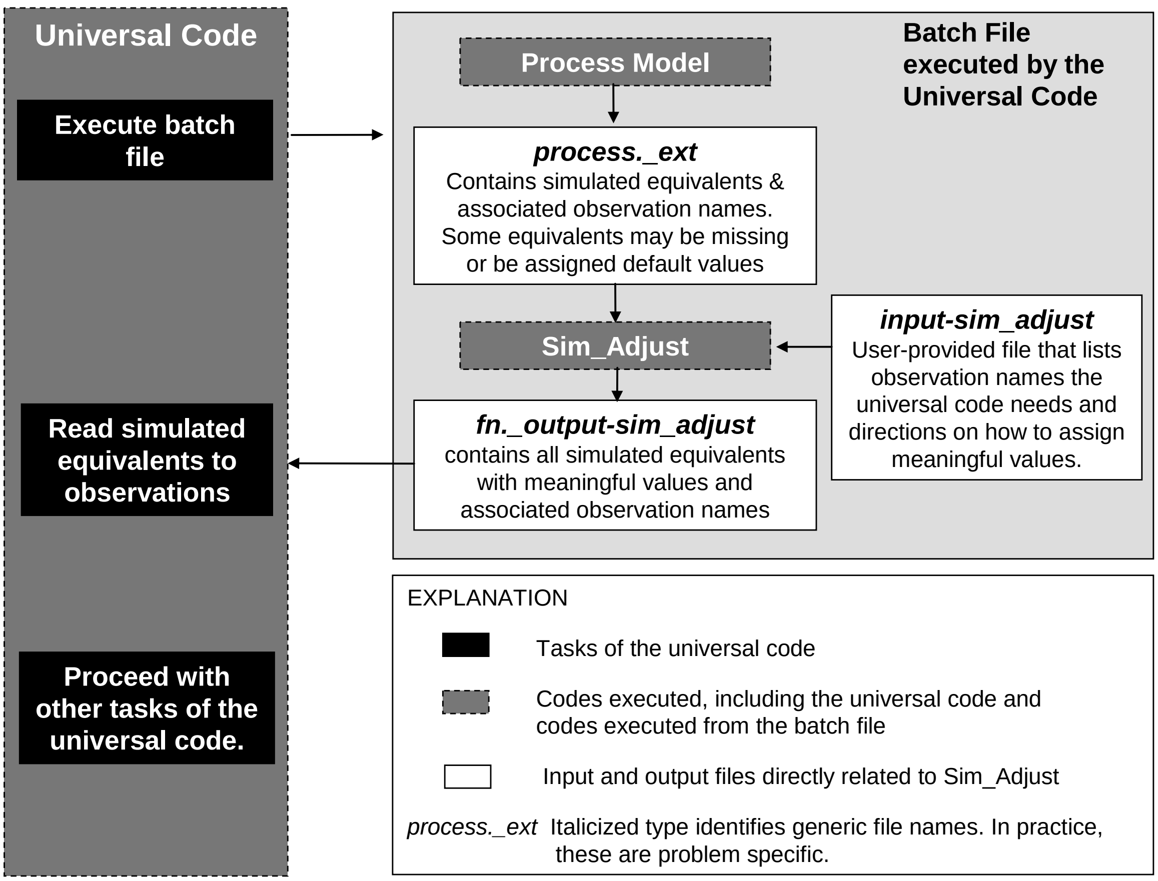

Figure 2. Universal codes usually execute batch files, as indicated. To use SIM_ADJUST, include it in the batch file. Then, instead of using simulated equivalents from the output of the process model (here, *process._ext)*, the universal code uses output from SIM_ADJUST (here, *fn.*_output-sim_adjust).

Here we italicize portions of file names to indicate names that will be specified by the user. The name of the file produced by the process model depends on the process model and choices made in its execution; in this report it is referred to as *process._ext*. The user of SIM_ADJUST supplies the name of the SIM_ADJUST input file, which is referred to in this report as *input-sim_adjust*. This file contains directions for converting simulated equivalents that may be omitted from or assigned a default value in the *process._ext* file. The root (prefix) of the SIM_ADJUST output file is represented by *fn* and is assigned a specific name by the user when executing SIM_ADJUST. SIM_ADJUST adds the extension "._output-sim_adjust" to form the complete output file name *fn*._output-sim_adjust. The files are described in Chapter 2.

As an example, process model files containing observed and simulated values are produced by the Observation Process of MODFLOW-2000 or MODFLOW-2005 (Harbaugh and others, 2000; Harbaugh, 2005). In MODFLOW-2000, this file is assigned a filename with the extension "_os", where the "o" and "s" indicate that observed and simulated vales are listed in the file. In MODFLOW-2005, the file is similar but the filename is defined by the user through the MODFLOW name file. If other programs produce files with lists of observation names and simulated values, they also could be adjusted with the SIM_ADJUST program.

In the event that a sequence of simulated equivalents specified by the user via SIM_ADJUST are missing from the *process._ext* file or are assigned process-model default values, a SIM_ADJUST global default value (specified by the user in *input-sim_adjust*) is assigned, and a message is written to both the screen and the bottom of the *fn*._output-sim_adjust file. Some codes that extract values (such as UCODE and UCODE_2005) allow the user to specify a value that, when equal to the value read as a simulated equivalent, indicates observations or predictions that should be omitted from consideration. This can be specified as the global process model default value of SIM_ADJUST.

The observation or prediction names used in the *input-sim_adjust* file need to be consistent with those listed in the *process._ext* file. These may not be the same as the names defined for the universal code.

Purpose and Scope

This report documents SIM_ADJUST, a code for adjustment of process model output which is problematic when read by a universal parameter-estimation code.

This report begins with an overview of SIM_ADJUST. The remainder of the report describes how to run SIM_ADJUST, construct input files, and use the SIM_ADJUST output files. Appendix 1 includes an example application with SIM_ADJUST input and output files for a simple problem. Appendix 2 describes the connection between SIM_ADJUST and the JUPITER API. Appendix 3 contains information about the distributed files, including source code files.

Files for SIM_ADJUST are available on the World Wide Web at URL http://water.usgs.gov/software/ground_water.html/ and http://water.usgs.gov/software/general.html/.

Expertise of the authors is primarily in the simulation of ground-water systems, so examples in this report come from this field. However, models of nearly any type of system can be evaluated.

Users of SIM_ADJUST need to be knowledgeable about the process model(s) being investigated.

Acknowledgements

The authors would like to acknowledge Kimberly Fisher, Clint Carney, Michael le Francois, and Stephanie Schmidt, students at the Colorado School of Mines in Golden, Colorado; and William Wingle of NewFields in Denver, Colorado for testing the programs using their data sets. Beta testing programs is always frustrating and these colleagues brought good ideas and good humor to the process. The documentation was reviewed by William Wingle of NewFields and Charles Heywood of the U.S. Geological Survey.

Chapter 2: SIM_ADJUST Execution

This section (1) describes the command used to run SIM_ADJUST, (2) contains information on filename restrictions that need to be respected for SIM_ADJUST to perform correctly; and (3) provides brief explanations of the files used by SIM_ADJUST. Additional information on the input and output files is presented in subsequent sections.

