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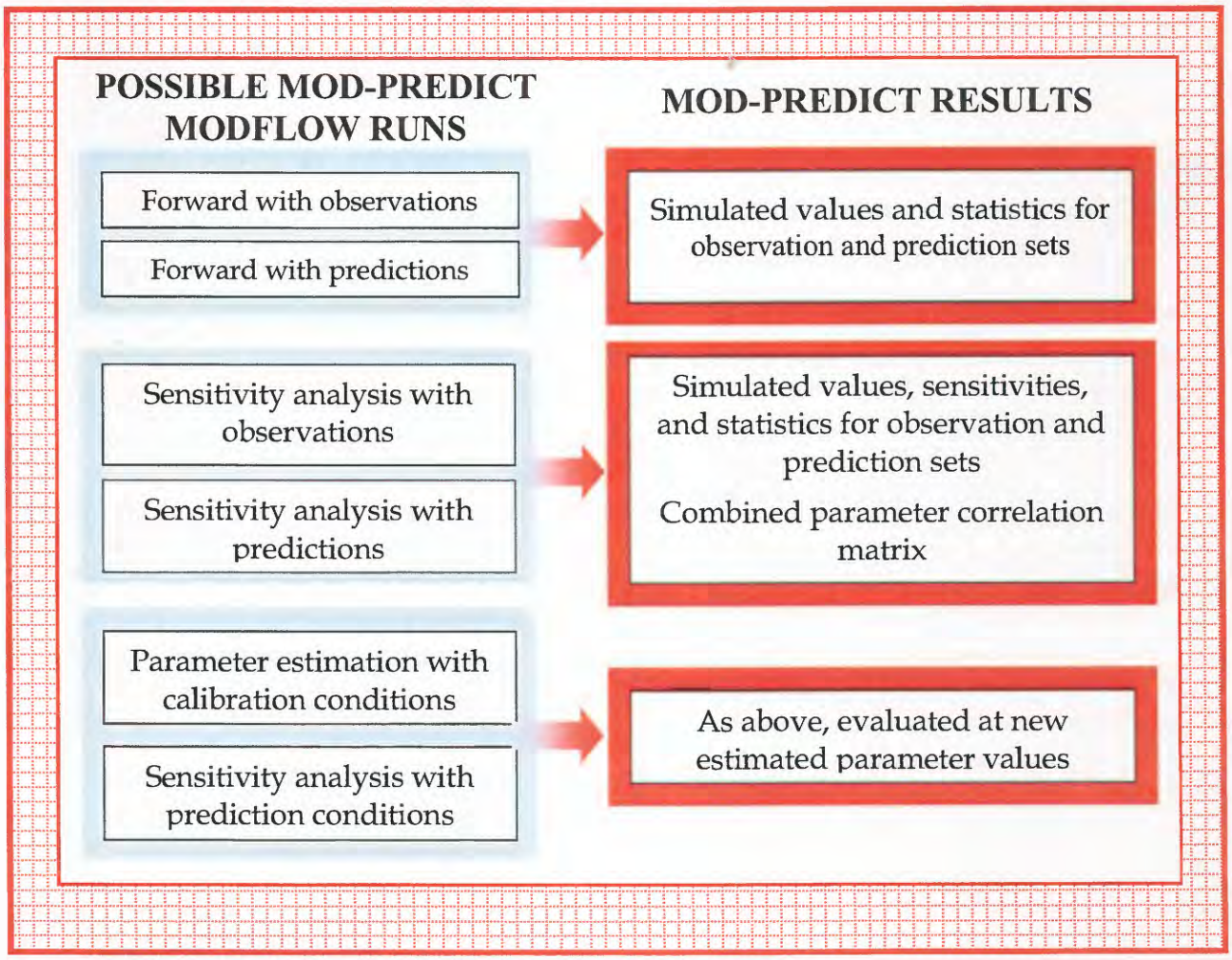
MODFLOW-2000, THE U.S. GEOLOGICAL SURVEY MODULAR GROUND-WATER MODEL -- DOCUMENTATION OF MOD-PREDICT FOR PREDICTIONS, PREDICTION SENSITIVITY ANALYSIS, AND ENHANCED ANALYSIS OF MODEL FIT

Open-File Report 03-385



U.S. Department of the Interior
U.S. Geological Survey

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By Matthew J. Tonkin[1], Mary C. Hill[2], and John E. Doherty[3]

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PREFACE

This document describes the MOD-PREDICT program, which helps evaluate user-defined sets of observations, prior information, and predictions, using the ground-water model MODFLOW-2000. MOD-PREDICT takes advantage of the existing Observation and Sensitivity Processes (Hill and others, 2000) by initiating runs of MODFLOW-2000 and using the output files produced. The names and formats of the MODFLOW-2000 input files are unchanged, such that full backward compatibility is maintained. A new name file and input files are required for MOD-PREDICT.

The performance of MOD-PREDICT 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 U.S. Geological Survey of any errors found in this document or the computer program using the email address available at the web address below. Updates might occasionally be made to this document, to the MOD-PREDICT program, and to MODFLOW-2000. Users can check for updates on the Internet at URL http://water.usgs.gov/software/ground_water.html/.

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ABSTRACT

Ground-water models often are constructed to produce predictions of hydraulic heads, drawdowns, flows, transport, and so on at an unmeasured location or time or under altered stresses such as increased pumpage or changed climate. This document describes MOD-PREDICT, a program that makes definition and analysis of predictions easier for users of MODFLOW-2000 and enhances the analysis capabilities of model fit to observations and prior information, using the concept of sets. Sets can be created that are composed of observations and prior information, or predictions. Supported predictions include the types of quantities presently supported by the MODFLOW-2000 Observation Process. MOD-PREDICT uses a name file analogous in design to the MODFLOW-2000 name file. The MOD-PREDICT name file identifies (1) a PRD input file that lists the MODFLOW-2000 name file, the MODFLOW-2000 execution command, and some optional file-naming conventions; (2) a SETS input file that defines set characteristics, including whether the members are used in calibration, are predictions, or are omitted from consideration; (3) input files that contain predictions, observations, and prior information; and (4) additional file(s) required to simulate prediction conditions if they differ from the calibration conditions. MOD-PREDICT prepares input files for MODFLOW-2000 and

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automatically executes MODFLOW-2000 runs, possibly including forward, sensitivity, and (or) calibration calculations. Predictions and their sensitivity-equation sensitivities are calculated using the capabilities of the existing MODFLOW-2000 Observation and Sensitivity Processes. Results of the MODFLOW-2000 runs are automatically post-processed by MOD-PREDICT to provide a comprehensive suite of set-specific summary statistics that supplement the statistics reported by MODFLOW-2000. These statistics include composite scaled sensitivities for sets of observations and prior information. Other statistics can be used to analyze model fit and predictions, and identify parameters most important to the simulated predictions. MOD-PREDICT also can be helpful in constructing the files required for the MODFLOW-2000 post-processing programs YCINT-2000 and BEALE-2000, which calculate linear confidence intervals on predictions and test whether the model is linear enough for these intervals to be valid.

MODFLOW-2000 and MOD-PREDICT are intended for use on any computer operating system. They are programmed in Fortran 90, which efficiently performs numerical calculations and is fully compatible with the newer Fortran 95.

Chapter 1. INTRODUCTION

Ground-water models are conceived, constructed, and calibrated with the objective of understanding a physical system, testing hypotheses, and making predictions to support environmental management decisions. In this respect, the predictions made with ground-water models may be of paramount importance. Yet, in MODFLOW-2000, the most widely used ground-water model in the world, the existing capabilities for evaluating predictions described by Hill and others (2000, p. 87-91) are limited and awkward.

Another difficulty with MODFLOW-2000 is that summary statistics with which model fit is evaluated are calculated for all observations and items of prior information together. In many circumstances, statistics of model fit for user-defined subsets of the observations and prior information are of interest.

To address these limitations of MODFLOW-2000, the U.S. Geological Survey, in cooperation with the U.S. Department of Energy, developed the supplemental computer program MOD-PREDICT.

Purpose and Scope

This report describes enhanced capabilities of MODFLOW-2000 for making and testing predictions, implemented through the supplementary program MOD-PREDICT.

Sets of observations and prior information, predictions, and quantities that are to be omitted from a given evaluation are defined. Each set is identified by a set name. Certain properties can be assigned to all members of a set. One of those properties is whether members are used for calibration or prediction, or are omitted. Summary measures are calculated for each set. Set definitions are activated through a new SETS input file read by MOD-PREDICT

MOD-PREDICT is designed to simplify and automate the analysis of predictions by (1) managing MODFLOW-2000 input and output files, (2) attributing user-specified properties to observations, prior information, and predictions that have been grouped using sets, (3) controlling the necessary MODFLOW-2000 runs, and (4) detailing results of the analysis in a small group of files designed specifically for the purpose of analyzing predictions. MOD-PREDICT can generate up to two runs of MODFLOW-2000 to obtain information concerning the observations,, prior information, and predictions. These runs are depicted in figure 1, with the output concerning observations and predictions noted.

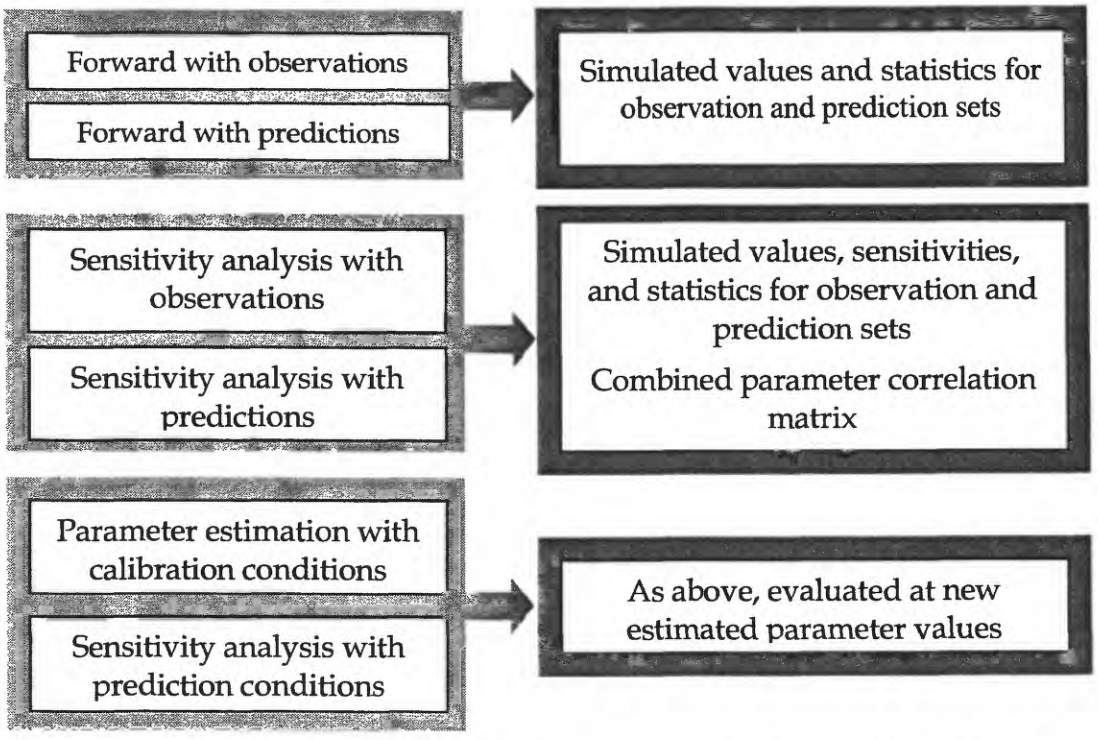

Figure 1. The three MODFLOW-2000 execution options that can be initiated by MOD-PREDICT and associated MOD-PREDICT results. Calibration and prediction conditions can be combined into one set of MODFLOW-2000 input files or the input files may differ.

The calculated prediction sensitivities are used to calculate the prediction scaled sensitivities of Hill (1998, p. 16), with scaling defined by the user. The prediction scaled sensitivities can be used to indicate the importance of each parameter to the predictions. Also included is the combined parameter correlation matrix, which can be used to determine whether parameters that could not be estimated uniquely are individually important to the predictions.

It is expected that this report will be used in conjunction with the documentation of the Ground-Water Flow Process of MODFLOW-2000 (Harbaugh and others, 2000), and the Observation, Sensitivity and Parameter Estimation Processes (Hill and others, 2000). The theory behind parameter estimation and guidelines for undertaking model calibration as described by Cooley and Naff (1990), Hill (1992, 1998), Poeter and Hill (1997), and Hill and Tiedeman (2003) provide the foundation for understanding and implementing the methods described in this report.

Previous Works

The Ground-Water Flow, Observation, Sensitivity and Parameter-Estimation Processes of MODFLOW-2000 together provide functionality for automated ground-water model calibration. Following calibration, the model can be used to make predictions for resource management or other purposes. Presently, predictions can be analyzed by constructing modified Observation Process input files containing the predictions of interest, and using the MODFLOW-2000 Processes to simulate equivalents of the values listed in the modified Observation Process files. The post-processing programs BEALE-2000 and YCINT-2000 that accompany MODFLOW-2000 can be used to test model linearity and interpret predictions, differences, and their linear confidence and prediction intervals (Hill and others, 2000). These can be useful indicators of the uncertainty with which prediction or differences have been determined (Hill, 1998; Hill and others, 2000). This approach to analyzing predictions using the MODFLOW-2000 Processes typically requires a sequence of calibration and prediction model runs, which in turn generates a large number of output files which must all be manipulated and reviewed in order to correctly summarize and interpret the simulation results, as discussed by Hill and others (2000, p. 87-91).

Chapter 2. MOD-PREDICT OVERVIEW AND COMPATIBILITY

This chapter briefly discusses important aspects of MODFLOW-2000 and MOD-PREDICT and compatibility with the Packages and Processes of MODFLOW-2000.

Overview of MODFLOW-2000 and MOD-PREDICT

MODLOW-2000 combines solution of the ground-water flow equation with sensitivity and parameter-estimation capabilities necessary to estimate parameter values that produce the best fit of simulated to observed values, as reflected by a least-squares objective function. These capabilities are embodied in four Processes – the Ground-Water Flow (GWF), Observation (OBS), Sensitivity (SEN), and Parameter-Estimation (PES) Processes (Harbaugh and others, 2000; Hill and others, 2000). The Observation Process determines and reports simulated equivalents to listed observations. The Sensitivity and Observation Processes together calculate derivatives of the simulated equivalents of observation with respect to defined parameters using the accurate sensitivity-equation method. These derivatives are commonly called sensitivities. The Parameter-Estimation Process uses these sensitivities to estimate parameter values using modified Gauss-Newton non-linear regression. The MODFLOW-2000 name file is used to activate these capabilities and define input and output files for MODFLOW-2000 (Harbaugh and others, 2000, p. 7, 43-44). Example name files are shown in Appendix A of Hill and others (2000) and Appendix B of this report. A generalized flowchart of MODFLOW-2000 is presented in figure 1 of Hill and others (2000), and the sequence of possible operations undertaken by MODFLOW-2000 depending on the Processes active in the name file is detailed in table 3 of that report. Briefly, MODFLOW-2000 initializes a parameter-estimation (calibration) problem by reading input from the following:

1. Ground-Water Flow Process input files, which define the ground-water flow simulation. Parameter values listed in the Sensitivity Process input file instead of the Ground-Water Flow Process input files can be used at the discretion of the modeler.

2. Observation Process input files, which define observed values and provides information to calculate simulated equivalents to which the observed values are compared.

3. Sensitivity Process input file, which lists the parameters for which (a) values are controlled by the Sensitivity Process, (b) sensitivities are to be calculated, and (c) values are to be estimated through the Parameter-Estimation Process.

4. Parameter-Estimation Process input file, which lists values for variables that control the modified Gauss-Newton nonlinear regression used to estimate parameter values.

MODFLOW-2000 output is used to evaluate model fit and regression performance (Hill, 2000, chapter 8).

MOD-PREDICT facilitates model calibration by making it easier to evaluate model fit to user-defined sets of observations and prior information, and facilitates the analysis of predictions by organizing some of the input-file manipulation and MODFLOW-2000 runs required to calculate predictions and their sensitivities. MOD-PREDICT accomplished the first using sets described in Chapter 3 of this report. MOD-PREDICT accomplishes the latter by (1) manipulating the files listed in the MOD-PREDICT and MODFLOW-2000 name files and the entries in the Observation Process input files, (2) managing the MODFLOW-2000 input and output files, (3) controlling the necessary MODFLOW-2000 runs, (4) calculating statistics customized for evaluating predictions, and (5) summarizing the outputs in a small group of files designed to analyze predictions. The options available for running MODFLOW-2000 using MOD-PREDICT are shown in figure 1. Table 1 shows MODFLOW-2000 modes of operation used by MOD-PREDICT; the complete list can be found in Hill and others (2000, p. 12). A more detailed description of MOD-PREDICT operations under a variety of circumstances is given in chapter 4. The format and type of outputs produced by the MODFLOW-2000 runs are unchanged from the outputs produced by typical MODFLOW-2000 runs executed through the command prompt, or through a Graphical User Interface. However, interpretation of these outputs is different for calibration and prediction runs, as described in Section 5 of this report.

