Chapter 3. USER GUIDE TO THE UNC PROCESS

When to Use the UNC Process

If one is confident that a linear confidence or prediction interval will be an accurate approximation for the actual interval, then a parameter confidence interval can be computed by the Parameter-Estimation Process of MODFLOW-2000, and a confidence or prediction interval for dependent variables like hydraulic heads or head-dependent flows can be computed by YCINT-2000. Otherwise the UNC Process should be used with MODFLOW-2000 to compute nonlinear approximations for the confidence or prediction intervals for both parameters and dependent variables.

Significant bias in the model can cause a non-random distribution of residuals. To check residuals for randomness, the graphical procedures described by Cooley and Naff (1990, p. 167-171) can be used. If these analyses show that the residuals do not appear to be random, the model is likely to be biased. In this case the model should be modified in order to better describe the properties and processes of the actual physical system.

To check for a normal distribution of residuals, standard statistical procedures such as the normal probability plot can be used. In this context it is important to note that residuals usually are correlated and have unequal variances because of the regression method (Cooley and Naff, 1990, p. 167-168). Therefore, if residuals analysis indicates that the residuals are correlated and (or) have unequal variances (for example, if the normal probability plot for the weighted residuals does not exhibit a linear trend), a control group should be developed for comparison with the weighted residuals. For this purpose Cooley and Naff (1990, p. 168-170) described a graphical procedure, but it is better to use the measure of weighted residuals correlation and the percentiles computed by the RESAN2-2k program described in this report.

In ground-water modeling whether or not a linear confidence or prediction interval is a good approximation of the actual interval depends on the degree of total nonlinearity of the regression model (also called the total model nonlinearity). If the total model nonlinearity is significant, then linearized methods (of, for example, YCINT-2000) should not be used to compute confidence or prediction intervals, and MODFLOW-2000 with the UNC Process should be used to compute the more accurate nonlinear intervals. However, Cooley (2004, p. 66) has shown that, if model intrinsic nonlinearity and model combined intrinsic nonlinearity both are small, then linear intervals should be good approximations. (See remark near the end of this sub-section on the need to use correction factors for calculation of linear intervals.)

Beale's (1960, p. 54-55) empirical measure of nonlinearity as corrected by Linssen (1975) quantifies the total model nonlinearity. Cooley and Naff (1990) published a code that can be used to compute the modified (corrected) Beale's measure, and Hill (1994) and Hill and others (2000) modified the code of Cooley and Naff (1990) to work with MODFLOWP and

MODFLOW-2000 (termed BEALE-2000), respectively. The present report describes a significantly expanded version called BEALE2-2k that also works with MODFLOW-2000. BEALE2-2k not only computes measures of total model nonlinearity, but also measures of intrinsic and combined intrinsic nonlinearity that are important for the computation of the critical value that is described by equation 86 given in this section. A comparison of the modified Beale's measure of total model nonlinearity with the ranges summarized in chapter 2 will indicate whether or not the regression model is approximately linear. If the model appears to be approximately linear, then linear intervals might not differ much from intervals computed by UNC. However, note from Hill (1994, p. 47) that, if the quantities for which confidence or prediction intervals are to be calculated are very different from the observations used in the regression, then the modified Beale's measure may be an inadequate measure of model linearity. Therefore, if, for example, hydraulic head observations were the only type of data used for nonlinear regression, then linear intervals for model parameters or head dependent flows may not be good approximations of the actual intervals. A better indication than Beale's measure of total model nonlinearity is whether or not the intrinsic nonlinearity and combined intrinsic nonlinearity both are small.

Model intrinsic nonlinearity and model combined intrinsic nonlinearity should be quantified using both RESAN2-2k and BEALE2-2k. If the tests indicate that both types of intrinsic nonlinearity are small, then linear confidence or prediction intervals can be used instead of nonlinear intervals calculated by UNC. However, it must be remembered that correction factors defined by equations 22-24 also must be used to correct the likelihood region from which linear confidence or prediction intervals are calculated. (For individual confidence intervals, $c_c t_{\alpha/2}^2$ should be used instead of $t_{\alpha/2}^2$; for Scheffé type confidence intervals, $c_r F_\alpha(p, n-p)$ should be used instead of $F_\alpha(p, n-p)$; for individual prediction intervals, $c_p t_{\alpha/2}^2$ should be used instead of $t_{\alpha/2}^2$.)