Run Command

The run command needs to be executed in the folder containing the SIM_ADJUST input file, *input-sim_adjust*, and in which the output *fn.*_output-sim_adjust will appear. An example run command is:

“path”\sim_adjust.exe *input-sim_adjust fn*

where "path” is the full or relative path to the SIM_ADJUST executable, *input-sim_adjust* is the name of the input file for SIM_ADJUST and *fn* represents a filename prefix for the output file (which may include a path to the file). The specifications for *input-sim_adjust* and *fn* can include full or relative paths and need to conform to filename restrictions of the operating system being used. If there are spaces in *input-sim_adjust* or *fn*, then they need to be enclosed in double quotation marks. For operating systems with case-sensitivity, the case used in *input-sim_adjust* and *fn* on the command line must be consistent with the filenames. The output file extension that is added to *fn*, “._output-sim_adjust”, is always lower case.

Input and Output Files

SIM_ADJUST reads two input files and one output file, as shown in figure 2. One input file is produced by the process model and is referred to in this report as *process._ext*. The italicized letters indicate that the actual filename is defined by the user; it is defined in the first line of the input file described in Chapter 3. The filename can not include spaces and on case-sensitive operating systems the same case needs to be used as the file generated by the process model. SIM_ADJUST is designed for use with output files from the Observation Process of MODFLOW-2000 or MODFLOW-2005, but is basic enough that it may be used with other process models for which similar files are produced.

The other SIM_ADJUST input file is produced by the modeler and is referred to in this report as *input-sim_adjust*, where *input-sim_adjust* is defined in the SIM_ADJUST run command, as described in the previous section of this report. The *input-sim_adjust* file identifies the observations or predictions for which simulated equivalents appear in the *fn.*_output-sim_adjust file and defines a sequence of alternatives that can be used to generate useful simulated equivalents if one or more simulated equivalents are omitted from the *process._ext* file, or if one or more of the simulated equivalent values indicate a valid value was not simulated by the process model.

The output file is *fn.*_output-sim_adjust. It contains two columns: the first column lists the simulated equivalents and the second column lists the associated observation or prediction names.

The output file, *fn.*_output-sim_adjust, is overwritten in subsequent runs of SIM_ADJUST. To preserve output files, they can be moved to another directory or their name can be changed. JUPITER "data exchange" files, such as *fn.*_output-sim_adjust, contain data with little or no explanatory text because they are intended for use by another computer program.

Contents of the files containing simulated equivalents are listed in Table 1.

Table 1. Content of files containing simulated equivalents read and produced by SIM_ADJUST.

Name used to refer to file in this report[1]	**Input or Output**	**Column**	
process._ext	Input	*process._ext* may or may not have header lines	
		Any Column[2]	Any Column[2]
		Simulated Equivalent	Observation or prediction name
*fn.*_output-sim_adjust	Output	*fn.*_output-sim_adjust header line has "Column Tags" surrounded by double quotes as indicated	
		Column 1	Column 2
		"SIMULATED EQUIVALENT"	"OBSERVATION NAME"

[1] Italicized filenames and the prefix *fn* are replaced by user-defined names and a prefix. "*process._ext*" is replaced by a name specified in the SIM_ADJUST input file described in Chapter 3. "*fn*" is replaced by the filename prefix defined in the SIM_ADJUST run command, as described in the beginning of Chapter 2.

[2] The process._ext file may include columns of simulated equivalents in any order. The column containing the observation or prediction names need not be to the right of the simulated equivalents.

Chapter 3: SIM_ADJUST Input Instructions

SIM_ADJUST requires a primary input file, *input-sim_adjust*, including the name of the process model file (e.g. *process._ext*) containing the simulated equivalent values (some of which may be missing or replaced by default values), information about the contents of the *process._ext* file generated by the process model, and definition of defaults. The *input-sim_adjust* input instructions are as follows:

Blank lines and comment lines are not permitted, however comments may be written to the right of any line.

Line 1: **NAME_PROCESS_OUTPUT**

NAME_PROCESS_OUTPUT is the file name of the process-model output file to be evaluated. Relative or absolute path information needs to be included if the process model file resides in a directory other than the one in which the SIM_ADJUST code is invoked. If NAME_PROCESS_OUTPUT includes any spaces, then it needs to be surrounded by quotation marks. This file is referred to in this report as *process._ext*.

Line 2: **NSKIP COL_SIM COL_NAME Process_Model_Default SIM_ADJUST_Default**

NSKIP is the number of lines to skip in the *process._ext* file before reading data. It needs to be an integer value.

COL_SIM is the column of the *process._ext* file that contains the simulated value (for example, COL_SIM is 1 when using the _os file of MODFLOW-2000 or the Observation Process output file of MODFLOW-2005). It needs to be an integer.

COL_NAME is the column in the *process._ext* file that contains the name of the observation or prediction (for example, COL_NAME is 4 when using the _os file of MODFLOW-2000 and 3 when using the Observation Process output file of MODFLOW-2005). It needs to be an integer.

Process_Model_Default is a default value printed in the *process._ext* file when the simulated value can not be produced (for example the value of HDRY for all versions of MODFLOW).

SIM_ADJUST_Default is the value assigned in the *fn.*_output-sim_adjust file to an observation or prediction in the event that the alternatives specified by the user do not produce a replacement value.

Line 3 **ObsorPred_Name STATUS TYPE [ALTERNATIVE]**

Repeat item 3 as many times as needed to list all observations or predictions and to define all alternatives.

ObsorPred_Name is a character string (maximum length 20 characters including upper and lower case letters, numerals and underscore, hyphen, and decimal point). The name must exactly match the name of an observation or prediction that may be written by the process model.

STATUS is a single character (not case sensitive) that determines ObsorPred_Names that will appear in the *fn.*_output-sim_adjust file. The options are:

L – ObsorPred_Name will be listed in the *fn.*_output-sim_adjust file

or

X – ObsorPred_Name will not be listed in the *fn.*_output-sim_adjust file. Instead, it is being used to define an alternate.

Note: Observations or predictions with ‘L’s will appear in the *fn.*_output-sim_adjust file in the order they are elisted in the *input-sim_adjust* file. This is important because in universal codes, such as UCODE_2005 and PEST, the names and order of observations and predictions are defined by the user and the simulated values read need be in the defined order.

TYPE is a single character (not case sensitive) that determines whether ALTERNATIVE is not read, is read as an observation or prediction name, or is read as a value. The options are as follows.