Two of the MODFLOW-2000 post-processing programs, YCINT-2000 and BEALE-2000 presented by Hill and others (2000) are likely to be important to users of MOD-PREDICT. YCINT-2000 calculates linear confidence and prediction intervals that approximate the likely uncertainty in predictions simulated using the calibrated model and optimized parameter values (Christensen and Cooley, 1999; Hill and others, 2000). These intervals must be interpreted and presented with a full understanding and presentation of the underlying assumptions (Hill, 1994 and 1998; Hill and others, 2000; Christensen and Cooley, 1999). In particular these interval statistics depend on the model being linear near the optimized parameter values. Model linearity can be tested with the post processor BEALE-2000.

Table 1. Modes of MODFLOW-2000 used by MOD-PREDICT produced by activating different combinations of the Observations (OBS), Sensitivity (SEN), and Parameter-Estimation (PES) Processes, the source of parameter values, and commonly used model output. (modified from table 3, p. 12, Hill and others, 2000)

Active?[1]			Mode [2]	Source Of Parameter Values	Model Output Used by MOD-PREDICT
OBS	**SEN**	**PES**			
Forward Modes					
YES	NO	NO	Forward with observations and Forward with predictions	Package files	• Observation run: Simulated equivalents to the observations • Prediction run: Simulated predictions
YES	YES[3]	NO or YES[4]	Forward with observations and Forward with predictions Parameter-Value Substitution	SEN input file for parameters listed there	• As above
Parameter-Sensitivity Modes					
YES	YES	NO	Parameter sensitivity with observations and Parameter sensitivity with predictions	SEN input file for parameters listed there	• Observation run: Simulated equivalents to the observations and their sensitivities. • Prediction run: Simulated predictions and their sensitivities.
YES	YES	YES[4]	Sensitivity Analysis	SEN input file for parameters listed there	• As above
Parameter-Estimation Mode					
YES	YES	YES	Parameter estimation with observations only and Parameter sensitivity with predictions	First, values from SEN input file for parameters listed there; then, values calculated by regression	• Optimal parameter values or, if optimal values are not achieved, data from parameter-estimation iterations to diagnose problems. • If optimal values are achieved, the same output as described above.

[1]The processes are made active by being listed in the MOD-PREDICT name file.
[2]The most commonly used modes are shaded. "Forward with Observations and Parameter-Value Substitution" is like PHASE=1 of UCODE; "Sensitivity Analysis" is like PHASE=22; "Parameter Estimation" is like PHASE=3.
[3]ISENALL<0 in the Sensitivity Process input file.
[4]MAX-ITER=0 in the Parameter-Estimation Process input file.

Compatibility with MODFLOW-2000 Processes and Packages

MOD-PREDICT is compatible with the Observation, Sensitivity, and Parameter Estimation Processes and the Observation packages listed in table 2, and is compatible with all aspects of the Ground-Water Flow Process. Because obtaining the parameter sensitivities necessary for non-linear parameter estimation may require many model runs, MODFLOW-2000 is distributed with a parallel-processing capability for the Sensitivity Process in computing environments with multiple processors (Hill and others, 2000, p. 7). MOD-PREDICT is compatible with the parallel version of MODFLOW-2000.

Table 2. File types compatible with MOD-PREDICT that control the Observation, Sensitivity, and Parameter-Estimation Processes (All documented by Hill and others, 2000, except as noted)

Package or Process	File Type
Observation Process	
Input file for all observations; needed whenever observations are defined.	OBS
Hydraulic heads or changes in hydraulic head over time. Part of the Basic Package.	HOB
Flow to or from a feature represented by the River Package.	RVOB
Flow to a feature represented by the Drain Package.	DROB
Flow to or from a feature represented by the General-Head Boundary Package.	GBOB
Flow to or from a set of constant-head finite-difference cells. Part of the Basic Package.	CHOB
Advective transport represented by the ADV2 Package.[1]	ADV
Sensitivity Process input file.	SEN
Parameter-Estimation Process input file.	PES

[1]Documented by Anderman and Hill (1997, 2001)

Chapter 3. OBSERVATIONS, PRIOR INFORMATION, AND PREDICTIONS, AND CALIBRATION, PREDICTION, AND OMITTED SETS

This chapter discusses how observations, prior information, and predictions are defined, how they are included as members in calibration and prediction sets, and sets comprised of members that are to be omitted from all calculations, and the options that are available for the different sets.

Define Predictions and Observations in the Observation Process Input Files Listed in the MOD-PREDICT Name File

Presently within MODFLOW-2000 the Observation Process does the following:

1. Calculates simulated equivalents of observations specified in the Observation Process input files (table 2);
2. Compares observed values with the simulated equivalent values; and
3. When used with the Sensitivity Process, calculates observation sensitivities (the derivative of the simulated equivalent to the observations with respect to the parameters).

MODFLOW-2000 supports observations of the following types (Hill and others, 2000, except as noted):

- Hydraulic head;
- Changes in hydraulic head over time;
- Flow to and from surface-water bodies (represented by the General-Head Boundary (GHB), Drain (DRN) and River (RIV) Packages);
- Flow to and from a set of constant-head finite-difference cells; and
- Advective transport (described by Anderman and Hill, 2001).

For each observation defined in a MODFLOW-2000 Observation Process input file, the variables read are described by Hill and others, 2000, p. 38, 47, 51, 55, 63). The variables read in addition to those required to define how the simulated value is to be calculated include the following:

OBSNAM HOBS STATISTIC STAT-FLAG PLOT-SYMBOL

These variables are described briefly in table 3, and defined and described completely in Hill and others (2000). For predictions, the same number, type, and sequence of variables are read, but the variables have different uses and meanings, as shown in table 3. Predictions have a prediction name instead of an observation name; a reference value instead of an observed value; a scale value instead of a statistic; and a scale flag instead of a statistic flag. The variable names of table 3 are used to refer to these entities in the MOD-PREDICT main output file. The value of PLOT-SYMBOL is used to allocate the quantities to sets that are then designated as being used for calibration or prediction. PLOT-SYMBOL is used to differentiate observations and predictions, and to identify members of sets, and is discussed first. Then the other variables used for predictions are described.

PLOT-SYMBOL –The Variable Shared by Observations and Predictions

Within MODFLOW-2000, the value of the integer variable PLOT-SYMBOL is defined by modelers for each observation, and this value is repeated in the underscore files produced by MODFLOW-2000 for use by plotting routines, enabling modeler-defined groups of observations to have the same plot symbol (Hill and others, 2000, p. 28). When using MOD-PREDICT, PLOT-SYMBOL retains the current functionality within MODFLOW-2000 and for post-processing programs.

MOD-PREDICT uses PLOT-SYMBOL to identify observations and predictions as members of sets described in the SETS file. One or multiple PLOT-SYMBOL values can be assigned to a single set. Use of multiple PLOT-SYMBOL values allows subsets to be identified with different plot-symbols in graphs, while MOD-PREDICT's fit and sensitivity statistics are calculated for the entire set.

Table 3. Parallel quantities for observations and predictions in the Observation Process input files listed in the MOD-PREDICT Name File, their variable names and descriptions

Variable Name	Observations[1] Description	Variable Name	Predictions Description
OBSNAM	Observation name used to identify the observation. Needs to be unique for each observation[2] and cannot be the same as any of the prediction names.	PREDNAM	Prediction name used to identify the prediction. Needs to be unique for each prediction and cannot be the same as any of the observation names.
HOBS	Value compared to the simulated equivalent to the observation.	REFERENCE	Value compared to the simulated prediction.
STATISTIC[3]	Value used to calculate the observation weighting used in the objective function. Ideally reflects observation error.	SCALE[3]	Scaling factor used to calculate prediction scaled sensitivities and some summary statistics.
STAT-FLAG	Flag that governs how the observation STATISTIC is used to calculate the weight for observations.	SCALE-FLAG	Flag that governs how the prediction scaling factor stored in STATISTIC is used to calculate scaled sensitivities and other statistics.
PLOT-SYMBOL	Defines the set[3] and the plot symbol used in graphs. The default or the set options define that this is an observation.	PLOT-SYMBOL	Defines the set[4] and the plot symbol used in graphs. The set options define that this is a prediction.

[1]The variable name and description for the observations are the same as those described by Hill and others (2000). Additional information about these variables can be found in that work.
[2]This became required for observations in MODFLOW-2000 with version 1.12
[3]The values specified in the Observation Process input files can be modified by MULT defined for each set, as described in the section "The Multiplier (MULT) for Changing the Weighting and Scaling of All Set Members"
[4]This is a new role for this variable.

Two issues arise when transient head data at a well location are defined together in the Hydraulic-Head Observation input file. To begin, consider a few aspects of the data input described by (Hill and others, 2000, p. 38-39). Transient head data at a well location are defined together by setting the reference stress period (variable IREFSP) in item 3 to be negative and the following |IREFSP| repetitions of item 6 each define an observation or a prediction. Here, |IREFSP| equals the absolute value of IREFSP. The two issues of concern are as follows.

First, the value of PLOT-SYMBOL read in line 3 is ignored, and values of PLOT-SYMBOL read from the subsequent repetitions of item 6 are used. This is consistent with the present use of PLOT-SYMBOL in MODFLOW-2000, and is what allows some of the repetitions of item 6 to define observations and others to define predictions.

Understanding of the second issue requires further consideration of the MODFLOW-2000 capabilities. The variable ITT (item 5 in the Hydraulic-Head Observation input file) Indicates whether hydraulic heads or changes in hydraulic head are defined. If changes in hydraulic head are defined (ITT=2), then the first item 6 defines a hydraulic head and this hydraulic head may be either an observation or a prediction. Subsequent repetitions of item 6 define hydraulic heads from which the first hydraulic head is subtracted to obtain the change. The changes may be observations or predictions, depending on the PLOT-SYIMBOL for the subsequent repetitions of item 6. Of concern is how to calculate the sensitivity for the change when the two heads used to calculate the change are not the same type (that is, one is an observation and one is a prediction). In this circumstance, MOD-PREDICT ignores the sensitivity calculated for the first repetition of item 6, and uses only the sensitivity for the subsequent head (or head difference). This difficulty can be eliminated by defining the predictions under a separate item 3 in which all repetitions of item 6 are either observations or predictions.

Prediction Input Variables

Prediction Name (PREDNAM)

The prediction name is used as a unique identifier for predictions in the same way that observation names are used for observations. The prediction names need to be unique and different from the observation names.

Reference Value (REFERENCE)

In some circumstances comparing the reference values to predictions can be very useful. For example:

- To calculate summary statistics about the predictions;
- To compare to a simulated prediction and its linear confidence and prediction intervals, if they are calculated; and

- To investigate what conditions would have to exist for the model to achieve specific values for one or more predictions. If conditions necessary to match the reference value are implausible, the reference value is less likely to occur than if the required conditions are reasonable. This option is accomplished by (a) changing the set type from prediction to calibration, (b) setting what are now weights to emphasize the predictions in the model fit, and (c) executing a calibration run of MODFLOW-2000. The calibration and prediction conditions need to be defined in one set of MODFLOW-2000 files.

Scale Factor (SCALE)

The scale factor is used to calculate scaled sensitivities for predictions using equations presented in Chapter 5. The value specified is modified by the value of MULT specified for the set of which this observation is a member (see section "User-Defined Set Characteristics").

Scale Flag (SCALE-FLAG)

The SCALE-FLAG governs how the prediction scale factor is used to calculate scaled sensitivities and other statistics pertaining to predictions.

Define Prior Information in the Parameter-Estimation Process Input File

Prior information is used in parameter-estimation as described by Cooley (1982, 1983) and Hill (1998, p. 4, 13-14). In MODFLOW-2000, prior information is defined in the Parameter-Estimation Process input file as described by Hill and others (2000, p. 77-78). For prior information to be included in sets, the Parameter-Estimation Process input file needs to be listed in the MOD-PREDICT name file.

The value of the prior information PLOT-SYMBOL variable is used to assign the prior information to a set, as described above for observations and predictions. Prior information can only be assigned to sets of type CALIBRATION and OMIT. Prior information can be combined in a set with observations.

As for observations and predictions, the value of STATISTIC is modified using MULT as described in the section of this report entitled "User-Defined Set Characteristics".

Define Sets in the SETS Input File

The SETS input file is used to identify set name(s) and type(s), determine the members of the named sets, and provide information used to manage, process, and summarize the data related to the members of each set. Detailed input instructions for the SETS input file are provided in appendix A.

Sets that Contain Predictions or Observations

Predictions and observations defined in the Observation Process input files listed in the MOD-PREDICT name file are linked to sets defined in the SETS input file using values of PLOT-SYMBOL. One or more PLOT-SYMBOL values can be included in each set. Each value may be shared by one or more predictions or observations. A single set cannot include both predictions and observations. Four points about sets that contain predictions or observations are listed below.

1. All sets of predictions need to be listed in the SETS input file and the set type specified as PREDICTION. Otherwise the quantity will not be treated as a prediction.

2. As mentioned above, one set can include observations or predictions simulated using different packages. For example, hydraulic heads and gains and losses simulated using the General-Head Boundary and River Packages can be included in the same set.

3. For some types of observations, MODFLOW-2000 supports full weight matrices. For example, a full weight matrix can be used for head-dependent flow observations simulated using a single package, such as the General-Head Boundary or the River Package. The full weight matrices are not specified directly. Rather, the user specifies variance-covariance matrices that reflect the observation error and the correlation between errors in different observations. For predictions, the same capability can be used to define a full matrix by which to scale statistics. A situation that warrants such a matrix has not been encountered by the authors of this work, but the capability is inherited because it exists for observations. When both observations and predictions are defined in one of these Observation Process input files, it is possible to define a matrix related both to the weighting of observations and the scaling of predictions, but the utility of such a matrix is unclear. In MOD-PREDICT, if such a matrix is defined, the off-diagonal components are ignored if they are related to pairs comprised of a prediction and an observation.

Sets that Contain Prior Information

As for predictions and observations, set members are defined using PLOT-SYMBOL values.

Two restrictions apply for defining sets of prior information. First, sets that include prior information need to be designated in the Sets input file as being of type CALIBRATION or OMIT (see table 4 and Appendix A). Second, if prior information is correlated (Hill and others, 2000, p. 78, item 8 and 9), all inter-correlated prior information items must be assigned to the same set.

Composite scaled sensitivities are calculated for all sets of type CALIBRATION, including those that include prior information. This allows the prior information to be included in an evaluation of what parameters are likely to be successfully estimated. Inclusion of prior information in the calculation of composite scaled sensitivities is an expansion of the analysis supported by MODFLOW-2000.

User-Defined Set Characteristics

User-defined set characteristics are described in table 4; detailed data input instructions are provided in appendix A. Definition of the MULT variable is less straightforward than the other variables and is discussed in the following section.

Table 4. Set characteristics that can be defined by the user

Variable Name	Description	Options[2]
SETNAME	Name of the set	Any name up to 12 characters long. Spaces can be included if the name is in double quotes.
PLOT-SYMBOL or PLOT-SYMBOLS	PLOT-SYMBOL value(s) included in the set	Any of the PLOT-SYMBOL values that appear in the Observation Process input files listed in the MOD-PREDICT name file. More than one number is expected if PLOT-SYMBOLS is used.
PRINT-FLAG [1]	Defines printing options	PRINT/**NOPRINT**
TYPE-FLAG [1]	Defines how the quantity is used	PREDICTION/**CALIBRATION**/OMIT
MULT [1]	Modifies the weighting (for observations) or scaling (for predictions) used for all set members	Any non-zero, positive real number. **By default, MULT=1.0.**

[1]These variables are optional; if not included, the defaults apply.
[2]The option in bold is the default.

The Multiplier (MULT) for Changing the Weighting or Scaling of all Set Members

The multiplier (MULT) enables the weighting for sets of observations and prior information, and the scaling for predictions to be easily modified, performing a similar role to that of the EVH and EVF variables appearing in Observation Process input files for the various MODFLOW-2000 packages. MULT is used by MOD-PREDICT to change the value of STATISTIC or SCALE (table 3) and these changed values are used by MOD-PREDICT. How MULT is used to change STATISTIC or SCALE depends on the value of STAT_FLAG or SCALE_FLAG:

- If STAT_FLAG or SCALE_FLAG equals 0, STATISTIC or SCALE are multiplied by MULT.
- If STAT_FLAG or SCALE_FLAG equals 1 or 2, STATISTIC or SCALE are multiplied by the square root of MULT.