Changes to MODFLOW-2000 to Include the UNC Process

The UNC Process consists of a number of subroutines (called modules in MODFLOW) necessary to compute confidence and prediction intervals by the Vecchia and Cooley (1987) method. UNC subroutines that are called from the MAIN program of MODFLOW-2000 have names that begin with UNC1NLI1. Subroutines called from within the UNC1NLI1 subroutines have names beginning with SUNC1NLI1.

The UNC Process has been incorporated into MODFLOW-2000 by making a few changes to the MAIN program: "UNC" was added to element 50 of the CUNIT array; calls to ten UNC1NLI1 subroutines were added; and calls to OBS1BAS6SS and OBS1BAS6OT are cancelled when the UNC process is active. Minor modifications were made in the following seven MODFLOW-2000 subroutines: OBS1BAS6HAL, OBS1BAS6FAL, OBS1DRN6AL, OBS1DRT1AL, OBS1GHB6AL, OBS1RIV6AL, and OBS1STR6AL. For each of these subroutines two calling arguments were added that have to do with the reading of dependent variables for which confidence or prediction intervals are to be computed. This is explained in the ‘Hydraulic Heads and Head-Dependent Flows’ section.

Activation of the UNC Process

To activate the UNC Process of MODFLOW-2000 the name file must include a short input file of type UNC that contains information necessary for the uncertainty calculations. The input instructions are given in the ‘Input Instructions’ section. When the UNC Process is activated, the Observations (OBS), Sensitivity (SEN), and Parameter-Estimation (PES) Processes also must be activated.

The UNC Process is used for three different actions that should be carried out in the following sequence:

1. Generation of the input file for the CORFAC-2k program.
2. Generation of the input files for the BEALE2-2k program.
3. Computation of the confidence or prediction intervals.

BEALE2-2k (and RESAN2-2k) should be used to study the significance of total nonlinearity, model intrinsic nonlinearity, and model combined intrinsic nonlinearity. The correction factors computed by CORFAC-2k are based on the assumption that both types of intrinsic nonlinearity are small. If testing using BEALE2-2k and RESAN2-2k indicates that this is not the case, then the correction factors computed by CORFAC-2k can be inaccurate. The correction factors are used in action 3. The desired action of UNC is set by the input variable IACT described in the ‘Explanation of Variables in UNC Input File’ section.

Types of Parameter-Dependent Functions For Which Intervals Can Be Computed By the UNC Process

MODFLOW-2000 with the UNC Process can be used to compute confidence or prediction intervals for parameters of the Parameter-Estimation Process, and for most types of predictions that can be computed by a MODFLOW-2000 model calibrated by the Parameter-Estimation Process. The types of predictions for which the package works include hydraulic heads, hydraulic head differences, head-dependent flows computed by various head-dependent flow packages, and differences between flows computed by a flow package. The computation of intervals for the difference between flows computed by two different flow packages is not allowed. The UNC Process is prepared for the head-dependent flow packages for drains (DRN6), rivers (RIV6), general-head boundaries (GHB6), streams (STR6), drain-return cells (DRT1), and constant-head boundaries (CHD).

If MODFLOW-2000 with the UNC Process is used to compute confidence or prediction intervals for predictions, and if the calibration simulation period and/or stresses are different from the prediction simulation period and/or stresses, then MODFLOW-2000 must be set up to run the calibration simulation and the prediction simulation in sequence. (This is for example seen from equation 8 where $g(\boldsymbol{\gamma\theta})$ is the prediction modeled by the prediction simulation and $S(\boldsymbol{\theta})$, which is defined in equation 1, quantifies the fit of the model to the observation data from the calibration period.)