N –ALTERNATIVE is not read. Use this option when it is certain that the ObsorPred_Name will be found in the *process._ext* file and that the related simulated value can always be used for sensitivity analysis, calibration, and so on.

or

O –ALTERNATIVE is read as ObsorPred_Name_Alt, which is a name that may be listed in the *process._ext* file. The simulated value associated with ObsorPred_Name_Alt is used if ObsorPred_Name is not listed in the *process._ext* file or if the value listed as the simulated value indicates a useful value was not calculated.

or

V –ALTERNATIVE is a numerical value to be used if ObsorPred_Name is not listed in the *process._ext* file or if the value listed as the simulated value indicates a useful value could not be calculated

ALTERNATIVE has a form that depends on TYPE. Options are:

(1) Not read when TYPE=N.

or

(2) Read as a character string when TYPE = O. In this situation, ALTERNATIVE defines ObsorPred_Name_Alt, an alternative name listed in the *process._ext* file. The simulated value associated with ObsorPred_Name_Alt replaces the simulated value of ObsorPred_Name if (1) ObsorPred_Name is not listed in the *process._ext* file or (2) the simulated value listed for ObsorPred_Name indicates that a useful solution was not obtained.

or

(3) Read as a numerical value when TYPE = V. In this situation, ALTERNATIVE defines a value that will be used as the default value if (1) ObsorPred_Name is omitted from the *process._ext* file or (2) the value listed for ObsorPred_Name indicates a useful solution was not obtained.

Commonly, a name that appears as ObsorPred_Name_Alt in one occurrence of line 3 then appears as ObsorPred_Name in a subsequent occurrence. This is how a sequence of alternatives is defined.

An example *input-sim_adjust* file is provided in Appendix A.

Chapter 4: Using SIM_ADJUST Output

The file *fn.*_output-sim_adjust is generally used by a universal application code such as UCODE_2005 or PEST for extracting alternative values for observations or predictions that were omitted from the *process._ext* file during a process model simulation. Messages that may lead the user to find errors in their default definitions are written at the end of the *fn.*_output-sim_adjust file. This allows the automated program to proceed by printing the global defaults while documenting potential problems in the same file. It is advisable to check these messages when first setting up the SIM_ADJUST files.

Chapter 5: References

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Appendix 1: Example Files

Use of SIM_ADJUST is illustrated for a modified version of test case 1 presented in Appendix C of the UCODE_2005 users' manual (Poeter and others, 2005). An illustration of that system is presented here as Figure A1-1. Files for the test case are distributed with the SIM_ADJUST code in folder \test\tc1-3layer.

To obtain a substantial number of omitted observations, model layers were modified from the problem presented in the UCODE_2005 documentation. That test case was simulated using MODFLOW-2000, which also is used here.

The test case was modified as follows. Instead of confined layers, all layers were specified as convertible with specific yields approximately two orders of magnitude greater than the specific storage. The first layer was divided into a thin upper layer that would readily go dry during the simulation. Layer tops and bottoms were defined so that layer 2 and 3 would go dry at some locations (Figure A1-2). Specifically, the bottom elevations of layer two (lower portion of aquifer 1) and the confining bed were raised so they would each be thin at the location of observations 3, 5, and 8 (Figure A1-2). This caused the second layer to go dry at those locations. The bottom elevation of layer 3 was raised so it would be thin at the location of observations 3 and 8, which caused layer 3 to go dry so that SIM_ADJUST used the elevation of the layer bottom (118m) for the simulated equivalent at that location. These adjustments required changes to the tc1-fwd.bas, tc1-fwd.dis, tc1-fwd.lpf, and tc1-fwd.ohd files as compared with those provided for the UCODE_2005 test case. Those files are printed (for the MODFLOW-2000 version) along with the SIM_ADJUST input and output files at the end of this Appendix.

The MODFLOW input file tc1-fwd.ohd contains the same observations defined for the confined test case and alternative observations referred to in the SIM_ADJUST input file. Additional observations were included in tc1-fwd.ohd at the locations of the observations in layer 1, but identify heads from the new layer 2 (the lower portion of the original layer 1), and the third layer which was originally layer 2.

In all of the examples, the MODFLOW simulation is executed to generate a tc1-fwd._os file, which is then processed by SIM_ADJUST. The tc1.input-sim_adjust file specifies that for any head observation of layer 1 missing from the tc1-fwd._os file (this is *process._ext* in this case), the head value at the same location in layer 2 should be used, and if that is missing from the tc1-fwd._os file, then the head value from layer 3 should be used, and finally if that is missing a default value equal to the bottom elevation of layer 3 is used. The elevation of the bottom of layer 3 is 40m everywhere except at observations 3 and 8 where it is 118m.

An error-free example is provided in folder tc1-3layer distributed with the SIM_ADJUST code. A folder named tc1-3layer-example-input-error is provided to illustrate the character of SIM_ADJUST error messages. In that folder, the SIM_ADJUST input file tc1.input-sim_adjust includes two purposefully incorrect entries so as to illustrate that the global SIM_ADJUST default would be used and error messages would be printed to help the user identify potential problems. These are observation obs2.2 (this is the sixth observation listed in the tc1.input-sim_adjust file) which was identified with 'n' indicating the value should be found in the tc1-fwd._os file when it is actually omitted; and observation obs3.12d1, which is specified as a default for obs3.12 and should default to obs3.12d2, but is entered as an 'n', thus resulting in a sequence of defaults that leads nowhere. Both of these situations result in the simulated equivalent being assigned the global default value (-1.E-50) specified by the user in the SIM_ADJUST input file, tc1.input-sim_adjust, and caused warnings to be printed to the screen and at the end of the tc1.output-sim_adjust file. Note that the universal code could proceed by using these global SIM_ADJUST default values, but the results may not be useful, so we recommend the SIM_ADJUST output be reviewed for such messages before using it with a universal code.

The same exercise is performed using MODFLOW-2005 in folder tc1-3layer-mf2005. MODFLOW-2000 does not write a default value for dry observations, while MODFLOW-2005 does. The MODFLOW-2005 example illustrates how a process-model default value can be identified and replaced by SIM_ADJUST.