When a variance-covariance matrix is supplied to determine the weights for a set of observations, the terms are multiplied by the square root of the row-index MULT and the square root of the column-index MULT, such that if the row- and column-indexes pertain to the same set (that is, along the diagonal where I=J), the value is effectively multiplied by MULT. Multiplication by MULT does not supersede the role of EVH and EVF of MODFLOW-2000; EVH or EVF maintain their values in the generated Observation Process input files and are used by MODFLOW-2000 as usual.

In each case, MULT is applied to the pertinent entries in the Observation Process files that are processed by MOD-PREDICT, in accordance with STAT-FLAG and SCALE-FLAG. In this manner the MULT-adjusted values are used in the MODFLOW-2000 runs initiated by MOD-PREDICT.

Assigning a PLOT-SYMBOL Value and Thereby Members to Multiple Sets

MOD-PREDICT allows one PLOT-SYMBOL value to be a member of multiple sets. This enables summary statistics to be calculated for different combinations of observations and prior information, or predictions. For example, a modeler may wish to obtain summary statistics for all calibration observations in an area of a model, and also for one (or more) subset(s) of those observations. The sets involved need to be of a consistent type – all calibration, all prediction, or all omit.

If a PLOT-SYMBOL value is listed as a member of more than one set, only the value of MULT listed with the first set listed in the SETS file is used in the weighting or scaling of the identified members. For example - if PLOT-SYMBOL=10 is a member of two sets listed in the SETS file, only the value for MULT specified for the first set read sequentially from the SETS file is applied to the relevant values of STATISTIC or SCALE.

Chapter 4. MOD-PREDICT EXECUTION, NAME FILE, INPUT FILES, AND RUN TYPES

This chapter describes the MOD-PREDICT name file and input files, the modes of operation referred to as Run Types, and the contents of the MODFLOW-2000 name file(s) manipulated and used by MOD-PREDICT.

Execution

MOD-PREDICT can be run from any directory when a pathname is used to specify the MOD-PREDICT name file. If MOD-PREDICT is in the same directory as the name file, the full path for the name file is not needed and MOD=PREDICT can be executed by simply typing:

MODPREDICT

at the Command Prompt.

The MOD-PREDICT Name File

When MOD-PREDICT is executed a prompt will appear for the MOD-PREDICT name file. This file lists the names and locations of files in a format analogous to the MODFLOW-2000 name file, as detailed in appendix A. The MOD-PREDICT name file lists the PRD and SETS input files described in the following section and in appendix A, and additional files that may include:

- Observation, Sensitivity, and Parameter-Estimation Process input files that are to be used by MOD-PREDICT to construct the necessary MODFLOW-2000 runs. The Observation Process input files need to be constructed to define both predictions and observations, as discussed in chapter 3 and appendix A.
- The names of any Ground-Water Flow Process input files that are to be used for prediction runs; that is, files that replace or supplement Ground-Water Flow Process input files listed in the MODFLOW-2000 name file.

MOD-PREDICT Input Files

The MOD-PREDICT input files include two input files that are unique to MOD-PREDICT, and additional input files that are modified versions of MODFLOW-2000 input files. The two files unique to MOD-PREDICT are described in this section.

The PRD Input File

The PRD input file identifies a MODFLOW-2000 name file, provides the command required to execute MODFLOW-2000, and provides an opportunity for the user to specify file-name precursors to identify the outputs of the prediction model runs. In the PRD input file, the MODFLOW-2000 name file needs to be designed to simulate calibration conditions. The files may be augmented to simulate prediction conditions, as discussed in the section 'Files to Simulate Different Calibration and prediction Conditions'. Detailed input instructions for the PRD input file are provided together with an example in appendix A.

The SETS Input File

The SETS input file contains information necessary for MOD-PREDICT to identify observation, prior information, and prediction sets; to relate these sets to the contents of the MODFLOW-2000 input files; and to summarize the results of the prediction analysis. The variables defined for each set were described in table 4.

Observation Process Input Files Listed in the MOD-PREDICT Name File

When using MOD-PREDICT, observations, prior information, predictions, and quantities that will be omitted from all calculations are defined through files that are consistent in format with the Observation Process input files listed in table 2. Defining the observations and predictions together in this manner enables the modeler to take advantage of the definitions used in the Observation Process input files. For example, to simulate a river flow prediction for a reach for which observations were defined in the River Observation Package input file, the modeler simply adds one line to those entries to define the time of the prediction, and increments the item 1 variables appropriately (Hill and others, 2000, p. 55). The presence of the prediction in the edited Observation Process input file(s) is identified using the PLOT-SYMBOL variable, and the relation between this prediction and other predictions listed in additional Observation Process input files is determined using sets definitions provided by the modeler through the Sets input

file. Reference stress periods for the predictions need to be coordinated with how the predictions are simulated. This sequence is detailed in the next section.

Files Used to Simulate Different Calibration and Predictions Conditions

MOD-PREDICT is designed to run prediction simulations using either the same conditions as the calibration run or using different conditions. If the calibration and prediction conditions are the same, the same Ground-Water Flow Process input files can be used. Different prediction conditions can be defined using augmented and(or) supplemental Ground-Water Flow Process input files. Augmented and supplemental files are discussed in the following paragraphs.

In augmented files, the prediction conditions are represented using stress periods that are added to the input files used to simulate calibration conditions. In MODFLOW-2000, the number of time steps simulated depends on the quantities defined in the Observation Process input files used. In MODFLOW-2000 runs for which MOD-PREDICT constructs Observation Process input files that contain only observations, MODFLOW-2000 simulates time steps until simulated equivalents for all the observations calculated. In MODFLOW-2000 runs for which MOD-PREDICT constructs Observation Process input files that contain predictions, MODFLOW-2000 simulates time steps until all the predictions are simulated. Using augmented files in circumstances in which they are not required generally results in longer than necessary execution times, because calibration conditions will unnecessarily be simulated every time predictions are simulated.

Supplemental files are additional or replacement files that represent different system stresses under prediction conditions than calibration conditions; for example, different pumping or recharge conditions. Supplemental Ground-Water Flow Process input files need to be listed in the MOD-PREDICT name file. For different pumping conditions, a supplemental WEL file can be listed in the MOD-PREDICT name file, and MOD-PREDICT will include it in the MODFLOW-2000 name file when predictions are simulated. If the file type involved already exists in the MODFLOW-2000 name file listed in the PRD file, the supplemental file replaces the existing file. If the file type is new, the supplemental file and its file type are added to the MODFLOW-2000 name file when predictions are simulated.

Supplemental Ground-Water Flow Process input files listed in the MOD-PREDICT name file that replace existing files can have the same Unit Number, because the two files will not be accessed by MODFLOW-2000 at the same time. For new supplemental Ground-Water Flow

Process input files, MOD-PREDICT checks the unit numbers and reports conflicts in the main MOD-PREDICT output file. If conflicts occur, execution stops.

Run Types

Figure 2 details the actions taken by MOD-PREDICT based upon the active MODFLOW-2000 Processes and the values of certain variables in the Sensitivity and Parameter-Estimation Process input files. Table 5 summarizes how the Run Type relates to the active Processes. For all modes, statistics that compare simulated values to prediction reference values will be printed as defined for sets of predictions. Coordination of the Observation, Sensitivity, and Parameter-Estimation Processes is presented in figure 1 of Hill and others (2000).

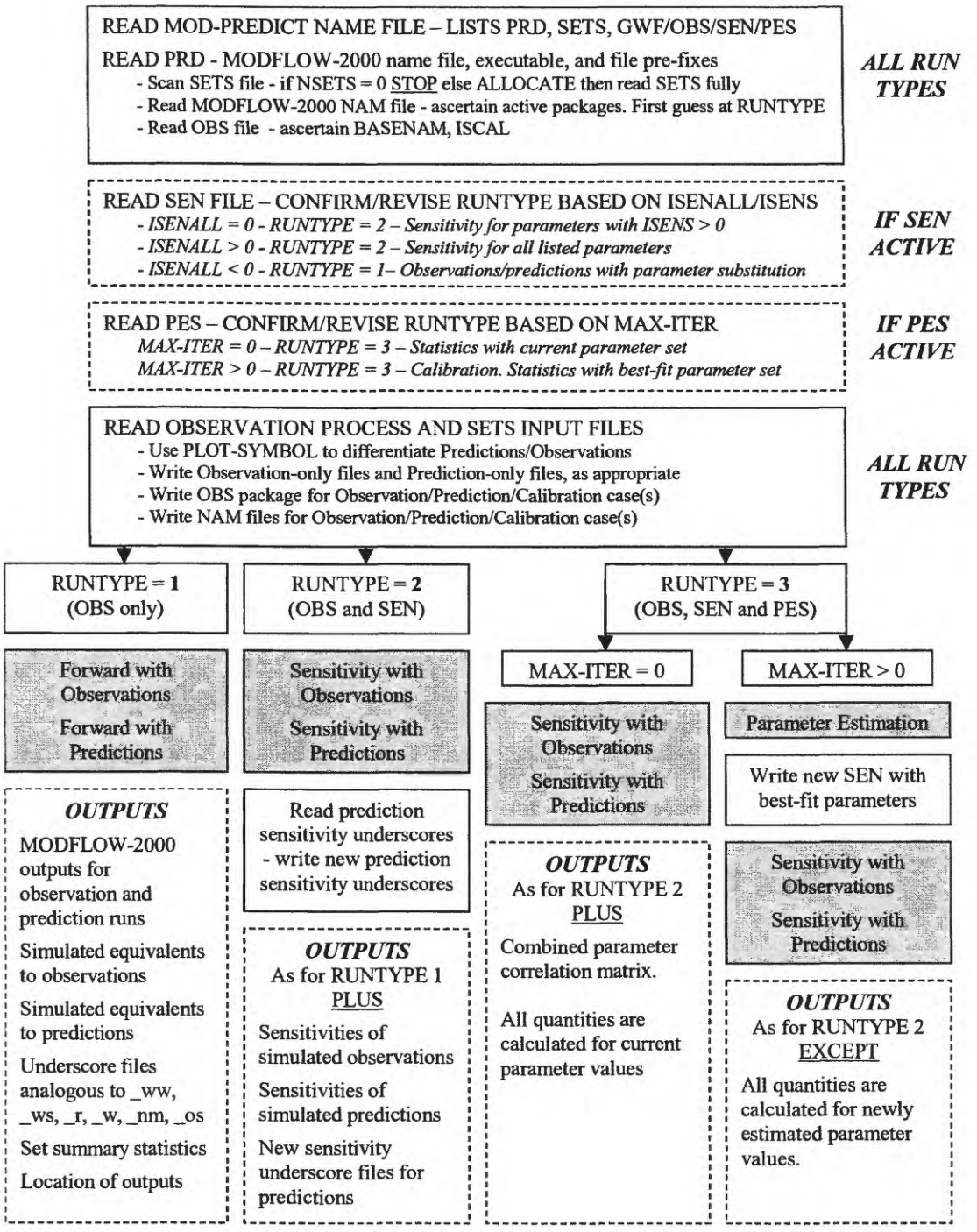

Figure 2. Flowchart showing performance of MOD-PREDICT for its three run types. Shaded boxes describe runs of MODFLOW-2000 conducted by MOD-PREDICT in which the Observations (OBS), Sensitivity (SEN), and(or) Parameter-Estimation (PES) Processes are active.

Table 5. Run type based on active processes detected in the MODFLOW-2000 name file. [The Observations (OBS), Sensitivity (SEN), and(or) Parameter-Estimation (PES) Processes are noted].

Active Processes	*Description*	*Run Type*
OBS	All forward with observation modes	1
OBS and SEN	All sensitivity modes	2
OBS, SEN, and PES	Parameter estimation mode	3

MOD-PREDICT needs to be used with versions of MODFLOW-2000 that write out the unscaled sensitivities in an underscore file with the suffix "_su". These sensitivities are used by MOD-PREDICT to calculate the combined parameter correlation matrix when executing a Run Type = 2 or 3 analysis of predictions.

Run Type 1: Observation Process Only Active

Observation Process input files are listed in the MOD-PREDICT name file. Input instructions for the Observation Process are detailed in Hill and others (2000). For Run Type = 1, MOD-PREDICT does the following.

- Creates two MODFLOW-2000 name files - one to run MODFLOW-2000 with observations only, and one to run it with predictions only. The name files are identical except they cite different Observation Process input files, different GLOBAL and LIST output files, and possibly one or more different Ground-Water Flow Process input files. The name files are identified by user-defined or default filename prefixes, identified through the PRD file.
- Reads the reference value and scale value for all predictions.
- Creates two sets of Observation Process input files with user-defined or default filename prefixes. One contains only observations; one contains only predictions.
- Uses a different filename base for the underscore files pertaining to each of these new runs. The filename base is user-defined or a default.
- Runs MODFLOW-2000 using each of the name files.
- Reads resulting underscore files. For each set included in the SETS input file, lists summary statistics to the MOD-PREDICT output file.
- Reports to the MOD-PREDICT output file the location of all pertinent output files.

Run Type 2: Sensitivity Process Also Active

List the Sensitivity Process input files in the MOD-PREDICT name file. Input instructions for the Sensitivity Process are detailed in Hill and others (2000). For Run Type = 2, MOD-PREDICT executes as for Run Type = 1 PLUS the following.

- Writes different grid sensitivity output file names to the MODFLOW-2000 name files for each of the observation and prediction runs respectively, using the user-defined or default filename prefixes. Grid sensitivities are discussed by Hill and others (2000, p. 67)
- Reads the prediction sensitivity underscore files, and produces the three new prediction sensitivity underscore files with the same filename base. The new prediction sensitivity underscore files are described in Chapter 5.
- Calculates and reports the combined correlation matrix for the current parameters, using the prediction and observation sensitivities.
- Reports to the MOD-PREDICT output file the location of all pertinent output files.

Run Type 3: Parameter-Estimation Process Also Active

List the Parameter-Estimation Process input files in the MOD-PREDICT name file. Input instructions for the Parameter-Estimation Process are detailed in Hill and others (2000). For Run Type = 3, execution of MOD-PREDICT executes as for Run Type = 2 PLUS the following, depending on the value of MAX-ITER, which is specified in item 1 of the Parameter-Estimation Process input file.

If *MAX-ITER* = 0

- Performs as described for Run Type = 2.

If *MAX-ITER* > 0

- Creates a MODFLOW-2000 name file for a Parameter-Estimation mode run, listing calibration-specific Global and List files.
- Using only calibration sets, runs MODFLOW-2000 with the Parameter-Estimation Process active.
- Reads the best-fit parameters from the _pa output file.

- Creates a new MODFLOW-2000 name file, and a set of Observation Process files containing Predictions only, and:
    - Creates a new Parameter-Estimation input file with MAX-ITER=0
    - Creates a new Sensitivity process input file containing the optimized parameters
- Runs MODFLOW-2000 to calculate prediction sensitivities.
- Produces the three new prediction sensitivity underscore files (see Chapter 5).
- Reads the pertinent underscore files and for each identified set lists summary statistics (table 9 and table 10, Chapter 5) to the MOD-PREDICT output file.
- Calculates and reports the combined correlation matrix pertaining to both predictions and observations for the best-fit parameters, using the prediction and observation sensitivities and the weight matrix constructed by MOD-PREDICT.
- Reports to the MOD-PREDICT output file the location of all pertinent output files.

File Protocols

MOD-PREDICT reads all input files pertaining to the Observation, Sensitivity, and parameter-Estimation Processes, to determine the Run Type and differentiate observations from predictions. Where necessary – for example, where an Observation Process input file contains both observations and predictions, or where a new MODFLOW-2000 name file is required for a parameter-estimation run – MOD-PREDICT prepares the files necessary for the run(s). To clearly distinguish these files from user-prepared files, MODFLOW-2000 input files generated for MODFLOW-2000 by MOD-PREDICT are modified with the appropriate user-supplied (using the "PRD" file) or default ("OB_", "PR_", "PE_") prefixes detailed in appendix A. In this manner, input files generated by MOD-PREDICT for prediction-only, observation-only, and parameter estimation simulations can be identified by an alphabetical sorting of files in the model directory. In addition, a header line is written to the file indicating that it was produced by MOD-PREDICT and giving a brief comment indicating the purpose of the file. Three example header lines are provided in table 6 for the Observation, Sensitivity, and Parameter-Estimation Processes with Run Type 3.

Table 6. Example header lines as written by MOD-PREDICT to various MODFLOW-2000 files for the case "TC1OBSEN" presented in Appendix B.