Determination of the Critical Value

As mentioned in chapter 2, a confidence or prediction interval for a parameter-dependent function is defined by two limits, the maximum and minimum values of the function over a likelihood region. Definition of the likelihood region depends on the type of interval being computed. UNC needs an input value that defines the likelihood region for each interval to be computed. This input value is called the critical value and is computed as

$$D_{1-\alpha}^2 = S(\hat{\boldsymbol{\theta}}) + d_{1-\alpha}^2 = S(\hat{\boldsymbol{\theta}}) + \frac{S(\hat{\boldsymbol{\theta}})}{n-p} C\,\Sigma_{n,p,\alpha} = S(\hat{\boldsymbol{\theta}}) \left(1 + \frac{C\,\Sigma_{n,p,\alpha}}{n-p} \right), \tag{86}$$

where $S(\hat{\boldsymbol{\theta}})$ is the weighted sum of squared residuals computed by MODFLOW-2000 using the weighted least-squares estimated parameter values, $\hat{\boldsymbol{\theta}}$; n is the number of observations used to estimate $\hat{\boldsymbol{\theta}}$; p is the number of estimated parameters (the number of elements in $\hat{\boldsymbol{\theta}}$); C is a correction factor explained below; and $\Sigma_{n,p,\alpha}$ is $t_{\alpha/2}^2(n-p)$ for individual confidence and prediction intervals and is $F_\alpha(p, n-p)$ for Scheffé-type confidence intervals.

As described in chapter 2, a correction factor is necessary to correct the likelihood region for intrinsic nonlinearity and for the difference between the inverse of the observation covariance matrix, $\boldsymbol{\Omega}^{-1}$, and the weight matrix, $\boldsymbol{\omega}$, used in the regression to compute the parameter estimates, $\hat{\boldsymbol{\theta}}$. The CORFAC-2k program can be used to compute this correction factor (labeled C in equation 86) assuming that model intrinsic nonlinearity and model combined intrinsic nonlinearity are negligible. For an individual confidence interval the correction factor C is C=c_c; for a Scheffé-type confidence interval, C=c_r; and for an individual prediction interval, C=c_p. The correction factors are defined by equations 22-24, calculated exactly by equations 66, 68, and 70, and approximated by equations 82-84.

Three steps are used to determine whether or not the assumption of negligible model and model combined types of intrinsic nonlinearity is plausible for a specific case. The first step is to use BEALE2-2k to compute measures of intrinsic nonlinearity and combined intrinsic nonlinearity. Use of these measures is explained in the user guide to BEALE2-2k. The second step is to use RESAN2-2k to compute intrinsic nonlinearity test statistics. Use of these statistics is explained in the user guide to RESAN2-2k. The first two steps should be carried out before UNC is used to compute the confidence or prediction interval. If these results indicate that intrinsic nonlinearity and combined intrinsic nonlinearity are insignificant, then the third step is to use MODFLOW-2000 with UNC to compute the confidence or prediction interval with UNC set to print the weighted residuals from the constrained regression. (How to set UNC to do this is explained in the ‘Checking for Intrinsic Nonlinearity Using Weighted Residuals Produced By the UNC Process’ section.) After the computation, the weighted residuals from the constrained regression should be compared with the weighted residuals from the Parameter Estimation Process of MODFLOW-2000. The two sets of weighted residuals should be nearly the same if the intrinsic nonlinearity and combined intrinsic nonlinearity both are negligible. The model intrinsic nonlinearity and model combined intrinsic nonlinearity have been found to be negligible for all the ground-water models the authors have analyzed.

Setting the Starting Values for the Parameters

Starting values for the parameters used in the computation of a limit of a confidence or prediction interval can be specified in two ways. If NIB>0 in the UNC input file, then the starting values also are read as the B2 array from this file. (See the ‘Input Instructions’ section.) Otherwise the starting parameter values equal the values given as B in item 3 of the SEN file.

Normally it is advantageous to use the parameter values estimated by nonlinear regression as starting values for the UNC computations. However, as described in the ‘Searching for the Global Extreme Value’ section, other starting values sometimes may be preferred in a search for a global extreme value.