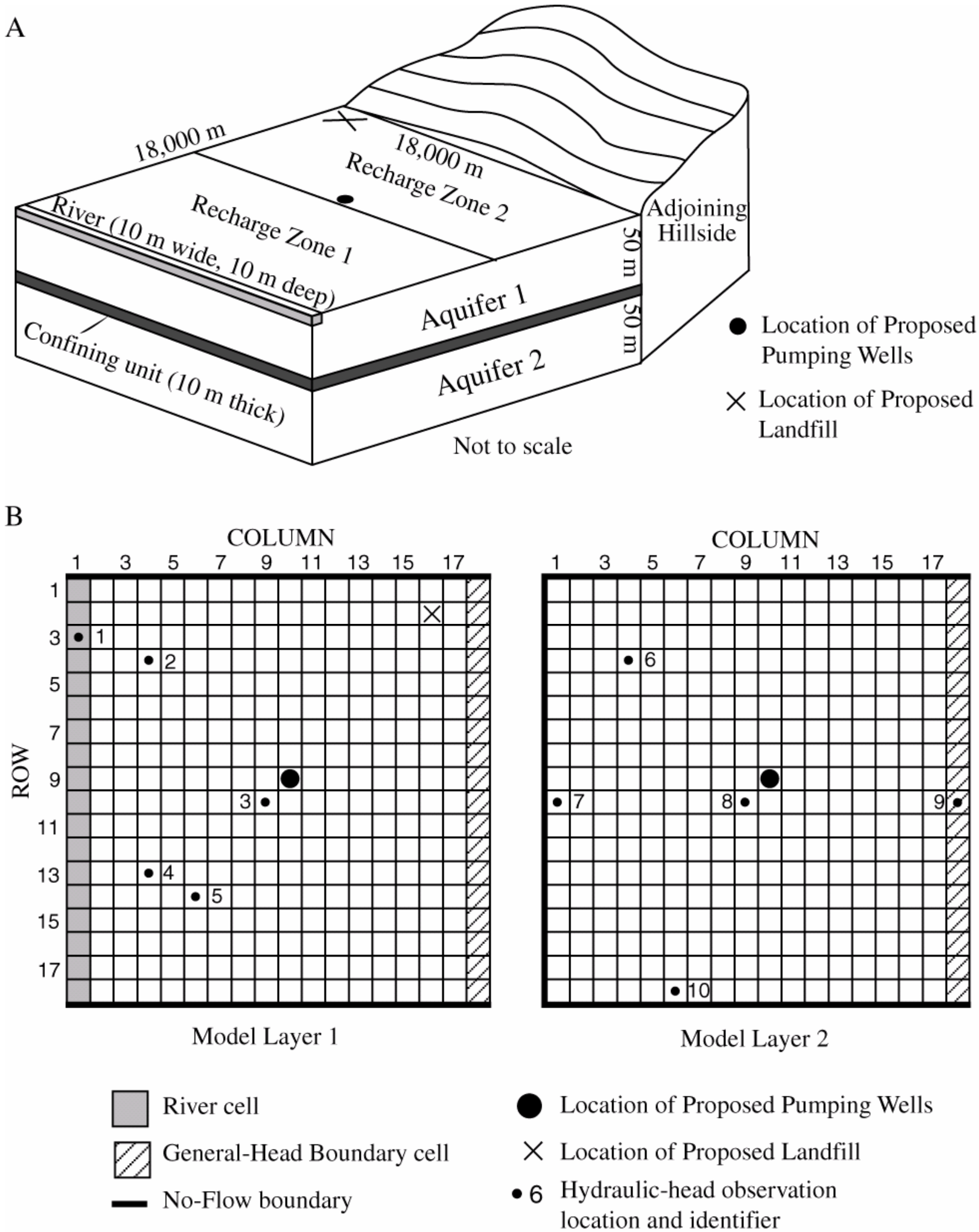

Figure A1-1. (A) Physical system and (B) model grid for test case 1 of Poeter and others (2005) reproduced here with permission of author.

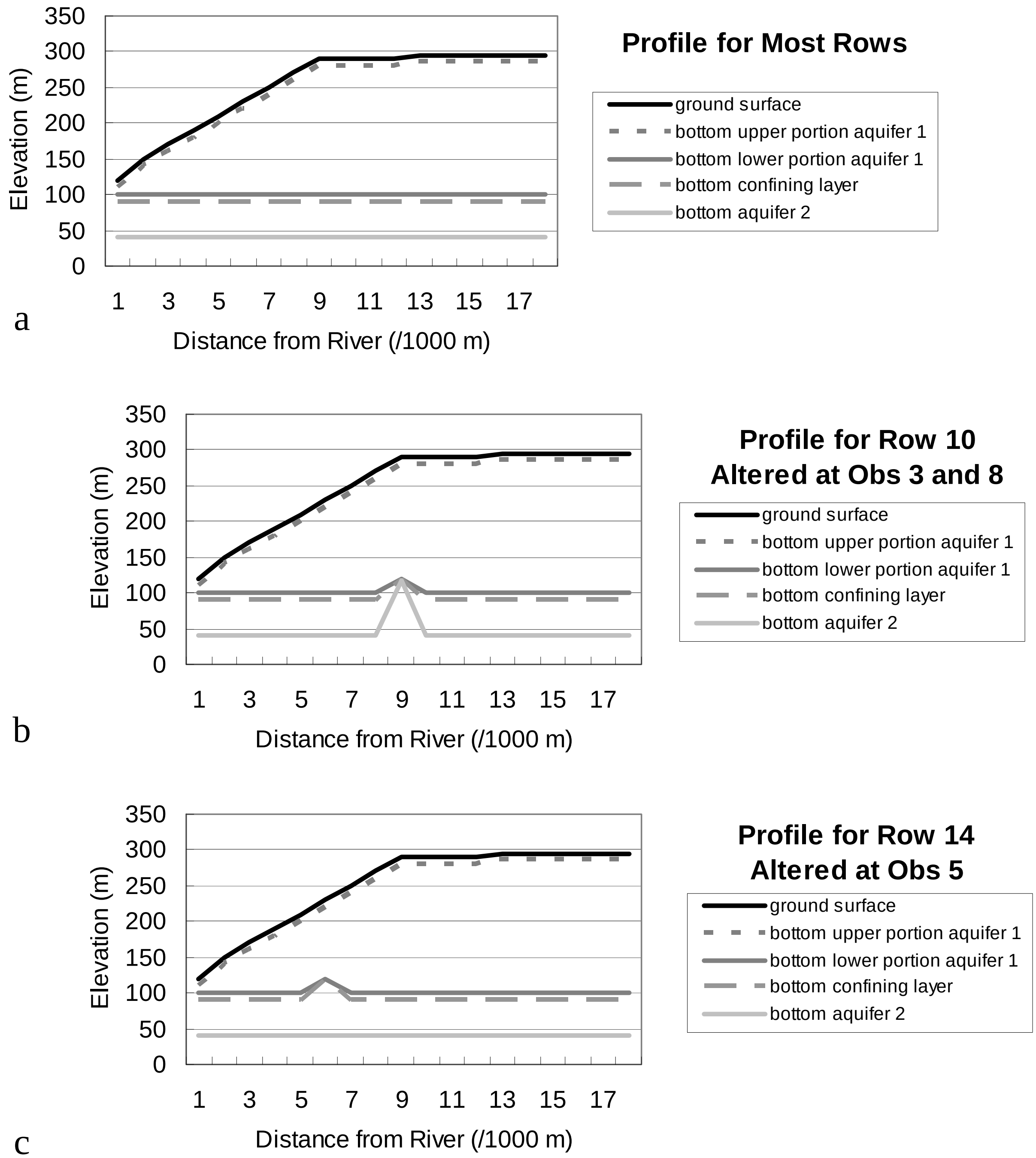

Figure A1-2. Layering used in the test case to produce dry cells at observation locations. Pumping occurs at row 9, column 10. The illustrated layer elevations cause cells to go dry at observation locations 3, 5, and 8.