Name File	# MOD-PREDICT PRODUCED THIS CALIBRATION NAME FILE
OBS File	# MOD-PREDICT PRODUCED THIS OBSERVATION PROCESS INPUT FILE FOR ALL OBSERVATIONS
HOB File	# MOD-PREDICT PRODUCED THIS HOB OBSERVATION PROCESS INPUT FILE FOR HEAD OBSERVATIONS

Output Files Named Using OUTNAM

The Observation Process input file for all observations (table 2) includes the character variable OUTNAM, which is used to name some of the output files (Hill and others, 2000, p. 28-29). When using MOD-PREDICT, OUTNAM is modified with the appropriate user-supplied or default prefixes as described in appendix A. In this manner, underscore files from observations-only and predictions-only simulations are clearly identified.

Chapter 5. MOD-PREDICT OUTPUTS

MOD-PREDICT operates by controlling MODFLOW-2000 runs. These runs produce the output files described by Harbaugh and others (2000) and Hill and others (2000). These include the List and Global files, and auxiliary files designed for use by plotting routines and other programs (Hill and others, 2000, p. 13, 28-29). In addition, there is a MOD-PREDICT main output file and auxiliary files.

MODFLOW-2000 Global and List Output Files

Use of the MODFLOW-2000 Global and List output files is described by Hill and others (2000, p. 95-97). Care is needed when interpreting results for runs in which predictions are defined because of how the reference values are defined. This difficulty is discussed in the following section.

MODFLOW-2000 Auxiliary Files

For MODFLOW-2000 runs that simulate predictions, the underscore files and the contents of the Global and List files must be interpreted differently, because the reference values specified for predictions do not perform the same function as observations, and statistics such as objective-function values generally are not meaningful. For predictions, the statistics presented in the MOD-PREDICT output file are designed to be more useful than the statistics presented in the MODFLOW-2000 output files. However, some of the auxiliary output files also are useful for predictions, in particular the files with suffixes _os, _r, _ww, _w, described in table 7.

Table 7. Auxiliary output files produced by MODFLOW-2000 that are likely to be useful in the analysis of predictions

[The files are identified using the suffixes of Hill and others (2000, p. 28); all files also contain the prediction name and the PLOT-SYMBOL. The PLOT-SYMBOL can be used to produce graphs in which predictions within a set are identified.]

File suffix	Use of contents for predictions
_os	Unscaled reference values and the associated predictions
_r	Unscaled difference between reference values and the associated predictions calculated as (ref_i-$pred_i$)
_ww	Scaled reference values and the associated predictions
_w	Scaled difference between reference values and the associated predictions.

MOD-PREDICT Main Output File

The MOD-PREDICT main output file is named MODPREDICT.OUT and is divided into a series of sections shown in table 8. Example MOD-PREDICT output files are shown in appendix B. The statistics reported in the MOD-PREDICT main output file are described below.

Table 8. Summary of contents of the MOD-PREDICT main output file

SECTION	CONTENTS
INITIALIZE	• Echo of items read from the PRD input file • Echo of packages/processes listed in MODFLOW-2000 name file
READ MODFLOW SIMULATION FILES	• Echo of Run Type determined from active packages listed in the MODFLOW-2000 name file • Echo of pertinent entries in the Observation, Sensitivity, and parameter-Estimation Process input files as they are read in sequence • The number of observations, predictions, and omitted quantities defined in each Observation Process input file and in total • If there are both observations and predictions, the names of the new Observation Process input files • List the new MODFLOW-2000 name files created by the MOD-PREDICT • Tabulate the Calibration, Prediction, and Omitted sets identified in the "SETS" file
RUN MODFLOW SIMULATIONS	• List MODFLOW-2000 runs as they begin and end • Report the underscore files read from the MODFLOW-2000 runs
CALCULATE SET SUMMARY STATISTICS	• Table that reports the results of comparing the quantities listed in the Observation Process input files and those listed in the MODFLOW-2000 underscore files. The underscore files will have fewer entries if dry cells prohibit calculation of a simulated equivalent. The Observation or Prediction name, the Set name, and the value of PLOT_SYMBOL are listed. • If Run Type = 2 or 3: Print out the combined parameter correlation matrix. • Tabulate Prediction Statistics (table 10)
RUN FILES SUMMARY	• Summary of the location/names of pertinent output files from the analysis

Statistics for Sets of Observations, Prior Information, and Predictions

Summary statistics are calculated for each set listed in the Sets input file for which members are defined. The statistics calculated depend on whether the wet type is calibration or prediction.

The statistics reported for calibration sets are listed in table 9 and focus on evaluating model fit. They include the statistics reported by MODFLOW-2000 and a few additional statistics calculated by MOD-PREDICT.

Table 9. Statistics for sets of observations and prior information.

[y_i, the ith observation in the set; $y'_i(\underline{b})$, value simulated using the parameter values represented by $\underline{b}$ and which is to be compared with the ith observation; Max, the largest of the values in parentheses in the set; Min, the smallest of the values in parentheses in the set; Σ, the sum of the values in parentheses in the set; n, the number of members in the set.]

Statistic name	Column Heading for this Statistic in "modpredict.out"	Equation or the page in Hill (1998) where the equation can be found
Unweighted (UW_)		
Maximum unweighted residual	UW_RES-MAX	$Max(y_i-y'_i(\underline{b}))$
Minimum unweighted residual	UW_RES-MIN	$Min(y_i-y'_i(\underline{b}))$
Average of unweighted residuals[1]	UW_RES-AVG	$\Sigma(y_i-y'_i(\underline{b}))/n$
Weighted		
Maximum weighted residual	RES-MAX	p. 20-21
Minimum weighted residual	RES-MIN	p. 20-21
Average of weighted residuals	RES-AVG	p. 20-21
Positives and Negatives		
Number of residuals larger than zero	NRESGT0	p. 22
Number of residuals less than zero	NRESLT0	p. 22
Regression Statistics		
Contribution to the total least-squares objective function	SOSWR	p. 4, 17-18
Calculated error variance	EV	p. 18-19
Standard error of the regression	SE	p. 18-19

1. Can be meaningful only if all observations involved have the same units.

The statistics reported for predictions focus on issues typically encountered for predictions, such as the value of the largest prediction, and the maximum difference between the user-supplied reference values and their associated predictions. User-defined scaling can be used

to make these statistics more meaningful to the situation involved. Table 10 lists statistics presented for sets of predictions.

Table 10. Statistics for sets of predictions.

[$pred_i$, prediction number i in the set; ref_i, reference value for prediction number i in the set; $scal_i$, scaling factor for prediction number i (adjusted from input variable SCALE using MULT as described in the text); n, the number of predictions in the set; Σ, sum the following for all predictions in the set]

Statistic name	Column Heading for this Statistic in "modpredict.out"	Equation
Unscaled (US_)		
Maximum predicted value	US_LARGEST	$Max(pred_i)$
Minimum predicted value	US_SMALLEST	$Max(pred_i)$
Average predicted value[1]	US_AVERAGE	$\Sigma\ (pred_i)/n$
Scaled		
Maximum scaled predicted value	LARGEST	$Max(pred_i/scal_i)$
Minimum scaled predicted value	SMALLEST	$Min(pred_i/scal_i)$
Average scaled predicted value	AVERAGE	$\Sigma\ (pred_i/scal_i)/n$
Unscaled comparison to reference values (US_)		
Maximum difference between reference values and predictions	US_DIFF-MAX	$Max(ref_i\text{-}pred_i)$
Minimum difference between reference values and predictions	US_DIFF-MIN	$Min(ref_i\text{-}pred_i)$
Mean difference between reference values and predictions	US_DIFF-AVG	$\Sigma(ref_i\text{-}pred_i)/n$
Scaled comparison to reference values		
Maximum scaled difference between reference values and predictions	DIFF-MAX	$Max[(ref_i\text{-}pred_i)/scal_i]$
Minimum scaled difference between reference values and predictions	DIFF-MIN	$Min[(ref_i\text{-}pred_i)/scal_i]$
Mean scaled difference between reference values and predictions	DIFF-AVG	$\Sigma[(ref_i\text{-}pred_i)/scal_i]/n$
Other comparison to reference values		
No. of predictions greater than their reference values	NGTREF	
No. of predictions less than their reference values	NLTREF	

1. Can be meaningful only if all predictions involved have the same units.

Interpretation of Tabulated Summary Statistics

Calibration summary statistics can be used to indicate the model fit for sets, and the contribution of the various sets to the total least-squares objective function.

Prediction summary statistics can be used to indicate the deviation of simulated predictions from expected, regulatory, or other meaningful values, and the range of predictions. If there is no basis for specifying a reference value, then statistics that refer to the differences between reference and simulated values are meaningless. In this situation, only statistics referring to the absolute value of the prediction are interpretable. This includes USLARGEST, USSMALLEST, USAVERAGE, LARGEST, SMALLEST, and AVERAGE. For prediction reference values that equal zero, NGTREF and NLTREF will equal the number of positive and negative predictions in each set.

Examples of both Calibration and Prediction set summary statistics are provided for the test cases in appendix B.

Combined Parameter Correlation Matrix

A parameter correlation matrix calculated using members of both calibration and prediction sets is calculated. This matrix can be compared with the parameter correlation matrix calculated using only calibration quantities to determine if the predictions depend on individual parameter values that have not been estimated uniquely. This analysis is generally most useful if all of the defined parameters are included.

MOD-PREDICT Auxiliary Files

As noted by Hill (1998) and many statistics texts such as Helsel and Hirsch (2002), it is important to look at graphical depictions as well as summary statistics when evaluating simulated results. Sets of observations, prior information, and predictions can be evaluated graphically using the underscore files produced by MODFLOW-2000 (generally those listed in table 7), and additional files produced by MOD-PREDICT.

New underscore files printed by MOD-PREDICT are listed in table 11. The new files are analogous in form to the underscore files printed by MODFLOW-2000 when the Sensitivity Process is active and OUTNAM is not "NONE" (Hill and others, 2000, p. 27-28). The files can be read as space-delimited free format. The scaling of the sensitivities presented in the MOD-PREDICT underscore files is detailed in table 11.

Table 11. Underscore files containing prediction scaled sensitivities produced by MOD-PREDICT when OUTNAM is not "NONE"

Extension	Meaning of the scaled sensitivity given the scaling used
_spp	The percent change in the prediction given a one percent change in the parameter value. Calculated by multiplying the sensitivity by $(b_j/100)\times(100/\text{prediction value})$
_spr	The change in prediction expressed as a percent of the reference value given a one percent change in the parameter value. Calculated by multiplying the sensitivity by $(b_j/100)\times(100/\text{reference value})$
_sps	The change in prediction expressed as a percent of the scale value given a one percent change in the parameter value. Calculated by multiplying the sensitivity by $(b_j/100)\times(100/\text{scale value})$. Calculation of the scale value is dependent on the value of SCALE-FLAG[1]: If SCAL-FLAG = 1, scale value = scaling factor If SCAL-FLAG = 2, scale value = scaling factor *x* prediction If SCAL-FLAG = 3, scale value = scaling factor *x* reference value

1. The scaling factor has been modified using MULT.

A Note on Dry Cells

The MODFLOW-2000 Observation Process may not be able to calculate some observation simulated equivalents or some predictions if selected cells go dry during the simulation (Hill and others, 2000, p.36-37). In the event that a simulated equivalent can not be determined, MODFLOW-2000 does not list a simulated equivalent in the underscore files. To identify observations (or predictions) affected by dry cells, MOD-PREDICT compares the quantities defined in the Observation Process files to the quantities defined in the underscore files. For quantities present in the Observation Process input files and absent in the underscore files, the observation or prediction name, set type (Calibration or Prediction; Calibration includes observations and prior information), the Observation Process file involved (HOB, GBOB, DROB, RVOB, CHOB, or ADV2), and PLOT-SYMBOL are listed. Quantities in sets with set type Omit are not considered. The missing quantities are excluded from the summary statistics calculated for the run.

Run-Time Screen Output

MOD-PREDICT reports to the screen the name of the MODFLOW-2000 name file that is being run; the sequence of MODFLOW-2000 runs that it is managing as they start and finish, and when output from a MODFLOW-2000 run is being read. If MOD-PREDICT terminates with an error, the following message is reported to the screen:

```
MOD-PREDICT TERMINATED WITH ERRORS - CHECK MODPREDICT.OUT
```

If MOD-PREDICT terminates without errors, the following message is reported to the screen:

```
PREDICTION RUN COMPLETED SUCCESSFULLY
NORMAL TERMINATION OF MOD-PREDICT
```

Because MOD-PREDICT may run a sequence of several MODFLOW-2000 runs, MOD-PREDICT as compiled and provided executes the runs necessary for the Run Type using the "> NUL" command. This directs screen output from MODFLOW-2000 to a nul file. An example of MOD-PREDICT run-time screen output is provided for the first test case in appendix B.

Error Reporting

MOD-PREDICT may not execute successfully for a number of reasons – for example, an error in accessing the MODFLOW-2000 executable listed in the PRD file, an error in processing an input or output file, or non-convergence of a MODFLOW-2000 run. If MODFLOW-2000 fails to execute due to a file-access or run-time error, the error encountered by MODFLOW-2000 will be reported to the screen. MODFLOW-2000 non-convergence errors and file-access errors encountered by MOD-PREDICT are reported to the MOD-PREDICT output file. These errors are generated by MODFLOW-2000 and generally are accompanied by the subroutine name and a block number indicating the location within MOD-PREDICT that the error was raised. Remaining run-time errors are reported to the screen.

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APPENDIX A. MOD-PREDICT INPUT INSTRUCTIONS

The files required by MOD-PREDICT include a name file and PRD and SETS input files. The MOD-PREDICT name file lists files constructed according to the instructions for the Observation Process input files (Hill and others, 2000, Chapter 4). These files define both observations and predictions. The MOD-PREDICT name file also may list files for the Ground-Water Flow Process as needed to simulate prediction conditions.

MOD-PREDICT Name File

Input Instructions

The name file contains the names of the input files required by MOD-PREDICT. The name file is read on unit 99. The name file is constructed as follows:

FOR EACH SIMULATION

```
0. [#Text]
```

Item 0 is optional -- "#" must be in column 1. Item 0 can be repeated multiple times.

```
1. FTYPE NUNIT FNAME
```

Repeat Item 1 for each file included in the name file. All variables are read in free format. The length of each record must be 199 characters or less. At least two files must be listed in the name file: file type "SETS" and file type "PRD". The following files also may be listed, and these will determine the MOD-PREDICT Run Type:

- OBS Process "OBS" file and one or more Observation Process input files analogous to those listed in table 2.
- Sensitivity (SEN) and Parameter Estimation (PES) Process files.
- Replacement or supplementary GWF Process files to be used for predictions-only MODFLOW-2000 simulations.

Explanation of Variables Read from the Name File

FTYPE — the file type. Can be any combination of lower-upper case characters. Must be one of the following character values:

SETS for the "SETS" input file

PRD for the MOD-PREDICT input file

OBS, ***SEN***, and ***PES*** for the Observation, Sensitivity, and Parameter-Estimation Processes;

HOB, CHOB, GBOB, RVOB, DROB, and -ADV for the observation packages supported by MOD-PREDICT

Any of the **GWF** Process files

NUNIT — the Fortran unit to be used when reading from the file. Any legal unit number can be specified except units 96-99 which are reserved in MOD-PREDICT and in MODFLOW-2000 (Harbaugh and others, 2000, p. 44).

FNAME— the file name. Can be any combination of lower-upper case characters. Can include pathnames.

```
# MODPREDICT NAME FILE FOR TEST CASE TC1OBSEN
# NOTE: The files contained in the MODPREDICT name file
# comprise OBS-SEN-PES files required for calibration runs; and
# OBSERVATION  PROCESS files (similar in form to MODFLOW2000
observation package
# files) containing some combination of observations and predictions.
#
# All Global input files and GWF Process input files can be read
# from the MODFLOW-2000 name file UNLESS stresses are different
# for the prediction scenario, in which case the prediction GWF Process
# input file must be included here.
#
# PRD file for prediction scenario
PRD     95  tc1obsen.prd
#
# SETS file for prediction scenario
SETS    50  TEST.SETS
#
# OBS-SEN-PES process input files for prediction scenario
OBS     21  tc1obsen.obs
HOB     22  tc1obsenPRED.ohd
RVOB    23  tc1obsen_COV.orv
SEN     24  tc1obsen.sen
PES     25  tc1obsen.pes
#
# GWF Process input file for prediction scenario
WEL     43  tc1obsenPRED.wel
```

Figure A- 1. Example MOD-PREDICT Name File

PRD Input File

Entries in the MOD-PREDICT PRD input file are based on the concept of blocks, each proceeded by a block-header and followed by a block-footer. The PRD file should contain a minimum of one block, with the block-header "START MF2K_DATA" and block-footer "END MF2K_DATA". The first block contains information necessary for MOD-PREDICT to identify the MODFLOW-2000 name file and to execute MODFLOW-2000.

The PRD may also include an optional second block. If the second block is provided, the block-header is "START FILENAMES" and the block-footer is "END FILENAMES". This block defines prefixes for MODFLOW-2000 input and output files for observation-only, prediction-only, and parameter-estimation runs. These prefixes may be three characters or less. If the "START FILENAMES" block is not included, MOD-PREDICT uses the defaults "OB_", "PR_", and "PE_", respectively.

Input Instructions

Free format is used for reading all entries. The PRD file is constructed as follows:

FOR EACH SIMULATION

0. [#Text]

Item 0 is optional -- "#" must be in column 1. Item 0 can be repeated multiple times.

1. START [*blockname*]

2. Item 2 depends on *blockname* and may include more than one record.

If blockname = "MF2K_DATA"

MODFLOW_NAME_FILE

MODFLOW_COMMAND

If blockname = "FILENAMES"

OBSERVATION_RUN_FILENAME_BASE cal

PREDICTION_RUN_FILENAME_BASE pre

PARAMETER_ESTIMATION_FILENAME_BASE pes

3. END [*blockname*]

Repeat Items 1 to 3 for each BLOCK included in the input file. The input file must contain the block with the block-header "START MF2K_DATA", and may contain an optional second block with the block-header "START FILENAMES". The maximum record length for an entry in the "PRD" file is 199 characters.

Explanation of Variables Read from the MOD-PREDICT (PRD) File

BLOCK *"MF2K_DATA"*

MODFLOW_NAME_FILE – Can be upper or lower case characters. The MODFLOW-2000 name file that lists the simulation files for the analysis. This name file must at a minimum list Ground-Water Flow Process input files that define calibration conditions and Observation Process input files, and may include Sensitivity and Parameter Estimation Process input files.

MODFLOW_COMMAND – Can be upper or lower case characters, and can include a path statement. The name and path for the MODFLOW-2000 executable. Read and stored as MF2KCOM by MOD-PREDICT. If a value is not provided, a default of MF2KCOM = "MF2K.EXE" is used by MOD-PREDICT.

BLOCK *"FILENAMES"*

OBSERVATION_RUN_FILENAME_BASE – Up to three characters. Can be upper or lower case characters. Read and stored as OBS_PREF by MOD-PREDICT. The character prefix used to identify simulation input and output files as relating to *ONLY* observations. If a value is not provided, a default of OBS_PREF = "OB_" is used by MOD-PREDICT.

PREDICTION_RUN_FILENAME_BASE – Up to three characters. Can be upper or lower case characters. Read and stored as PRE_PREF by MOD-PREDICT. The character prefix used to identify simulation input and output files as relating to *ONLY* predictions. If a value is not provided, a default of PRE_PREF = "PR_" is used by MOD-PREDICT.

PARAMETER_ESTIMATION_FILENAME_BASE – Up to three characters. Can be upper or lower case characters. Read and stored as PAR_PREF by MOD-PREDICT. The character prefix used to identify simulation input and output files related to parameter estimation (calibration) runs, and therefore containing *ONLY* observations. If a value is not provided, a default of PAR_PREF = "PE_" is used by MOD-PREDICT.

The example MOD-PREDICT "PRD" file shown below tells MOD-PREDICT that the MODFLOW-2000 name file is "TC3.NAM" (example 1 in appendix B); the MODFLOW executable is "MF2KSEN.EXE". These three items are required for MOD-PREDICT to execute.

```
# MOD-PREDICT INPUT FILE - EXAMPLE
# NOTE: IF "START FILENAMES" IS NOT INCLUDED THE FOLLOWING DEFAULTS ARE
# USED
#
# PREDICTIONS_ONLY:       'PR_'
# OBSERVATIONS ONLY:      'OB_'
# PARAMETER ESTIMATION:   'PE_'

START MF2K_DATA
  MODFLOW_NAME_FILE TC3.NAM
  MODFLOW_COMMAND MF2KSEN.exe
END MF2K_DATA

START FILENAMES
  OBSERVATION_RUN_FILENAME_BASE cal
  PREDICTION_RUN_FILENAME_BASE pre
  PARAMETER_ESTIMATION_FILENAME_BASE pes
END FILENAMES
```

Figure A- 2. Example MOD-PREDICT "PRD" File

SETS Input File

The SETS input file lists sets and defines the set characteristics. Calibration sets can include observations and prior information. Prediction sets can only include predictions. The same PLOT-SYMBOL value can occur in more than one set, but for a single value all the sets need to be the same type – CALIBRATION, PREDICTION, or OMIT.

Input File Instructions

Inputs for defining sets are read from the file that has file type SETS in the MOD-PREDICT name file. Free format is used for reading all entries. The SETS file is constructed as follows:

FOR EACH SIMULATION

0. [#Text]

Item 0 is optional -- "#" must be in column 1. Item 0 can be repeated multiple times.

1. NSETS

2. SETNAME PLOT-SYMBOL/PLOT-SYMBOLS ["PRINT"/"**NOPRINT**" "PREDICTION"/"**CALIBRATION**"/"OMIT" "MULT="MULT]

Repeat Item 2 for each set to be defined (that is, NSETS times). The SETNAME variable must be first; all other entries can be supplied in any order, or can be omitted, wherein the default option identified in bold or the default value described below is used.

Explanation of Variables Read from the SETS Input File

NSETS – is an integer variable equal to the number of sets defined on the following lines of the SETS file. If it is omitted, a default value of zero is assumed, and MOD-PREDICT will terminate.

SETNAME – is the name of an observation set. This can be up to twelve characters in length. Each set name must be unique. SETNAME has the same restrictions imposed on the OBSNAM variable. That is, blanks are not be allowed unless double quotes proceed and follow the SETNAME.

"PRINT"/"NOPRINT" – Can be upper or lower case characters. Controls printing related to sets. If neither is specified, "NOPRINT" is used.

PRINT – Statistical and sensitivity information for this set is recorded in the MOD-PREDICT output file and pertinent underscore files.

NOPRINT – For observations and prior information, only the output from MODFLOW-2000 is printed (Hill and others, 2000). For predictions, reference and prediction

values are recorded in the MODFLOW-2000 underscore files (table 7) and summary statistics for each set (table 10) are tabulated in the MOD-PREDICT output file.

"CALIBRATION"/"PREDICTION"/"OMIT" – Specifies whether the observation set includes data to be used in the calibration (observations or prior information), for predictive simulations, or not at all. If none of these are specified, CALIBRATION is assumed. Lower case letters can be used.

MULT – A multiplier that can be used to control the weighting of sets of observations and prior information or the scaling of predictions. The default value for MULT is 1.0. Lower case letters can be used. The use of this variable is explained in more detail below.

- If STAT_FLAG or SCALE_FLAG equals 0, STATISTIC or SCALE are multiplied by MULT.
- If STAT_FLAG or SCALE_FLAG equals 1 or 2, STATISTIC or SCALE are multiplied by the square root of MULT.

PLOT-SYMBOL/PLOT-SYMBOLS – Defines the value(s) of PLOT-SYMBL used to identify set members. If PLOT-SYMBOL is specified, it needs to be followed by an equal sign bounded by spaces and a single integer. If PLOT-SYMBOLS is specified, it needs to be followed by an equal sign bounded by spaces, a single integer, and then a sequence of integers, where the first integer (ISYMBOL) indicates the number of subsequent integers. All observations, prior information (or) predictions identified in the Observation Process files that have a PLOT-SYMBOL equivalent to any of the ISYMBOL PLOT-SYMBOLS will be assigned to that set. For example:

Example Sets input file: PLOT-SYMBOL

```
# MOD-PREDICT: SETS FILE
2
HEADS   PRINT   PREDICTION   MULT = 1.0   PLOT-SYMBOL = 1000
FLOWS   PRINT   PREDICTION   MULT = 1.0   PLOT-SYMBOL = 2000
```

Example Sets input file: PLOT-SYMBOLS

```
# MOD-PREDICT: SETS FILE
1
HEADS   PRINT   PREDICTION   MULT = 1.0   PLOT-SYMBOLS = 2 100 150
```

Observation, Sensitivity and Parameter-Estimation Process Input Files Listed in the MOD-PREDICT Name File

Instructions for the Observation, Sensitivity, and Parameter-Estimation Process input files are unchanged from those described in Hill and others (2000). The Observation, Sensitivity and Parameter-Estimation Process input files should be listed in the MOD-PREDICT name file, and should not be listed in the MODFLOW-2000 name file. MOD-PREDICT will detect and report conflicts that occur if Observation, Sensitivity and (or) Parameter Estimation Process input files are listed in both the MOD-PREDICT name file and the MODFLOW-2000 name file, and will use the file(s) listed in the MOD-PREDICT name file. If conflicts occur, MOD-PREDICT will report the conflict, and terminate execution.

Ground-Water Flow Process Input Files Listed in the MOD-PREDICT Name File

Ground-Water Flow Process input files can be listed in the MOD-PREDICT name file to define prediction conditions. The input instructions are unchanged from those described by Harbaugh and others (2000). The listed files are used to replace files in the MODFLOW-2000 name file if the same file type occurs there. Otherwise the listed files are added to the MODFLOW-2000 name file. Replacement files can have the same unit number as the file being replaced, but added files need to have unit numbers that are different than others used in the file. MOD-PREDICT looks for conflicts. If any occur a message is written to the MOD-PREDICT main output file and execution stops.

APPENDIX B. EXAMPLE SIMULATIONS

The test cases presented in this section are intended to provide example input and output files using MOD-PREDICT, and demonstrate that the calculations performed by MOD-PREDICT are correct. The test cases provided are based upon test cases provided by Hill and others (2000), illustrating the use of the Observation, Sensitivity, and Parameter Estimation Processes with the Ground-Water Flow Process of MODFLOW-2000.

Two test cases are provided here. Test case 1 involves hydraulic head and head-dependent observations and predictions. Test case 2 includes hydraulic head and advective-transport observations and predictions. Outputs from MOD-PREDICT for each of the two test cases are presented. Input and output files for these test cases from the Parameter-Estimation mode (table 3) are presented in Hill and others (2000). MODFLOW-2000 outputs from these and additional test cases and modes are provided in electronic files with distributions of MODFLOW-2000 (see the Distributed Files and Directories section of Appendix B, Hill and others, 2000).

One purpose of the example simulations provided is to demonstrate that the calculations made by MOD-PREDICT are correct. To evaluate the statistical analyses, this includes demonstrating that for a given set of input values, the correct result was obtained. The tables written to the output file MODPREDICT.OUT can be used, together with a spreadsheet program such as Excel™ or Lotus™ to verify the statistics printed to the summary statistic tables for the example simulations provided.

Test Case 1

Description

The base name for Test Case 1 is TC1OBSEN. This test case is based upon Test Case 1 in Hill and others (2000) that is described in detail in appendix A of that report. This test case is used here to demonstrate the following features of MOD-PREDICT:

1. The format and contents of the files required by MOD-PREDICT to run a Run Type 3 analysis. This includes the MODFLOW-2000 name files, the MOD-PREDICT name file, and the contents of the PRD and SETS files.
2. How MOD-PREDICT differentiates observations and predictions using PLOT-SYMBOL, and how multiple PLOT-SYMBOLS can be assigned to a set.
3. How observations can be defined by excluding them from any set.
4. How MOD-PREDICT controls a sequence of MODFLOW-2000 forward and sensitivity runs for a Run Type 3 analysis of predictions.

Input Files

In this test case, hydraulic-head observations are listed in an HOB file (that is, a file with file type HOB in the name file), and flow observations are listed in an Observation Process, River Package (RVOB) file. Head observations are listed in the file "TC1OBSENPRED.OHD", where the name indicates that there are also predictions listed in the file. Flow observations for boundaries simulated using the River Package are listed in the file "TC1OBSEN.ORV". In repetitions of item 5 in the HOB file, ITT=2, so that initial hydraulic heads and subsequent changes in hydraulic head are used as observations and predictions.

For MOD-PREDICT to execute, the Ground-Water Flow Process input files necessary for a forward run of MODFLOW-2000 are listed in the MODFLOW-2000 name file. Note that parameters are defined in the input files for the packages to which the parameters apply (Harbaugh and others, 2000), and the parameter values are obtained from the Sensitivity Process (SEN) input file. The name of the MODFLOW-2000 name file is "TC1OBSEN.NAM". For a Run-Type 3 analysis of predictions, the MOD-PREDICT name file includes file types OBS, SEN, and PES, and the names of the Observation Process files containing observations and predictions differentiated by PLOT-SYMBOL. Starting estimates for parameters are listed in the Sensitivity

Process input file. The Sensitivity Process input file also controls which parameters are analyzed for sensitivity. The name of the MOD-PREDICT name file is "PREDICT.NAM". The MODFLOW-2000 and MOD-PREDICT name files are shown in this section.

The Ground-Water Flow, Sensitivity and Parameter-Estimation Process input files, and the Observation Process input file for all observations (OBS), are unchanged from those presented in Hill and others (2000). The river observation file "TC1OBSEN.ORV" and the head observation file "TC1OBSENPRED.OHD" are shown below.

Note that in the electronic files provided together with MOD-PREDICT, a modified version of the TC1OBSEN case is provided which includes a variance-covariance matrix for specifying weights in the RVOB river observation package. The name of the river observation file in that instance is "TC1OBSENPRED_COV.ORV", indicating that there are predictions listed in the file, and that a variance-covariance matrix is used for defining the observation weights.

MODFLOW-2000 Name File "TC1OBSEN.NAM" for Test Case TC1OBSEN

```
# MODFLOW2000 NAME FILE FOR TEST CASE TC1OBSEN
#
# NOTE: The files contained in the MODFLOW2000 name file
# comprise the GWF files for a forward run of MODFLOW2000.
# Obs-Sen-Pes process input files required for
# calibration/prediction runs are listed in the MODPREDICT
# name file PREDICT.NAM
#
# Output files
global  11  tc1obsen.glo
list    12  tc1obsen.lst
#
# Global input files
dis     31  tc1obsen.dis
zone    32  tc1obsen.zon
mult    33  tc1obsen.mlt
#
# Flow process input files
bas6    41  tc1obsen.bas
lpf     42  tc1obsen.lpf
wel     43  tc1obsen.wel
de4     44  tc1obsen.de4
oc      45  tc1obsen.oc
ghb     46  tc1obsen.ghb
riv     47  tc1obsen.riv
rch     48  tc1obsen.rch
```

MOD-PREDICT Name File "PREDICT.NAM" for Test Case TC1OBSEN

```
# MODPREDICT NAME FILE FOR TEST CASE TC1OBSEN
#
# NOTE: The files contained in the MODPREDICT name file
# comprise OBS-SEN-PES files required for calibration runs; and
# OBSPRED files (similar in form to MODFLOW2000 observation package
# files) containing some combination of observations and predictions.
#
# All Global input files and GWF Process input files can be read
# from the MODFLOW2000 name file UNLESS stresses are different
# for the prediction scenario, in which case the prediction GWF Process
# input file must be included here.
#
# PRD file for prediction scenario
PRD     80  tc1obsen.prd
#
# SETS file for prediction scenario
SETS    50  TEST.SETS
#
# Obs-Sen-Pes process input files for prediction scenario
obs     21  tc1obsen.obs
hob     22  tc1obsenPRED.ohd
rvob    23  tc1obsen.orv
sen     24  tc1obsen.sen
pes     25  tc1obsen.pes
#
# Dummy GWF Process input files for prediction scenario (as an example)
wel     43  tc1obsenPRED.wel
```

MOD-PREDICT SETS File "TEST.SETS" for Test Case TC1OBSEN

```
# SETS FILE
4
HEAD1   PRINT   OMIT          MULT = 1.00   PLOT-SYMBOL = 100
HEAD2   PRINT   PREDICTION    MULT = 1.00   PLOT-SYMBOLS = 3 1000 1100 1200
FLOW1   PRINT   PREDICTION    MULT = 1.00   PLOT-SYMBOL = 2000
FLOW2   PRINT   CALIBRATION   MULT = 1.00   PLOT-SYMBOL = 1
```

MOD-PREDICT PRD File "TC1OBSEN.PRD" for Test Case TC1OBSEN

```
# PREDICTION DRIVER INPUT FILE - EXAMPLE
# NOTE: IF "START FILENAMES" IS NOT INCLUDED, THE FOLLOWING DEFAULTS ARE USED
#
# PREDICTIONS_ONLY:        'PR_'
# OBSERVATIONS ONLY:       'OB_'
# PARAMETER ESTIMATION:    'PE_'

START MF2K_DATA
  MODFLOW_NAME_FILE tc1obsen.nam
  MODFLOW_COMMAND ..\..\bin\MF2KSEN.EXE
END MF2K_DATA
```