Input files:

tc1.input-sim_adjust (this is an example of the file generically referred to as *input-sim_adjust* in this report)

```
'tc1-fwd._os'
0  1  4  -888.  -1.E-50
obs1.0     L    o    obs1.0d1
obs1.1     L    o    obs1.1d1
obs1.12    L    o    obs1.12d1
obs2.0     L    o    obs2.0d1
obs2.1     L    o    obs2.1d1
obs2.2     L    o    obs2.2d1
obs2.8     L    o    obs2.8d1
obs2.12    L    o    obs2.12d1
obs3.0     L    o    obs3.0d1
obs3.1     L    o    obs3.1d1
obs3.12    L    o    obs3.12d1
obs4.0     L    o    obs4.0d1
obs4.1     L    o    obs4.1d1
obs4.12    L    o    obs4.12d1
obs5.0     L    o    obs5.0d1
obs5.1     L    o    obs5.1d1
obs5.12    L    o    obs5.12d1
```

First 17 observations have alternatives defined

```
obs1.0d1   X    o    obs1.0d2
obs1.1d1   X    o    obs1.1d2
obs1.12d1  X    o    obs1.12d2
obs2.0d1   X    o    obs2.0d2
obs2.1d1   X    o    obs2.1d2
obs2.2d1   X    o    obs2.2d2
obs2.8d1   X    o    obs2.8d2
obs2.12d1  X    o    obs2.12d2
obs3.0d1   X    o    obs3.0d2
obs3.1d1   X    o    obs3.1d2
obs3.12d1  X    o    obs3.12d2
obs4.0d1   X    o    obs4.0d2
obs4.1d1   X    o    obs4.1d2
obs4.12d1  X    o    obs4.12d2
obs5.0d1   X    o    obs5.0d2
obs5.1d1   X    o    obs5.1d2
obs5.12d1  X    o    obs5.12d2
```

First level alternatives for the first 17 observations are defined using additional repetitions of line 3

```
obs1.0d2   X    v    40.
obs1.1d2   X    v    40.
obs1.12d2  X    v    40.
obs2.0d2   X    v    40.
obs2.1d2   X    v    40.
obs2.2d2   X    v    40.
obs2.8d2   X    v    40.
obs2.12d2  X    v    40.
obs3.0d2   X    v    118.
obs3.1d2   X    v    118.
obs3.12d2  X    v    118.
obs4.0d2   X    v    40.
obs4.1d2   X    v    40.
obs4.12d2  X    v    40.
obs5.0d2   X    v    40.
obs5.1d2   X    v    40.
obs5.12d2  X    v    40.
```

Second level alternatives for the first 17 observations are defined as values. These values could have been listed as the first level alternatives, but this file shows how sequences of alternatives are defined.

```
obs6.0     L    v    40.
obs6.1     L    v    40.
obs6.12    L    v    40.
obs7.0     L    v    40.
obs7.1     L    v    40.
obs7.12    L    v    40.
```

The next 15 observations have alternative values defined

```
obs8.0      L    v    118.
obs8.1      L    v    118.
obs8.12     L    v    118.
obs9.0      L    v    40.
obs9.1      L    v    40.
obs9.12     L    v    40.
obs0.0      L    v    40.
obs0.1      L    v    40.
obs0.12     L    v    40.
obsSS       L    n
obsTR3      L    n
obsTR12     L    n
```

…continued

The last three observations have no alternatives defined

tc1._os (this is an example of the file generically referred to as *process._ext* in this report)

```
   100.0667        101.8040         1  obs1.0         0.000000
   104.1128        128.1170         1  obs2.0         0.000000
   104.1128        124.8930         1  obs4.0         0.000000
   100.0690        101.8040         1  obs1.0d1       0.000000
  0.1397247       -0.2899933E-01    1  obs1.1d1       87163.00
   3.531517       -0.1289978        1  obs1.12d1     0.2443906E+08
   104.1103        128.1170         1  obs2.0d1       0.000000
 -0.8554077E-01   -0.4100037E-01    1  obs2.1d1       87163.00
 -0.2619858       -0.5570068        1  obs2.2d1       348649.0
 -0.6630936        -11.53101        1  obs2.8d1       9303771.
 -0.4744186        -14.18401        1  obs2.12d1     0.2443906E+08
   104.0871        156.6780         1  obs3.0d1       0.000000
   104.1103        124.8930         1  obs4.0d1       0.000000
 -0.8559418E-01   -0.6700134E-01    1  obs4.1d1       87163.00
 -0.4742050        -14.30400        1  obs4.12d1     0.2443906E+08
   104.0854        140.9610         1  obs5.0d1       0.000000
   100.4227        101.8040         1  obs1.0d2       0.000000
  0.1004486       -0.2899933E-01    1  obs1.1d2       87163.00
   3.179291       -0.1289978        1  obs1.12d2     0.2443906E+08
   103.9412        128.1170         1  obs2.0d2       0.000000
 -0.5223846E-01   -0.4100037E-01    1  obs2.1d2       87163.00
 -0.1873093       -0.5570068        1  obs2.2d2       348649.0
 -0.4893188        -11.53101        1  obs2.8d2       9303771.
 -0.3039246        -14.18401        1  obs2.12d2     0.2443906E+08
   104.0871        156.6780         1  obs3.0d2       0.000000
   103.9414        124.8930         1  obs4.0d2       0.000000
 -0.5261230E-01   -0.6700134E-01    1  obs4.1d2       87163.00
 -0.3039169        -14.30400        1  obs4.12d2     0.2443906E+08
   104.0823        140.9610         1  obs5.0d2       0.000000
 -0.1990509E-01   -0.5999756E-01    1  obs5.1d2       87163.00
 -0.4158173        -21.67599        1  obs5.12d2     0.2443906E+08
   103.9412        126.5370         1  obs6.0         0.000000
 -0.5223846E-01    0.4997253E-02    1  obs6.1         87163.00
 -0.3039246        -14.36501        1  obs6.12       0.2443906E+08
   100.4227        101.1120         1  obs7.0         0.000000
  0.1004181        0.4800415E-01    1  obs7.1         87163.00
   3.178619       -0.5680008        1  obs7.12       0.2443906E+08
   104.0871        158.1350         1  obs8.0         0.000000
   104.0918        176.3740         1  obs9.0         0.000000
 -0.4776001E-02   -0.9918213E-03    1  obs9.1         87163.00
 -0.3380127        -38.24199        1  obs9.12       0.2443906E+08
   104.0769        142.0200         1  obs0.0         0.000000
 -0.8422852E-02   -0.1300049E-01    1  obs0.1         87163.00
 -0.4099197        -19.92101        1  obs0.12       0.2443906E+08
  -1.441222        -4.400000        2  obsSS          0.000000
   0.000000        -4.100000        2  obsTR3         871621.9
   0.000000        -2.200000        2  obsTR12       0.2443906E+08
```

tc1-fwd.bas

```
# MODULAR MODEL - TWO-LAYER EXAMPLE PROBLEM, TEST CASE TC1
#
FREE                Item 1: options
CONSTANT     1      Item 2: IBOUND, layer 1
CONSTANT     1      Item 2: IBOUND, layer 2
CONSTANT     1      Item 2: IBOUND, layer 3
   0.0              Item 3: HNOFLO
CONSTANT   200.     Item 4: STRT, layer 1
CONSTANT   200.     Item 4: STRT, layer 2
CONSTANT   200.     Item 4: STRT, layer 3
```

tc1-fwd.dis

```
# DIS file for test case tc1
  3  18  18  5  1  2      Item 1:  NLAY NROW NCOL NPER ITMUNI LENUNI
  0   1   0               Item 2:  LAYCBD
CONSTANT  1000.           Item 3:  DELR
CONSTANT  1000.           Item 4:  DELC
CONSTANT   300.           Item 5:  TOP,  layer1 - top of original layer 1 raised to allow bottom to be high in the unconfined
system
INTERNAL   100. (FREE) 0  Item 6:  BOTM, layer 1
   1.1   1.4   1.6   1.8   2.0   2.2   2.4   2.6   2.8   2.8   2.8   2.8   2.85   2.85   2.85  2.85   2.85   2.85
   1.1   1.4   1.6   1.8   2.0   2.2   2.4   2.6   2.8   2.8   2.8   2.8   2.85   2.85   2.85  2.85   2.85   2.85
   1.1   1.4   1.6   1.8   2.0   2.2   2.4   2.6   2.8   2.8   2.8   2.8   2.85   2.85   2.85  2.85   2.85   2.85
   1.1   1.4   1.6   1.8   2.0   2.2   2.4   2.6   2.8   2.8   2.8   2.8   2.85   2.85   2.85  2.85   2.85   2.85
   1.1   1.4   1.6   1.8   2.0   2.2   2.4   2.6   2.8   2.8   2.8   2.8   2.85   2.85   2.85  2.85   2.85   2.85
   1.1   1.4   1.6   1.8   2.0   2.2   2.4   2.6   2.8   2.8   2.8   2.8   2.85   2.85   2.85  2.85   2.85   2.85
   1.1   1.4   1.6   1.8   2.0   2.2   2.4   2.6   2.8   2.8   2.8   2.8   2.85   2.85   2.85  2.85   2.85   2.85
   1.1   1.4   1.6   1.8   2.0   2.2   2.4   2.6   2.8   2.8   2.8   2.8   2.85   2.85   2.85  2.85   2.85   2.85
   1.1   1.4   1.6   1.8   2.0   2.2   2.4   2.6   2.8   2.8   2.8   2.8   2.85   2.85   2.85  2.85   2.85   2.85
   1.1   1.4   1.6   1.8   2.0   2.2   2.4   2.6   2.8   2.8   2.8   2.8   2.85   2.85   2.85  2.85   2.85   2.85
   1.1   1.4   1.6   1.8   2.0   2.2   2.4   2.6   2.8   2.8   2.8   2.8   2.85   2.85   2.85  2.85   2.85   2.85
   1.1   1.4   1.6   1.8   2.0   2.2   2.4   2.6   2.8   2.8   2.8   2.8   2.85   2.85   2.85  2.85   2.85   2.85
   1.1   1.4   1.6   1.8   2.0   2.2   2.4   2.6   2.8   2.8   2.8   2.8   2.85   2.85   2.85  2.85   2.85   2.85
   1.1   1.4   1.6   1.8   2.0   2.2   2.4   2.6   2.8   2.8   2.8   2.8   2.85   2.85   2.85  2.85   2.85   2.85
   1.1   1.4   1.6   1.8   2.0   2.2   2.4   2.6   2.8   2.8   2.8   2.8   2.85   2.85   2.85  2.85   2.85   2.85
   1.1   1.4   1.6   1.8   2.0   2.2   2.4   2.6   2.8   2.8   2.8   2.8   2.85   2.85   2.85  2.85   2.85   2.85
   1.1   1.4   1.6   1.8   2.0   2.2   2.4   2.6   2.8   2.8   2.8   2.8   2.85   2.85   2.85  2.85   2.85   2.85
   1.1   1.4   1.6   1.8   2.0   2.2   2.4   2.6   2.8   2.8   2.8   2.8   2.85   2.85   2.85  2.85   2.85   2.85
INTERNAL   100. (FREE) 0  Item 6:  BOTM, of layer2 - bottom of original layer 1
   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.2   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
   1.0   1.0   1.0   1.0   1.0   1.2   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
```

```
   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
INTERNAL    90. (FREE) 0  Item 6:  BOTM, confining bed
   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.32  1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
   1.0   1.0   1.0   1.0   1.0   1.32  1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
INTERNAL    40. (FREE) 0  Item 6:  BOTM, layer 3, original layer 2
   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   2.95  1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
       1.0  1  1.0  SS    Item 7:  PERLEN NSTP TSMULT SS/TR, stress period 1
    87162.  1  1.0  TR    Item 7:  PERLEN NSTP TSMULT SS/TR, stress period 2
   261486.  1  1.0  TR    Item 7:  PERLEN NSTP TSMULT SS/TR, stress period 3
   522972.  1  1.0  TR    Item 7:  PERLEN NSTP TSMULT SS/TR, stress period 4
 23567450.  9  1.2  TR    Item 7:  PERLEN NSTP TSMULT SS/TR, stress period 5
```

tc1-fwd.lpf

```
# LPF input file for test case tc1
#
  0  -999.  9                Item 1:  ILPFCB HDRY NPLPF
  1    1    1                Item 2:  LAYTYP
  0    0    0                Item 3:  LAYAVG
1.0  1.0  1.0                Item 4:  CHANI
  1    1    1                Item 5:  LAYVKA: 0 = Kz of model layer; not 0 = Kx/Kz
  0    0    0                Item 6:  LAYWET
SS_1       SS   1.3E-3   2   Item 8:  PARNAM PARTYP PARVAL NCLU
  1        FIFTIETH   ALL    Item 9:  LAYER MARRAY ZARRAY [zones]
  2        FIFTIETH   ALL    Item 9:  LAYER MARRAY ZARRAY [zones]
SY_1       SY   1.0E-1   2   Item 8:  PARNAM PARTYP PARVAL NCLU
  1        FIFTIETH   ALL    Item 9:  LAYER MARRAY ZARRAY [zones]
  2        FIFTIETH   ALL    Item 9:  LAYER MARRAY ZARRAY [zones]
HK_1       HK   3.0E-4   2   Item 8:  PARNAM PARTYP PARVAL NCLU
  1        NONE       ALL    Item 9:  LAYER MARRAY ZARRAY [zones]
  2        NONE       ALL    Item 9:  LAYER MARRAY ZARRAY [zones]
VERT_ANI_1 VANI 1.0      2   Item 8:  PARNAM PARTYP PARVAL NCLU
  1        NONE       ALL    Item 9:  LAYER MARRAY ZARRAY [zones]
  2        NONE       ALL    Item 9:  LAYER MARRAY ZARRAY [zones]
VERT_K_CB  VKCB 1.0E-7   1   Item 8:  PARNAM PARTYP PARVAL NCLU
  2        NONE       ALL    Item 9:  LAYER MARRAY ZARRAY [zones]
SS_2       SS   2.0E-4   1   Item 8:  PARNAM PARTYP PARVAL NCLU
  3        FIFTIETH   ALL    Item 9:  LAYER MARRAY ZARRAY [zones]
SY_2       SY   2.3E-2   1   Item 8:  PARNAM PARTYP PARVAL NCLU
  3        FIFTIETH   ALL    Item 9:  LAYER MARRAY ZARRAY [zones]
HK_2       HK   4.0E-5   1   Item 8:  PARNAM PARTYP PARVAL NCLU
  3        MULTARR_3  ALL    Item 9:  LAYER MARRAY ZARRAY [zones]
VERT_ANI_2 VANI 1.0      1   Item 8:  PARNAM PARTYP PARVAL NCLU
  3        NONE       ALL    Item 9:  LAYER MARRAY ZARRAY [zones]
 21                          Item 10:  print code for HK, layer 1
 21                          Item 12:  print code for VKA, layer 1
 21                          Item 13:  print code for SS, layer 1
 21                          Item 13:  print code for SY, layer 1
 21                          Item 15:  print code for VKCB, layer 1
 21                          Item 10:  print code for HK, layer 2
 21                          Item 12:  print code for VKA, layer 2
 21                          Item 13:  print code for SS, layer 2
 21                          Item 13:  print code for SY, layer 2
 21                          Item 15:  print code for VKCB, layer 2
 21                          Item 10:  print code for HK, layer 3
 21                          Item 12:  print code for VKA, layer 3
 21                          Item 13:  print code for SS, layer 3
 21                          Item 13:  print code for SY, layer 3
```