RVOB file "TC1OBSEN.ORV" for Test Case TC1OBSEN

```
# RVOB file for test case tc1obsen
#
    1   18    3
   86400.0  1.0  0
    3  -18
SS     1       0.0  -4.4   .40   0   2
TR3    5       0.0  -4.1   .38   0   2
TR12   5 272.7713  -2.2   .21   0   2
    1    1    1        1.0
    1    2    1        1.0
    1    3    1        1.0
    1    4    1        1.0
    1    5    1        1.0
    1    6    1        1.0
    1    7    1        1.0
    1    8    1        1.0
    1    9    1        1.0
    1   10    1        1.0
    1   11    1        1.0
    1   12    1        1.0
    1   13    1        1.0
    1   14    1        1.0
    1   15    1        1.0
    1   16    1        1.0
    1   17    1        1.0
    1   18    1        1.0
```

HOB file "TC1OBSENPRED.OHD" for Test Case TC1OBSEN

```
# HOB file for test case tc1obsen
#
   32    0    0
   86400.0  1.0
1.0  1  3    1   -3  0.00    0.00    0.00     0.000    0.00    0 1000
    2
1.0           1    0.00     101.804    1.0025    0.0025    0    1000
1.1           3    0.00     101.775    1.0025    0.0025    0    1100
1.12          5  272.7713   101.675    1.0025    0.0025    0    1000
2.0  1  4    4   -5  0.00    0.00    0.00     0.000    0.00    0  1
    2
2.0           1    0.00     128.117    1.0025    0.0025    0    1
2.1           3    0.00     128.076    1.0025    0.0025    0    1
2.2           4    0.00     127.560    1.0025    0.0025    0    1
2.8           5  97.59433   116.586    1.0025    0.0025    0    1
2.12          5  272.7713   113.933    1.0025    0.0025    0    1
3.0  1   10   9   -3  0.00    0.00    0.00     0.000    0.00    0  1
    2
3.0           1    0.00     156.678    1.0025    0.0025    0    1
3.1           3    0.00     152.297    1.0025    0.0025    0    1
3.12          5  272.7713   114.138    1.0025    0.0025    0    1
4.0  1   13   4   -3  0.00    0.00    0.00     0.000    0.00    0  1
    2
4.0           1    0.00     124.893    1.0025    0.0025    0    1
4.1           3    0.00     124.826    1.0025    0.0025    0    1
4.12          5  272.7713   110.589    1.0025    0.0025    0    100
5.0  1   14   6   -3  0.00    0.00    0.00     0.000    0.00    0  1
    2
5.0           1    0.00     140.961    1.0025    0.0025    0    1
5.1           3    0.00     140.901    1.0025    0.0025    0    1
5.12          5  272.7713   119.285    1.0025    0.0025    0    1
6.0  2    4   4   -3  0.00    0.00    0.00     0.000    0.00    0  1
    2
6.0           1    0.00     126.537    1.0025    0.0025    0    1
6.1           3    0.00     126.542    1.0025    0.0025    0    1
6.12          5  272.7713   112.172    1.0025    0.0025    0    1
7.0  2   10   1   -3  0.00    0.00    0.00     0.000    0.00    0  1
    2
7.0           1    0.00     101.112    1.0025    0.0025    0    1
7.1           3    0.00     101.160    1.0025    0.0025    0    1
7.12          5  272.7713   100.544    1.0025    0.0025    0    1
8.0  2   10   9   -3  0.00    0.00    0.00     0.000    0.00    0  1
    2
8.0           1    0.00     158.135    1.0025    0.0025    0    1
8.1           3    0.00     152.602    1.0025    0.0025    0    1
8.12          5  272.7713   114.918    1.0025    0.0025    0    1
9.0  2   10   18  -3  0.00    0.00    0.00     0.000    0.00    0  1
    2
9.0           1    0.00     176.374    1.0025    0.0025    0    1
9.1           3    0.00     176.373    1.0025    0.0025    0    1
9.12          5  272.7713   138.132    1.0025    0.0025    0    1
0.0  2   18   6   -3  0.00    0.00    0.00     0.000    0.00    0  1
    2
0.0           1    0.00     142.020    1.0025    0.0025    0    1
0.1           3    0.00     142.007    1.0025    0.0025    0    1
0.12          5  272.7713   122.099    1.0025    0.0025    0    1
```

MOD-PREDICT Run-Time Screen Reporting for Test Case TC1OBSEN

```
RUNNING CALIBRATION CASE                  PE_tc1obsen.NAM
 - COMPLETED CALIBRATION CASE                   PE_tc1obsen.NAM
READING OUTPUT FOR CALIBRATION CASE             PE_tc1obsen.NAM
RUNNING OBSERVATIONS-ONLY CASE                  OB_tc1obsen.NAM
 - COMPLETED OBSERVATIONS-ONLY CASE             OB_tc1obsen.NAM
RUNNING PREDICTIONS-ONLY CASE                   PR_tc1obsen.NAM
 - COMPLETED PREDICTIONS-ONLY CASE              PR_tc1obsen.NAM
READING OUTPUT FOR OBSERVATIONS-ONLY CASE       OB_tc1obsen.NAM
READING OUTPUT FOR PREDICTIONS-ONLY CASE        OB_tc1obsen.NAM

RECORDING CALIBRATION SUMMARY STATISTICS:
RECORDING PREDICTION SUMMARY STATISTICS:

== PREDICTION RUN COMPLETED SUCCESSFULLY ==
============================================
NORMAL TERMINATION OF MOD-PREDICT
```

MOD-PREDICT Output File "MODPREDICT.OUT" for Test Case TC1OBSEN

```
                                MODFLOW-2000
                            MODPREDICT VERSION 1

 OPENING predict.nam
   CHECKING ACTIVE PACKAGES IN MODPREDICT NAME FILE
   CHECKING TEST.SETS TYPE:SETS UNIT:   50
   CHECKING tc1obsen.obs TYPE:OBS UNIT:   21
   CHECKING tc1obsenPRED.ohd TYPE:HOB UNIT:   22
   CHECKING tc1obsen.orv TYPE:RVOB UNIT:   23
   CHECKING tc1obsen.sen TYPE:SEN UNIT:   24
   CHECKING tc1obsen.pes TYPE:PES UNIT:   25
   CHECKING tc1obsenPRED.wel TYPE:WEL UNIT:   43
   READ predict.nam - OK

 READING PRD INPUT FILE tc1obsen.prd
 - READING BLOCK MF2K DATA
   MODFLOW NAME FILE                : tc1obsen.nam
   MODFLOW COMMAND                  : ..\..\bin\MF2KSEN.EXE
 - READ BLOCK MF2K_DATA

   "FILENAMES" BLOCK NOT FOUND IN FILE tc1obsen.prd
   THE FOLLOWING DEFAULTS WILL BE USED:
   PREDICTIONS_ONLY:        "PR_"
   OBSERVATIONS ONLY:       "OB_"
   PARAMETER ESTIMATION:    "PE_"

 OPENING tc1obsen.nam
   CHECKING ACTIVE PACKAGES IN MODFLOW NAME FILE
   GLOBAL FILE: tc1obsen.glo UNIT   11
   GLOBAL FILE: tc1obsen.lst UNIT   12
   CHECKING tc1obsen.dis TYPE:DIS UNIT:   31
   CHECKING tc1obsen.zon TYPE:ZONE UNIT:   32
   CHECKING tc1obsen.mlt TYPE:MULT UNIT:   33
   CHECKING tc1obsen.bas TYPE:BAS6 UNIT:   41
   CHECKING tc1obsen.lpf TYPE:LPF UNIT:   42
   CHECKING tc1obsen.wel TYPE:WEL UNIT:   43
   CHECKING tc1obsen.de4 TYPE:DE4 UNIT:   44
   CHECKING tc1obsen.oc TYPE:OC UNIT:   45
   CHECKING tc1obsen.ghb TYPE:GHB UNIT:   46
   CHECKING tc1obsen.riv TYPE:RIV UNIT:   47
   CHECKING tc1obsen.rch TYPE:RCH UNIT:   48
   READ tc1obsen.nam - OK


====================  READ MODFLOW SIMULATION FILES  ======================

 SELECTED RUN TYPE 3 - OBS, SEN, AND PES ACTIVATED

 READING OBS FILE tc1obsen.obs FOR OUTNAM AND ISCALS
   OBSERVATION GRAPH-DATA OUTPUT FILES
     WILL BE PRINTED AND NAMED USING THE BASE: tc1obsen
   OBSERVATION GRAPH-DATA OUTPUT FILES
     WILL BE PRINTED AND NAMED USING THE PATH: output\
   DIMENSIONLESS SCALED OBSERVATION SENSITIVITIES WILL  BE PRINTED
   ONE-PERCENT SCALED OBSERVATION SENSITIVITIES WILL BE PRINTED

 READING SETS FILE  FOR NSETS
   NUMBER OF SETS:     4
```

```
  INFORMATION ON CALIBRATION/PREDICTION/OMIT SETS LISTED IN THE SETS FILE.
  EXCEPT FOR SETNAME AND PLOT-SYMBOL, DEFAULTS ARE USED IF NO INFORMATION IS
     SUPPLIED.

  SET NAME TYPE          VARIANCE     PLOT-SYMBOL  PRINT?
                         MULTIPLIER
  -------- ------------  ----------   -----------  ------
  HEAD1    OMIT            1.0000         100       YES
  HEAD2    PREDICTION      1.0000         1000      YES
  HEAD2    PREDICTION      1.0000         1100      YES
  HEAD2    PREDICTION      1.0000         1200      YES
  FLOW1    PREDICTION      1.0000         2000      YES
  FLOW2    CALIBRATION     1.0000         1         YES

READING SEN FILE tc1obsen.sen FOR ISENSU, ISENPU
  SEN FILE tc1obsen.sen READ - OK
  SEN FILE tc1obsen.sen ISENALL = 0:
  ISENS INDICATES   2 PARAMETERS
  GRID SENSITIVITIES WILL NOT BE PRINTED

READING PES FILE tc1obsen.pes FOR MAX-ITER

READING ACTIVE OBSERVATION PACKAGES
HOB
  READ tc1obsenPRED.ohd - OK
  tc1obsenPRED.ohd NUMBER OF OBSERVATIONS:   29
  tc1obsenPRED.ohd NUMBER OF PREDICTIONS:     3
  tc1obsenPRED.ohd OMITTED QUANTITIES:        0
  FILE FOR OBSERVATIONS = OB_tc1obsenPRED.ohd
  FILE FOR PREDICTIONS  = PR_tc1obsenPRED.ohd
RVOB
  NUMBER OF FLOW-OBSERVATION CELL GROUPS...:      1
  NUMBER OF CELLS IN CELL GROUPS.....:           18
  NUMBER OF CELL FLOWS.....:                      3
  READ tc1obsen.orv - OK
  tc1obsen.orv NUMBER OF OBSERVATIONS:    3
  tc1obsen.orv NUMBER OF PREDICTIONS:     0
  tc1obsen.orv OMITTED QUANTITIES:        0

PROCESSED ALL OBSERVATION PACKAGES OKAY
  TOTAL NUMBER OF OBSERVATIONS:   32
  TOTAL NUMBER OF PREDICTIONS:     3
  TOTAL OMITTED QUANTITIES:        0

MAX-ITER>0 IN tc1obsen.pes - CALIBRATION WILL BE COMPLETED.
  A NEW .PES FILE WILL BE CREATED WITH MAX-ITER=0
  TO CALCULATE STATISTICS OF THE CALIBRATED MODEL.
  (NOTE: "OMIT" NOT ACTIVATED FOR PRIOR IN MODPREDICT VERSION-1)

  PES FILE tc1obsen.pes READ - OK
  "MAX-ITER=0" PES FILE PE_tc1obsen.pes WRITTEN - OK

WRITING OBS FILES
  OBS FILE FOR PES-RUN  - PE_tc1obsen.obs
  OBS FILE FOR OBS-RUN  - OB_tc1obsen.obs
  OBS FILE FOR PRED-RUN - PR_tc1obsen.obs
  WRITTEN OBS FILE(S) FOR OBS-SEN-PES CASE
```

```
PREPARING .NAM FILES FOR OBS-SEN-PES CASE
   NAME FILE FOR CALIBRATION RUN - PE_tc1obsen.NAM
   NAME FILE FOR OBSERVATIONS ONLY - OB_tc1obsen.NAM
   NAME FILE FOR PREDICTIONS ONLY - PR_tc1obsen.NAM
   MODFLOW .NAM FILES WRITTEN - OK

 DELETING HANGING UNDERSCORE FILES FOR RUNTYPE  3
   DELETING - output\OB_tc1obsen._os
   DELETING - output\PR_tc1obsen._os
   DELETING - output\OB_tc1obsen._ww
   DELETING - output\PR_tc1obsen._ww
   DELETING - output\OB_tc1obsen._ws
   DELETING - output\PR_tc1obsen._ws
   DELETING - output\OB_tc1obsen._r
   DELETING - output\PR_tc1obsen._r
   DELETING - output\OB_tc1obsen._w
   DELETING - output\PR_tc1obsen._w
   DELETING - output\OB_tc1obsen._nm
   DELETING - output\PR_tc1obsen._nm
   DELETING - output\OB_tc1obsen._sc
   DELETING - output\PR_tc1obsen._sc
   DELETING - output\OB_tc1obsen._sd
   DELETING - output\PR_tc1obsen._sd
   DELETING - output\OB_tc1obsen._s1
   DELETING - output\PR_tc1obsen._s1
   DELETING - output\OB_tc1obsen._ss
   DELETING - output\OB_tc1obsen._pa
   DELETING - output\OB_tc1obsen._b
 DELETED HANGING UNDERSCORE FILES FOR RUNTYPE  3

 ======================    RUN MODFLOW SIMULATIONS    ======================


 RUNNING CALIBRATION CASE                          PE_tc1obsen.NAM
 (COMMAND = ..\..\bin\MF2KSEN.EXE PE_tc1obsen.NAM > NUL)
  - CHECKING FOR output\PE_tc1obsen._sc
  - CHECK RUN OKAY

  - COMPLETED CALIBRATION CASE                     PE_tc1obsen.NAM

 READING OUTPUT FOR CALIBRATION CASE               PE_tc1obsen.NAM

   READING UNDERSCORES FOR    2 PARAMETERS
   PARAMETER ESTIMATION DID NOT CONVERGE - USING "FINAL PARAMETER ESTIMATES"
   - USING VALUES FROM ITERATION NO:   10
   - PARAMETER: RCH_ZONE_1  VALUE: 60.00000
   - PARAMETER: RCH_ZONE_2  VALUE: 30.00000
   - PARAMETER: WELLS_TR    VALUE: -.858587
   - PARAMETER: RIVERS      VALUE: 4.860560
   - PARAMETER: HK_1        VALUE: 30000E-8
   - PARAMETER: SS_1        VALUE: .0013000
   - PARAMETER: VERT_K_CB   VALUE: 1000E-10
   - PARAMETER: HK_2        VALUE: 40000E-9
   - PARAMETER: SS_2        VALUE: 20000E-8
   ALL PARAMETER-ESTIMATION UNDERSCORE FILES READ - OK
   WRITING OPTIMAL PARAMETERS TO SENFILE: PE_tc1obsen.sen
```

```
RUNNING OBSERVATIONS-ONLY CASE                    OB_tc1obsen.NAM
(COMMAND = ..\..\bin\MF2KSEN.EXE OB_tc1obsen.NAM > NUL)
 - CHECKING FOR output\OB_tc1obsen._sc
 - CHECK RUN OKAY

 - COMPLETED OBSERVATIONS-ONLY CASE               OB_tc1obsen.NAM

RUNNING PREDICTIONS-ONLY CASE                     PR_tc1obsen.NAM
(COMMAND = ..\..\bin\MF2KSEN.EXE PR_tc1obsen.NAM > NUL)
 - CHECKING FOR output\PR_tc1obsen._sc
 - CHECK RUN OKAY

 - COMPLETED PREDICTIONS-ONLY CASE                PR_tc1obsen.NAM

READING OUTPUT FOR SENSITIVITY RUNTYPE            OB_tc1obsen.NAM
                                                  PR_tc1obsen.NAM
  READING UNDERSCORES FOR   35 OBS-PRED-PRIOR
  FILE output\PR_tc1obsen._os READ - OK
  FILE output\PR_tc1obsen._ww READ - OK
  FILE output\PR_tc1obsen._ws READ - OK
  FILE output\PR_tc1obsen._r READ - OK
  FILE output\PR_tc1obsen._w READ - OK
  FILE output\PR_tc1obsen._nm READ - OK
  FILE output\OB_tc1obsen._os READ - OK
  FILE output\OB_tc1obsen._ww READ - OK
  FILE output\OB_tc1obsen._ws READ - OK
  FILE output\OB_tc1obsen._r READ - OK
  FILE output\OB_tc1obsen._w READ - OK
  FILE output\OB_tc1obsen._nm READ - OK
  ALL OBSERVATION UNDERSCORE FILES READ - OK

  READING UNDERSCORES FOR    2 PARAMETERS
  FILE output\PR_tc1obsen._sc READ - OK
  FILE output\PR_tc1obsen._sd READ - OK
  FILE output\PR_tc1obsen._s1 READ - OK
  FILE output\PR_tc1obsen._su READ - OK
  FILE output\OB_tc1obsen._sc READ - OK
  FILE output\OB_tc1obsen._sd READ - OK
  FILE output\OB_tc1obsen._s1 READ - OK
  FILE output\OB_tc1obsen._su READ - OK
  ALL SENSITIVITY UNDERSCORE FILES READ - OK

PROCESSING DATA FOR CALCULATION OF THE PREDICTION CORRELATION MATRIX

  PROCESSED WEIGHTS FOR HEAD OBS

  PROCESSED WEIGHT MATRIX FOR HEAD-DEP. AND ADV OBS

MATCHING DATA READ FROM UNDERSCORE FILES WITH NAMES/PLOT-SYMBOLS AS
READ FROM "OBS" FILES.

  ALL OBS/PRIOR/PRED LISTED IN THE MF2K FILES WERE
  FOUND IN "OBS" UNDERSCORE FILES PRODUCED BY MF2K

  ALL OBS/PRIOR/PRED LISTED IN THE MF2K FILES WERE
  FOUND IN "SEN" UNDERSCORE FILES PRODUCED BY MF2K
```

```
PREDICTION CORRELATION MATRIX

            WELLS_TR    RIVERS
 ..............................
 WELLS_TR      1.00      2.463E-04
 RIVERS      2.463E-04    1.00


 ==================== CALCULATE SET SUMMARY STATISTICS  ====================


 RECORDING CALIBRATION SUMMARY STATISTICS:

 == SUMMARY STATISTICS FOR CALIBRATION SETS ==

 ------------ ---------- ---------- ---------- ---------- ---------- ----------
 SET NAME      UWRES-MAX  UWRES-MIN  UWRES-AVG  NRESGT0    NRESLT0     RES-MAX
 ------------ ---------- ---------- ---------- ---------- ---------- ----------
 FLOW2        1.41400099 -13.849610 -3.1995790      17         12     21.0786896
 ------------ ---------- ---------- ---------- ---------- ---------- ----------

 ------------ ---------- ---------- ---------- ---------- ----------
 SET NAME       RES-MIN    RES-AVG    SOSWR       EVP         SE
 ------------ ---------- ---------- ---------- ---------- ----------
 FLOW2        -25.688890 -2.6934311 3542.01270 131.185654 11.4536304
 ------------ ---------- ---------- ---------- ---------- ----------


 RECORDING PREDICTION SUMMARY STATISTICS:

 == SUMMARY STATISTICS FOR PREDICTION SETS ==

 ------------ ---------- ---------- ---------- ---------- ----------
 SET NAME     USLARGEST  USSMALLEST USAVERAGE   LARGEST    SMALLEST
 ------------ ---------- ---------- ---------- ---------- ----------
 HEAD2        100.000099 -2.2888E-5 33.3333588 99.8752823 -3.4120E-4
 FLOW1        --- NO OBS/PRIOR/PRED BELONG TO THIS SET ---
 ------------ ---------- ---------- ---------- ---------- ----------

 ------------ ---------- ---------- ---------- ---------- ----------
 SET NAME      AVERAGE   USDIFF-MAX USDIFF-MIN USDIFF-AVG   NGTREF
 ------------ ---------- ---------- ---------- ---------- ----------
 HEAD2        33.2916451 1.80394697 -.12897490 .548657596       2
 FLOW1
 ------------ ---------- ---------- ---------- ---------- ----------

 ------------ ---------- ---------- ---------- ----------
 SET NAME       NLTREF    DIFF-MAX   DIFF-MIN   DIFF-AVG
 ------------ ---------- ---------- ---------- ----------
 HEAD2               1    1.80169702 -1.9226440 -.20370837
 FLOW1
 ------------ ---------- ---------- ---------- ----------


  *INTERPRETING RUN STATISTICS FOR PREDICTION SETS*

The MOD-PREDICT tabulation of summary statistics pertains to
predictions, observations and prior information identified in
the OBS-SEN-PES process input files, and listed as members of
SETS in the "SETS" input file. Statistics are presented for
each SET.  For PREDICTIONS, statistics are of three types:
```

```
   ABSOLUTE     - USLARGEST, USSMALLEST, USAVERAGE
                  LARGEST, SMALLEST, AVERAGE
   DEVIATIONAL - USDIFF-MAX, USDIFF-MIN, USDIFF-AVG
                  DIFF-MAX, DIFF-MIN, DIFF-AVG
   RELATIVE     - NGTREF, NLTREF

This summary table can be used to indicate the deviation of
simulated predictions from reference values. HOWEVER - if
there is no supportable basis for specifying a reference
value, DEVIATIONAL and RELATIVE statistics are meaningless.
THUS use only ABSOLUTE statistics for PREDICTIONS.
(Refer to MOD-PREDICT documentation).

======================      RUN FILES SUMMARY      ========================

 RUNTYPE = "CALIBRATION"
   "CALIBRATION" RUN OUTPUT (OBSERVATIONS ONLY)          output\PE_tc1obsen.*
   "MAXITER = 0" RUN OUTPUTS FOR OBSERVATIONS            output\OB_tc1obsen.*
   "MAXITER = 0" RUN OUTPUTS FOR PREDICTIONS             output\PR_tc1obsen.*

============================ MOD-PREDICT COMPLETE ============================
==============================================================================
```