tc1-fwd.ohd

```
   66    0    0   49 -888.
   86400.0  1.0
obs1.0        1    3    1   -3      0.00    0.00    0.00     0.000    0.00    0    1
    2
obs1.0        1    0.00     101.804    1.0025    0.0025    0    1
obs1.1        3    0.00     101.775    1.0025    0.0025    0    1
obs1.12       5  272.7713   101.675    1.0025    0.0025    0    1
obs2.0        1    4    4   -5      0.00    0.00    0.00     0.000    0.00    0    1
    2
obs2.0        1    0.00     128.117    1.0025    0.0025    0    1
obs2.1        3    0.00     128.076    1.0025    0.0025    0    1
obs2.2        4    0.00     127.560    1.0025    0.0025    0    1
obs2.8        5  97.59433   116.586    1.0025    0.0025    0    1
obs2.12       5  272.7713   113.933    1.0025    0.0025    0    1
obs3.0        1   10    9   -3      0.00    0.00    0.00     0.000    0.00    0    1
    2
obs3.0        1    0.00     156.678    1.0025    0.0025    0    1
obs3.1        3    0.00     152.297    1.0025    0.0025    0    1
obs3.12       5  272.7713   114.138    1.0025    0.0025    0    1
obs4.0        1   13    4   -3      0.00    0.00    0.00     0.000    0.00    0    1
    2
obs4.0        1    0.00     124.893    1.0025    0.0025    0    1
obs4.1        3    0.00     124.826    1.0025    0.0025    0    1
obs4.12       5  272.7713   110.589    1.0025    0.0025    0    1
obs5.0        1   14    6   -3      0.00    0.00    0.00     0.000    0.00    0    1
    2
obs5.0        1    0.00     140.961    1.0025    0.0025    0    1
obs5.1        3    0.00     140.901    1.0025    0.0025    0    1
obs5.12       5  272.7713   119.285    1.0025    0.0025    0    1
obs1.0d1      2    3    1   -3      0.00    0.00    0.00     0.000    0.00    0    1
    2
obs1.0d1      1    0.00     101.804    1.0025    0.0025    0    1
obs1.1d1      3    0.00     101.775    1.0025    0.0025    0    1
obs1.12d1     5  272.7713   101.675    1.0025    0.0025    0    1
obs2.0d1      2    4    4   -5      0.00    0.00    0.00     0.000    0.00    0    1
    2
obs2.0d1      1    0.00     128.117    1.0025    0.0025    0    1
obs2.1d1      3    0.00     128.076    1.0025    0.0025    0    1
obs2.2d1      4    0.00     127.560    1.0025    0.0025    0    1
obs2.8d1      5  97.59433   116.586    1.0025    0.0025    0    1
obs2.12d1     5  272.7713   113.933    1.0025    0.0025    0    1
obs3.0d1      2   10    9   -3      0.00    0.00    0.00     0.000    0.00    0    1
    2
obs3.0d1      1    0.00     156.678    1.0025    0.0025    0    1
obs3.1d1      3    0.00     152.297    1.0025    0.0025    0    1
obs3.12d1     5  272.7713   114.138    1.0025    0.0025    0    1
obs4.0d1      2   13    4   -3      0.00    0.00    0.00     0.000    0.00    0    1
    2
obs4.0d1      1    0.00     124.893    1.0025    0.0025    0    1
obs4.1d1      3    0.00     124.826    1.0025    0.0025    0    1
obs4.12d1     5  272.7713   110.589    1.0025    0.0025    0    1
obs5.0d1      2   14    6   -3      0.00    0.00    0.00     0.000    0.00    0    1
    2
obs5.0d1      1    0.00     140.961    1.0025    0.0025    0    1
obs5.1d1      3    0.00     140.901    1.0025    0.0025    0    1
obs5.12d1     5  272.7713   119.285    1.0025    0.0025    0    1
obs1.0d2      3    3    1   -3      0.00    0.00    0.00     0.000    0.00    0    1
    2
obs1.0d2      1    0.00     101.804    1.0025    0.0025    0    1
obs1.1d2      3    0.00     101.775    1.0025    0.0025    0    1
obs1.12d2     5  272.7713   101.675    1.0025    0.0025    0    1
obs2.0d2      3    4    4   -5      0.00    0.00    0.00     0.000    0.00    0    1
    2
obs2.0d2      1    0.00     128.117    1.0025    0.0025    0    1
obs2.1d2      3    0.00     128.076    1.0025    0.0025    0    1
obs2.2d2      4    0.00     127.560          1.0025    0.0025    0    1
```

```
obs2.8d2       5  97.59433   116.586    1.0025    0.0025    0    1
obs2.12d2      5  272.7713   113.933    1.0025    0.0025    0    1
obs3.0d2       3   10    9   -3      0.00    0.00    0.00     0.000    0.00    0    1
    2
obs3.0d2       1    0.00     156.678    1.0025    0.0025    0    1
obs3.1d2       3    0.00     152.297    1.0025    0.0025    0    1
obs3.12d2      5  272.7713   114.138    1.0025    0.0025    0    1
obs4.0d2       3   13    4   -3      0.00    0.00    0.00     0.000    0.00    0    1
    2
obs4.0d2       1    0.00     124.893    1.0025    0.0025    0    1
obs4.1d2       3    0.00     124.826    1.0025    0.0025    0    1
obs4.12d2      5  272.7713   110.589    1.0025    0.0025    0    1
obs5.0d2       3   14    6   -3      0.00    0.00    0.00     0.000    0.00    0    1
    2
obs5.0d2       1    0.00     140.961    1.0025    0.0025    0    1
obs5.1d2       3    0.00     140.901    1.0025    0.0025    0    1
obs5.12d2      5  272.7713   119.285    1.0025    0.0025    0    1
obs6.0         3    4    4   -3      0.00    0.00    0.00     0.000    0.00    0    1
    2
obs6.0         1    0.00     126.537    1.0025    0.0025    0    1
obs6.1         3    0.00     126.542    1.0025    0.0025    0    1
obs6.12        5  272.7713   112.172    1.0025    0.0025    0    1
obs7.0         3   10    1   -3      0.00    0.00    0.00     0.000    0.00    0    1
    2
obs7.0         1    0.00     101.112    1.0025    0.0025    0    1
obs7.1         3    0.00     101.160    1.0025    0.0025    0    1
obs7.12        5  272.7713   100.544    1.0025    0.0025    0    1
obs8.0         3   10    9   -3      0.00    0.00    0.00     0.000    0.00    0    1
    2
obs8.0         1    0.00     158.135    1.0025    0.0025    0    1
obs8.1         3    0.00     152.602    1.0025    0.0025    0    1
obs8.12        5  272.7713   114.918    1.0025    0.0025    0    1
obs9.0         3   10   18   -3      0.00    0.00    0.00     0.000    0.00    0    1
    2
obs9.0         1    0.00     176.374    1.0025    0.0025    0    1
obs9.1         3    0.00     176.373    1.0025    0.0025    0    1
obs9.12        5  272.7713   138.132    1.0025    0.0025    0    1
obs0.0         3   18    6   -3      0.00    0.00    0.00     0.000    0.00    0    1
    2
obs0.0         1    0.00     142.020    1.0025    0.0025    0    1
```

Output files:

tc1._ output-sim_adjust *(this report refers generically to the file as fn.*_output-sim_adjust*)*

```
“SIMULATED EQUIVALENT” "OBSERVATION NAME”
   100.0667      obs1.0
  0.1397247      obs1.1
   3.531517      obs1.12
   104.1128      obs2.0
 -0.8554077E-01 obs2.1
 -0.2619858      obs2.2
 -0.6630936      obs2.8
 -0.4744186      obs2.12
   104.0871      obs3.0
   118.0000      obs3.1
   118.0000      obs3.12
   104.1128      obs4.0
 -0.8559418E-01 obs4.1
 -0.4742050      obs4.12
   104.0854      obs5.0
 -0.1990509E-01 obs5.1
 -0.4158173      obs5.12
   103.9412      obs6.0
 -0.5223846E-01 obs6.1
 -0.3039246      obs6.12
   100.4227      obs7.0
  0.1004181      obs7.1
   3.178619      obs7.12
   104.0871      obs8.0
   118.0000      obs8.1
   118.0000      obs8.12
   104.0918      obs9.0
 -0.4776001E-02 obs9.1
 -0.3380127      obs9.12
   104.0769      obs0.0
 -0.8422852E-02 obs0.1
 -0.4099197      obs0.12
  -1.441222      obsSS
   0.000000      obsTR3
   0.000000      obsTR12


 tc1-fwd._os
      WAS EVALUATED FOR ITEMS OMITTED, OR ASSIGNED A DEFAULT VALUE,
      BY THE PROCESS MODEL

         0 OBSERVATIONS WERE ASSIGNED THE GLOBAL DEFAULT VALUE, -1.0000000E-50


 Run end date and time (yyyy/mm/dd hh:mm:ss): 2008/02/16  6:42:47
 Elapsed run time:  0.031 Seconds
```

References

Poeter, E.P., Hill, M.C., Banta, E.R., Mehl, Steffen, and Christensen, Steen, 2005, UCODE_2005 and six other computer codes for universal sensitivity analysis, calibration, and uncertainty evaluation: U.S. Geological Survey Techniques and Methods, book 6, chapter A11, 283 p

Appendix 2: Connection of SIM_ADJUST with Jupiter API

The JUPITER API is a computer programming environment that includes conventions and software components. It is designed to support the development of computer programs that perform model sensitivity analysis, data needs evaluation, sensitivity analysis, uncertainty evaluation, and(or) optimization. The goal of the JUPITER API is to allow scientists to be able to express their ideas in useful programs that can be readily applied to practical problems. It is hoped that this facilitation of the connection between research and application will accelerate the technical advance of using data to model natural systems and thereby improve the scientific basis of societal decisions about these systems.

SIM_ADJUST uses the JUPITER modules indicated in Table A2-1. The modules are described in chapters of Banta and others (2006). Unlike most JUPITER applications, including UCODE_2005 (Poeter and others, 2005), OPR-PPR (Tonkin and others, 2007), and MMA (Poeter and Hill, 2007), SIM_ADJUST does not use the JUPITER API input block and keyword conventions so that the SIM_ADJUST input file is structured differently than input files of the other applications.

Table A2-1. JUPITER API modules used by SIM_ADJUST and the related chapter and chapter authorship in Banta and others (2006).

Modules	**Chapter**	**Authorship of chapter**
Datatypes	3	Banta
Global Data	4	Banta and Doherty
Utilities	5	Banta, Doherty, and Poeter

References

Banta, E.R., Poeter, E.P., Doherty, J.E., and Hill, M.C., 2006, JUPITER: Joint Universal Parameter IdenTification and Estimation of Reliability – An application programming interface (API) for model analysis: U.S. Geological Survey Techniques and Methods, Book 6, Section E, Chapter 1, 268 p.

Poeter, E.P., Hill, M.C., Banta, E.R., Mehl, Steffen, and Christensen, Steen, 2005, UCODE_2005 and six other computer codes for universal sensitivity analysis, calibration, and uncertainty evaluation: U.S. Geological Survey Techniques and Methods, book 6, chapter A11, 283p.

Poeter, Eileen P., and Mary C. Hill, 2007, MMA, A computer code for Multi-Model Analysis: U.S. Geological Survey Techniques and Methods 6-E3, 113 p.

Tonkin Matthew J., Tiedeman Claire R., Ely D. Matthew, and Hill Mary C., 2007, OPR-PPR, a Computer Program for Assessing Data Importance to Model Predictions Using Linear Statistics: Reston Virginia, USGS, Techniques and Methods Report TM –6E2, 115 p.

Appendix 3: Distributed Files and Directories

SIM_ADJUST files are distributed in the directories listed in Table A3-1.

Table A3-1. Directories distributed with SIM_ADJUST

Directory	Subdirectories	Description
test-*os*[1]	**tc1-3layer**	Contains three batch files and associated SIM_ADJUST and process model input files. One batch file 1_m.bat executes the process model (MODFLOW-2000) which is designed to produce an output that is missing some simulated equivalents to the observations and has default values for others. The next batch file 2_sim_adjust.bat executes SIM_ADJUST to read the process model output tc1-fwd._os, find the problems, and correct them. The third batch file 3_clean.bat removes the output files produced when the first two batch files are executed.
	tc1-3layer-example-input-error	The SIM_ADJUST input in this folder is purposefully set up to encounter some problems so the user can see how those will be documented.
	tc1-3layer-mf2005	In this folder, the problem from the tc1-3layer subdirectory is executed using MODFLOW_2005 rather than MODFLOW-2000. Although the process model output files (tc1-fwd._os) differ, the resulting SIM_ADJUST output (tc1._output-sim_adjust) is the same except that more digits are printed for the calculated heads.
Doc		The pdf file for this document as well as text files explaining installation and updates.
bin		Executables used in the example simulations.
src	sim_adjust	Fortran files unique to the SIM_ADJUST program.
	api-modules	JUPITER API modules used by SIM_ADJUST.
		The source for the other executables included in the bin directory can be obtained through the web.[2]

[1] The content of this directory is operating-system dependent. The directory name is formed by substituting letters representing the operating system for "*os*". For example, test-win includes files for a Windows operating system.

[2] http://water.usgs.gov/nrp/gwsoftware/modflow2000/modflow2000.html