Test Case 2

Description

The base name for Test Case 2 is TC2. This test case is based upon Test Case 2 of Hill and others (2000) that is described in detail in appendix A of that document. This test case is used here to demonstrate the following features of MOD-PREDICT:

1. The use of the Advective-Transport Observation Package (Anderman and Hill, 2001).
2. The format and contents of the files required by MOD-PREDICT to run a Run Type 3 analysis. This includes the MODFLOW-2000 name files, the MOD-PREDICT name file, and the contents of the PRD and SETS files.
3. How MOD-PREDICT differentiates advective transport observations and predictions using PLOT-SYMBOL.
4. How MOD-PREDICT reports a combined parameter correlation matrix.

Input Files

In this test case, advective transport observations and predictions are listed in the Observation Process file "TC2_PRED.ADV", indicating that the file contains predictions. Head observations are listed in the Observation Process file "TC2.OHD". Flow observations are listed in the Observation Process files "TC2.ODR" and "TC2.OGB" for observations simulated with the Drain Package and the General Head Boundary package, respectively.

For MOD-PREDICT to execute, the Ground-Water Flow Process input files necessary for a forward run of MODFLOW-2000 are listed in the MODFLOW-2000 name file. Note that parameters are defined in the input files for the packages to which the parameters apply (Harbaugh and others, 2000), and the parameter values are obtained from the Sensitivity Process input file. The name of the MODFLOW-2000 name file is "TC2PRED_COV.NAM". The MOD-PREDICT name file includes the file type OBS, and the names of the Observation Process input files containing observations and predictions differentiated by PLOT-SYMBOL. The name of the MOD-PREDICT name file is "PREDICT.NAM". The MODFLOW-2000 and MOD-PREDICT name files are shown in this section. The Ground-Water Flow, Sensitivity and Parameter-Estimation Process input files, and the Observation Process input file for all observations, are unchanged from those presented in Hill and others (2000). The Advective-

Transport Observation Package input file "TC2_PRED.ADV" shown in this section defines one observation and one prediction.

MODFLOW-2000 Name File "TC2PRED.NAM" for Test Case TC2

```
# NAME file for test case tc2
#
# NOTE: The files contained in the MODFLOW2000 name file
# comprise the GWF files for a forward run of MODFLOW2000.
# Obs-Sen-Pes process input files required for
# calibration/prediction runs are listed in the MODPREDICT
# name file PREDICT.NAM
#
# Output files
global          11   tc2.glo
list            12   tc2.lst
data(BINARY)    13   tc2.bin
#
# Global input files
dis             31   tc2.dis
zone            32   tc2.zon
#
# Flow process input files
bas6            41   tc2.bas
lpf             42   tc2.lpf
wel             43   tc2.wel
drn             44   tc2.drn
evt             45   tc2.evt
ghb             46   tc2.ghb
rch             47   tc2.rch
oc              48   tc2.oc
pcg             49   tc2.pcg
data            60   data.out
```

MOD-PREDICT Name File "PREDICT.NAM" for Test Case TC2

```
# MODPREDICT NAME FILE FOR TEST CASE TC2PRED
#
# NOTE: The files contained in the MODPREDICT name file
# comprise OBS-SEN-PES files required for calibration runs; and
# OBSPRED files (similar in form to MODFLOW2000 observation package
# files) containing some combination of observations and predictions.
#
# All Global input files and GWF Process input files can be read
# from the MODFLOW2000 name file UNLESS stresses are different
# for the prediction scenario, in which case the prediction GWF Process
# input file must be included here.
#
# PRD file for prediction scenario
PRD     95  tc2pred.prd
#
# SETS file for prediction scenario
SETS    50  test_adv.sets
#
# Obs-Sen-Pes process input files for prediction scenario
obs     21  tc2.obs
hob     22  tc2_PRED.ohd
drob    23  tc2.odr
gbob    24  tc2.ogb
sen     25  tc2.sen
```

```
pes      26  tc2.pes
adv2     27  tc2_PRED.adv
```

MOD-PREDICT SETS File "TEST_ADV.SETS" File for Test Case TC2

```
# SETS FILE
3
PREDICT   PRINT PREDICTION    MULT = 1.0   PLOT-SYMBOL = 15
ADVECT2   PRINT CALIBRATION   MULT = 1.0   PLOT-SYMBOLS = 2 3 44
GHB       PRINT PREDICTION    MULT = 1.0   PLOT-SYMBOLS = 2 6 5
```

MOD-REDICT PRD File "TC2PRED.PRD" for Test Case tc2

```
# PREDICTION DRIVER INPUT FILE - EXAMPLE
# NOTE: IF "START FILENAMES" IS NOT INCLUDED, THE FOLLOWING DEFAULTS ARE USED
#
# PREDICTIONS_ONLY:        'PR_'
# OBSERVATIONS ONLY:       'OB_'
# PARAMETER ESTIMATION:    'PE_'

START MF2K_DATA
  MODFLOW_NAME_FILE tc2PRED.nam
  MODFLOW_COMMAND ..\..\bin\MF2Ksen.exe
END MF2K_DATA
```

ADV2 File "TC2_PRED.ADV" for Test Case TC2

```
    2    2   60    1    1    0        0.0
         0       0.30
         0       0.30
         0       0.30
    1    1   14   11  0.5   0.0   0.0
L_6      1   12    5  0.5 -0.09 -0.13 1500. 1 1500. 1 750. 1 5.59e+8     15
    1    1   13   12  0.5  0.0   0.0
C_5      1   10   11 0.48 -0.37 -0.35 1500. 1 1500. 1 750. 1 2.28e+6     44
    0
```

MOD-PREDICT Output File "MODPREDICT.OUT" for Test Case TC2

```
                                MODFLOW-2000
                             MODPREDICT VERSION 1

 OPENING predict.nam
   CHECKING ACTIVE PACKAGES IN MODPREDICT NAME FILE
   CHECKING test_adv.sets TYPE:SETS UNIT:    50
   CHECKING tc2.obs TYPE:OBS UNIT:    21
   CHECKING tc2_PRED.ohd TYPE:HOB UNIT:    22
   CHECKING tc2.odr TYPE:DROB UNIT:    23
   CHECKING tc2.ogb TYPE:GBOB UNIT:    24
   CHECKING tc2.sen TYPE:SEN UNIT:    25
   CHECKING tc2.pes TYPE:PES UNIT:    26
   CHECKING tc2_PRED.adv TYPE:ADV2 UNIT:    27
   READ predict.nam - OK

 READING PRD INPUT FILE tc2pred.prd
 - READING BLOCK MF2K DATA
   MODFLOW NAME FILE                : tc2PRED.nam
   MODFLOW COMMAND                  : ..\..\bin\MF2Ksen.exe
 - READ BLOCK MF2K_DATA

   "FILENAMES" BLOCK NOT FOUND IN FILE tc2pred.prd
   THE FOLLOWING DEFAULTS WILL BE USED:
   PREDICTIONS_ONLY:        "PR_"
   OBSERVATIONS ONLY:       "OB_"
   PARAMETER ESTIMATION:    "PE_"

 OPENING tc2PRED.nam
   CHECKING ACTIVE PACKAGES IN MODFLOW NAME FILE
   GLOBAL FILE: tc2.glo UNIT    11
   GLOBAL FILE: tc2.lst UNIT    12
   CHECKING tc2.bin TYPE:DATA(BINARY) UNIT:    13
   CHECKING tc2.dis TYPE:DIS UNIT:    31
   CHECKING tc2.zon TYPE:ZONE UNIT:    32
   CHECKING tc2.bas TYPE:BAS6 UNIT:    41
   CHECKING tc2.lpf TYPE:LPF UNIT:    42
   CHECKING tc2.wel TYPE:WEL UNIT:    43
   CHECKING tc2.drn TYPE:DRN UNIT:    44
   CHECKING tc2.evt TYPE:EVT UNIT:    45
   CHECKING tc2.ghb TYPE:GHB UNIT:    46
   CHECKING tc2.rch TYPE:RCH UNIT:    47
   CHECKING tc2.oc TYPE:OC UNIT:    48
   CHECKING tc2.pcg TYPE:PCG UNIT:    49
   CHECKING data.out TYPE:DATA UNIT:    60
   READ tc2PRED.nam - OK


 ======================  READ MODFLOW SIMULATION FILES  ======================

 SELECTED RUN TYPE 3 - OBS, SEN, AND PES ACTIVATED

 READING OBS FILE tc2.obs FOR OUTNAM AND ISCALS
   OBSERVATION GRAPH-DATA OUTPUT FILES
     WILL BE PRINTED AND NAMED USING THE BASE: tc2
   OBSERVATION GRAPH-DATA OUTPUT FILES
     WILL BE PRINTED AND NAMED USING THE PATH: OUTPUT\
   DIMENSIONLESS SCALED OBSERVATION SENSITIVITIES WILL  BE PRINTED
```

```
READING SETS FILE  FOR NSETS
  NUMBER OF SETS:     3

  INFORMATION ON CALIBRATION/PREDICTION/OMIT SETS LISTED IN THE SETS FILE.
  EXCEPT FOR SETNAME AND PLOT-SYMBOL, DEFAULTS ARE USED IF NO INFORMATION IS
     SUPPLIED.

  SET NAME TYPE          VARIANCE     PLOT-SYMBOL  PRINT?
                         MULTIPLIER
  -------- ------------  ----------   -----------  ------
  PREDICT  PREDICTION      1.0000         15         YES
  ADVECT2  CALIBRATION     1.0000         3          YES
  ADVECT2  CALIBRATION     1.0000         44         YES
  GHB      PREDICTION      1.0000         6          YES
  GHB      PREDICTION      1.0000         5          YES

READING SEN FILE tc2.sen FOR ISENSU, ISENPU
  SEN FILE tc2.sen READ - OK
  SEN FILE tc2.sen ISENALL = 0:
  ISENS INDICATES   9 PARAMETERS
  GRID SENSITIVITIES WILL NOT BE PRINTED

READING PES FILE tc2.pes FOR MAX-ITER

READING ACTIVE OBSERVATION PACKAGES
HOB
  READ tc2_PRED.ohd - OK
  tc2_PRED.ohd NUMBER OF OBSERVATIONS:    40
  tc2_PRED.ohd NUMBER OF PREDICTIONS:      2
  tc2_PRED.ohd OMITTED QUANTITIES:         0
  FILE FOR OBSERVATIONS = OB_tc2_PRED.ohd
  FILE FOR PREDICTIONS  = PR_tc2_PRED.ohd
ADV2
  IPRED > 0: WRITTEN NEW ADV FILES - OK
  READ tc2_PRED.adv - OK
  tc2_PRED.adv NUMBER OF OBSERVATIONS:     3
  tc2_PRED.adv NUMBER OF PREDICTIONS:      3
  tc2_PRED.adv OMITTED QUANTITIES:         0
  FILE FOR OBSERVATIONS = OB_tc2_PRED.adv
  FILE FOR PREDICTIONS  = PR_tc2_PRED.adv
DROB
  NUMBER OF FLOW-OBSERVATION CELL GROUPS...:       5
  NUMBER OF CELLS IN CELL GROUPS.....:             5
  NUMBER OF CELL FLOWS.....:                       5
  READ tc2.odr - OK
  tc2.odr NUMBER OF OBSERVATIONS:     5
  tc2.odr NUMBER OF PREDICTIONS:      0
  tc2.odr OMITTED QUANTITIES:         0
GBOB
  NUMBER OF FLOW-OBSERVATION CELL GROUPS...:       5
  NUMBER OF CELLS IN CELL GROUPS.....:             5
  NUMBER OF CELL FLOWS.....:                       5
  READ tc2.ogb - OK
  tc2.ogb NUMBER OF OBSERVATIONS:     4
  tc2.ogb NUMBER OF PREDICTIONS:      1
  tc2.ogb OMITTED QUANTITIES:         0
  FILE FOR OBSERVATIONS = OB_tc2.ogb
  FILE FOR PREDICTIONS  = PR_tc2.ogb
```

```
PROCESSED ALL OBSERVATION PACKAGES OKAY
   TOTAL NUMBER OF OBSERVATIONS:    52
   TOTAL NUMBER OF PREDICTIONS:      6
   TOTAL OMITTED QUANTITIES:         0
   MAX-ITER=0 IN tc2.pes - CALIBRATION WILL NOT BE COMPLETED.
   STATISTICS WITH RESPECT TO THE PARAMETERS LISTED
   IN THE .SEN FILE WILL BE CALCULATED.
   (NOTE: "OMIT" NOT ACTIVATED FOR PRIOR IN MODPREDICT VERSION-1)

   PES FILE tc2.pes READ - OK

 WRITING OBS FILES
   OBS FILE FOR PES-RUN  - PE_tc2.obs
   OBS FILE FOR OBS-RUN  - OB_tc2.obs
   OBS FILE FOR PRED-RUN - PR_tc2.obs
   WRITTEN OBS FILE(S) FOR OBS-SEN-PES CASE

 PREPARING .NAM FILES FOR OBS-SEN-PES CASE
   NAME FILE FOR OBSERVATIONS ONLY - OB_tc2.NAM
   NAME FILE FOR PREDICTIONS ONLY - PR_tc2.NAM
   MODFLOW .NAM FILES WRITTEN - OK

 DELETING HANGING UNDERSCORE FILES FOR RUNTYPE  3
   DELETING - OUTPUT\OB_tc2._os
   DELETING - OUTPUT\PR_tc2._os
   DELETING - OUTPUT\OB_tc2._ww
   DELETING - OUTPUT\PR_tc2._ww
   DELETING - OUTPUT\OB_tc2._ws
   DELETING - OUTPUT\PR_tc2._ws
   DELETING - OUTPUT\OB_tc2._r
   DELETING - OUTPUT\PR_tc2._r
   DELETING - OUTPUT\OB_tc2._w
   DELETING - OUTPUT\PR_tc2._w
   DELETING - OUTPUT\OB_tc2._nm
   DELETING - OUTPUT\PR_tc2._nm
   DELETING - OUTPUT\OB_tc2._sc
   DELETING - OUTPUT\PR_tc2._sc
   DELETING - OUTPUT\OB_tc2._sd
   DELETING - OUTPUT\PR_tc2._sd
   DELETING - OUTPUT\OB_tc2._s1
   DELETING - OUTPUT\PR_tc2._s1
   DELETING - OUTPUT\OB_tc2._b
 DELETED HANGING UNDERSCORE FILES FOR RUNTYPE  3

 ======================    RUN MODFLOW SIMULATIONS    ======================


 RUNNING OBSERVATIONS-ONLY CASE                  OB_tc2.NAM
 (COMMAND = ..\..\bin\MF2Ksen.exe OB_tc2.NAM > NUL)
  - CHECKING FOR OUTPUT\OB_tc2._sc
  - CHECK RUN OKAY

  - COMPLETED OBSERVATIONS-ONLY CASE             OB_tc2.NAM

 RUNNING PREDICTIONS-ONLY CASE                   PR_tc2.NAM
 (COMMAND = ..\..\bin\MF2Ksen.exe PR_tc2.NAM > NUL)
  - CHECKING FOR OUTPUT\PR_tc2._sc
  - CHECK RUN OKAY

  - COMPLETED PREDICTIONS-ONLY CASE              PR_tc2.NAM
```

```
READING OUTPUT FOR SENSITIVITY RUNTYPE          OB_tc2.NAM
                                                 PR_tc2.NAM
   READING UNDERSCORES FOR   58 OBS-PRED-PRIOR
   FILE OUTPUT\PR_tc2._os READ - OK
   FILE OUTPUT\PR_tc2._ww READ - OK
   FILE OUTPUT\PR_tc2._ws READ - OK
   FILE OUTPUT\PR_tc2._r READ - OK
   FILE OUTPUT\PR_tc2._w READ - OK
   FILE OUTPUT\PR_tc2._nm READ - OK
   FILE OUTPUT\OB_tc2._os READ - OK
   FILE OUTPUT\OB_tc2._ww READ - OK
   FILE OUTPUT\OB_tc2._ws READ - OK
   FILE OUTPUT\OB_tc2._r READ - OK
   FILE OUTPUT\OB_tc2._w READ - OK
   FILE OUTPUT\OB_tc2._nm READ - OK
   ALL OBSERVATION UNDERSCORE FILES READ - OK

   READING UNDERSCORES FOR    9 PARAMETERS
   FILE OUTPUT\PR_tc2._sc READ - OK
   FILE OUTPUT\PR_tc2._sd READ - OK
   FILE OUTPUT\PR_tc2._s1 READ - OK
   FILE OUTPUT\PR_tc2._su READ - OK
   FILE OUTPUT\OB_tc2._sc READ - OK
   FILE OUTPUT\OB_tc2._sd READ - OK
   FILE OUTPUT\OB_tc2._s1 READ - OK
   FILE OUTPUT\OB_tc2._su READ - OK
   ALL SENSITIVITY UNDERSCORE FILES READ - OK

 PROCESSING DATA FOR CALCULATION OF THE PREDICTION CORRELATION MATRIX

   PROCESSED WEIGHTS FOR HEAD OBS

   PROCESSED WEIGHT MATRIX FOR HEAD-DEP. AND ADV OBS

 MATCHING DATA READ FROM UNDERSCORE FILES WITH NAMES/PLOT-SYMBOLS AS
 READ FROM "OBS" FILES.

   ALL OBS/PRIOR/PRED LISTED IN THE MF2K FILES WERE
   FOUND IN "OBS" UNDERSCORE FILES PRODUCED BY MF2K

   ALL OBS/PRIOR/PRED LISTED IN THE MF2K FILES WERE
   FOUND IN "SEN" UNDERSCORE FILES PRODUCED BY MF2K

 PREDICTION CORRELATION MATRIX

            HK_1        HK_2        HK_3        HK_4        ANIV_12     ANIV_3
RCHRAT      ETMAX       C_GHB

.....................................................................................
.........................
 HK_1          1.00      -0.635       0.145       3.494E-03  0.362       5.371E-03 -
0.349       0.917       6.554E-02
 HK_2         -0.635        1.00       0.315       0.198      0.180      -2.164E-02
0.745      -0.470       0.219
 HK_3          0.145       0.315        1.00      -0.115      0.421       9.804E-02
0.241       0.163       0.180
 HK_4          3.494E-03   0.198      -0.115        1.00      1.577E-02   0.226
0.303      -2.184E-03 -5.301E-02
 ANIV_12       0.362       0.180       0.421       1.577E-02   1.00       -0.154      -
0.192       0.363       0.563
 ANIV_3        5.371E-03 -2.164E-02   9.804E-02   0.226      -0.154        1.00      -
0.167      -0.282      -6.684E-02
```

```
 RCHRAT      -0.349       0.745       0.241       0.303      -0.192      -0.167
1.00      -0.107       2.908E-02
 ETMAX        0.917      -0.470       0.163      -2.184E-03  0.363      -0.282      -
0.107        1.00       5.209E-02
 C_GHB        6.554E-02  0.219       0.180      -5.301E-02  0.563      -6.684E-02
2.908E-02   5.209E-02    1.00


 ==================== CALCULATE SET SUMMARY STATISTICS  ====================

 RECORDING CALIBRATION SUMMARY STATISTICS:

 == SUMMARY STATISTICS FOR CALIBRATION SETS ==

 ------------ ---------- ---------- ---------- ---------- ---------- ----------
 SET NAME      UWRES-MAX  UWRES-MIN  UWRES-AVG  NRESGT0    NRESLT0     RES-MAX
 ------------ ---------- ---------- ---------- ---------- ---------- ----------
 ADVECT2      6131.83203 -335.10339 809.865723       4          3    4.08788776
 ------------ ---------- ---------- ---------- ---------- ---------- ----------

 ------------ ---------- ---------- ---------- ---------- ----------
 SET NAME       RES-MIN    RES-AVG    SOSWR       EVP         SE
 ------------ ---------- ---------- ---------- ---------- ----------
 ADVECT2      -1.5661720 .432172954 37.1772881 -1.0000E35 -1.0000E35
 ------------ ---------- ---------- ---------- ---------- ----------

 RECORDING PREDICTION SUMMARY STATISTICS:

 == SUMMARY STATISTICS FOR PREDICTION SETS ==

 ------------ ---------- ---------- ---------- ---------- ----------
 SET NAME     USLARGEST  USSMALLEST USAVERAGE   LARGEST    SMALLEST
 ------------ ---------- ---------- ---------- ---------- ----------
 PREDICT      61439.0586 370.322296 13025.7490 199.535797 .246881500
 GHB          -289.46570 -289.46570 -289.46570 -1.5763330 -1.5763330
 ------------ ---------- ---------- ---------- ---------- ----------

 ------------ ---------- ---------- ---------- ---------- ----------
 SET NAME      AVERAGE   USDIFF-MAX USDIFF-MIN USDIFF-AVG   NGTREF
 ------------ ---------- ---------- ---------- ---------- ----------
 PREDICT      86.3670502 6184.67822 -44324.059 -7716.8760       2
 GHB          -1.5763330 0.00000000 -322.64221 -322.64221       1
 ------------ ---------- ---------- ---------- ---------- ----------

 ------------ ---------- ---------- ---------- ----------
 SET NAME       NLTREF    DIFF-MAX   DIFF-MIN   DIFF-AVG
 ------------ ---------- ---------- ---------- ----------
 PREDICT             3    7.42549992 -29.549370 -2.8688374
 GHB                 0    0.00000000 -1.7570000 -1.7570000
 ------------ ---------- ---------- ---------- ----------


 *INTERPRETING RUN STATISTICS FOR PREDICTION SETS*

The MOD-PREDICT tabulation of summary statistics pertains to
predictions, observations and prior information identified in
the OBS-SEN-PES process input files, and listed as members of
SETS in the "SETS" input file. Statistics are presented for
each SET.  For PREDICTIONS, statistics are of three types:

   ABSOLUTE     - USLARGEST, USSMALLEST, USAVERAGE
                  LARGEST, SMALLEST, AVERAGE
```

```
   DEVIATIONAL - USDIFF-MAX, USDIFF-MIN, USDIFF-AVG
                 DIFF-MAX, DIFF-MIN, DIFF-AVG
   RELATIVE    - NGTREF, NLTREF

This summary table can be used to indicate the deviation of
simulated predictions from reference values. HOWEVER - if
there is no supportable basis for specifying a reference
value, DEVIATIONAL and RELATIVE statistics are meaningless.
THUS use only ABSOLUTE statistics for PREDICTIONS.
(Refer to MOD-PREDICT documentation).

======================       RUN FILES SUMMARY      ========================

 "MAXITER = 0" RUNTYPE OUTPUT FILES
   "MAXITER = 0" RUN OUTPUTS FOR OBSERVATIONS              OUTPUT\OB_tc2.*
   "MAXITER = 0" RUN OUTPUTS FOR PREDICTIONS               OUTPUT\PR_tc2.*

============================ MOD-PREDICT COMPLETE ============================
==============================================================================
```

APPENDIX C. PROGRAM DISTRIBUTION AND INSTALLATION

Distributed Files and Directories

MOD-PREDICT can be downloaded from the Internet site listed in the preface of this report. MODFLOW-2000 VERSION 1.12 or later is needed. Pervious versions did not produce the _su output file needed by MOD-PREDICT. When uncompressed, a directory and four subdirectories listed in table C-1 are created.

Table C- 1. Contents of the subdirectories distributed with MOD-PREDICT.

Subdirectory	Contents
Bin	Contains DOS-compatible executables compiled with Lahey-95
Data	Input and output files for test cases, including the two described in appendix B.
Doc	Documentation in Portable Document Format (PDF).
Source	Source-code files with the extension "f".

Compiling and Linking

If changes to the source code are required, or if MOD-PREDICT will be used with an operating system other than those for which executable files are distributed, the programs need to be compiled. For MOD-PREDICT, all files with the extension ".f" in the "source" directory need to be included in the compilation. The distributed source code is compatible with standard Fortran 90 and Fortran 95, and it complies with the fixed source form, where specific columns are reserved for statement labels, indicator of a continuation line, and Fortran statements. Columns after 72 may be used for comments. The object files created during compilation must be linked to create an executable program. The linker program commonly is invoked as part of the compilation procedure.

Portability

MOD-PREDICT is written in standard Fortran 90. The modular style used is similar to that of previous versions of MODFLOW. Portability is discussed in detail by Harbaugh and others (2000).

Memory Requirements

Dynamic memory allocation is used for all arrays with the exception of the following:

MODPREDICT.F:	OBPAC (10), SUMSTAT (NSETS, 20)
MSUB.F	SUMMARY (18, 2)

APPENDIX D. PROGRAM DESCRIPTION

Variable Names

The names of many of the major variables used in MOD-PREDICT are listed in the text of this report. The variable names presented in table 3 for predictions are defined to provide the user with easy to use terminology. In the MOD-PREDICT program, the variable names listed for observations are used for both observations and predictions.

Listing of Principal MOD-PREDICT Routines

MOD-PREDICT comprises three sets of FORTRAN routines – the main program (MODPREDICT.F); a collection of subroutines for managing files, processing data, and summarizing simulations (MSUB.F); and a collection of utilities to facilitate file reading and writing (MUTIL.F). A summary of these routines is provided in table D-1.

Table D- 1. List of routines in the MOD-PREDICT program

Program File	Description	Routines	Description
MODPREDICT.F	Main Program	MODPREDICT	Main Program
		DRIVER (Module)	Holds some global variables
MSUB.F	Subroutines	SOBS1BAS6WF	Adds head-dependent and advection observation sensitivities to coefficient matrix
		SPES1GAU1IN	Completes inversion of the coefficient matrix
		SPRD1ADV2AL	Reads ADV2 for dimensions
		SPRD1ADV2RP	Reads-writes ADV2 files
		SPRD1DIS1AL	Reads MF2K discretization file for dimensions
		SPRD1HOB1AL	Reads HOB for dimensions
		SPRD1HOB1RP	Reads-writes HOB files
		SPRD1NAM1OPEN	Reads MF2K name files
		SPRD1NAM1WR	Writes MF2K name files
		SPRD1NAM1WR	Writes MF2K name files necessary for MOD-PREDICT analysis
		SPRD1NAM2OPEN	Reads MOD-PREDICT name file
		SPRD1OB1AL	Reads DROB, RVOB, GBOB, CHOB for dimensions
		SPRD1OB1RP	Reads-writes DROB, RVOB, GBOB, CHOB
		SPRD1OBS1AL	Reads OBS Process file
		SPRD1OBS1US	Reads underscore files
		SPRD1OBS1WR	Writes new OBS Process file(s)
		SPRD1PES1AL	Reads PES Process file for dimensions
		SPRD1PES1RP	Reads PES Process file fully
		SPRD1PES1WR	Writes new PES Process file
		SPRD1PRD1RD	Reads MODPREDICT PRD file
		SPRD1PRED1WR	Writes new prediction underscore files
		SPRD1PRI1WR	Calculates/writes CSS for prior information
		SPRD1SEN1AL	Reads SEN Process file for dimensions
		SPRD1SEN1COR	Manages and reports the construction, scaling and inversion of the coefficient matrix
		SPRD1SEN1RP	Reads SEN process file for parameters
		SPRD1SEN1SORT	Sorts and checks sensitivity data
		SPRD1SEN1WR	Writes SEN process file with optimal
		SPRD1SETS1AL	Reads SETS for dimensions
		SPRD1SETS1RP	Reads SETS file fully
		SPRD1SETS1RSS	Records/prints set summary statistics
		SPRD1SETS1SM	Calculates set summary statistics
		SPRD1SETS1VM	Applies MULT-scaling to members of SETS
MUTIL.F	Utilities	*not described*	*not described*