Setting the Scaling Vector

As discussed in chapter 2, a user-supplied scaling vector is used in the computation of the damping parameter that is used to damp the parameter displacements computed by the Vecchia and Cooley (1987) procedure. If IBSC≠0 in the UNC input file, the scaling vector is read as the BS array from the UNC input file, otherwise the scaling vector is set equal to the starting parameter values given as B in item 3 of the SEN file. Also, if LN>0 for a parameter (in item 3 of the SEN file), then the scaling value is log-transformed. If the scaling value for a parameter equals zero, then UNC automatically sets the scaling value equal to 1.

Searching for the Global Extreme Value

Vecchia and Cooley’s (1987) implementation of the likelihood method is based on the assumption that the set of parameters producing a confidence limit for a parameter-dependent function is located on the edge of the likelihood region. The validity of this assumption was investigated in the field case study of Christensen and Cooley (1996; 1999a) by using the following two-stage approach. First, each confidence limit was computed by using nine different sets of starting parameter values. The starting values were obtained by adding or subtracting as much as two linearized standard deviations to or from the values estimated by nonlinear regression. In the cases tested by Christensen and Cooley (1996; 1999a) the variation of starting values did not produce significant differences in the computed confidence limits for either the parameters or the simulated hydraulic heads. Next, the extreme values corresponding to the confidence limits were searched for inside the likelihood region by reducing the critical value, $D^2_{1-\alpha}$. Reduced critical values were obtained from equation 86 by varying $C\Sigma_{n,p,\alpha}$ between 0 and the theoretical value corresponding to the edge of the likelihood region. In all cases tested by Christensen and Cooley (1996; 1999a) the parameter sets giving the confidence limits were found on the edge of the region.

The UNC Process includes facilities making it easy to search for global extreme values by the described approach. Various starting parameter values can be specified and used to compute interval limits in a single model run. This is done by setting the input value NIB equal to the number of different parameter starting values and by specifying the various starting values in the B2 input array (see 'Input Instructions'). Similarly, interval limits for a parameter-dependent function corresponding to n_c various critical values, $D^2_{1-\alpha}$, can be computed in the same model run by doing the following: (1) Repeat the necessary information about the parameter-dependent function n_c times. For the hydraulic head at a specific point, for example, the MODFLOW-2000 Hydraulic-Head Observations input must be modified so that in item 1 NH is increased by n_c and NHI is set equal to n_c, and so that the list of Hydraulic-Head Observations in item 3 is appended (at the end) by n_c identical records of information for the hydraulic head at the point. (2) Set the value of IDSQ in the UNC input file equal to 1. (3) Set the n_c elements of the DSQ array in the UNC input file equal to the various values of $D^2_{1-\alpha}$.

Addressing Convergence Problems

The studies of Vecchia and Cooley (1987), Christensen and others (1998) and Christensen and Cooley (1996; 1999a) show that convergence problems sometimes occur when computing confidence intervals, even if convergence problems were not observed during the nonlinear regression estimation process. The convergence problems were caused either by parameter correlations or by lack of sensitivity to one or more parameters. Adjusting one parameter manually and computing the others by the regression algorithm often could rectify the problem. This procedure can be invoked automatically by UNC by allowing incremental adjustment of one parameter in an outer iteration loop, while the other parameters are computed in an inner iteration loop by the Vecchia and Cooley (1987) algorithm**.** A guide to how this can be done is given in the following paragraph.

Suppose that the ground-water flow model has NPE estimated parameters, and suppose that a confidence limit cannot be computed within a reasonable number of iterations. If ITPR≠1, then set ITPR to 1 in the UNC input file, and repeat the computation to print the iteration log in the output file. Check the iteration log to see if the convergence problem seems to be caused by a specific parameter or a specific pair of parameters. If this is the case, modify the SEN input file (Hill and others, 2000, p. 72-75) so the problem parameter (or one of the pair) is specified in item 3 as the last parameter with ISENS>0. In the UNC input file specify IMAN, BDEL and TOLDSQ according to the instructions given in 'Explanation of Variables in UNC Input File.' If

IMAN is not equal to 0, then the NPE'th parameter (with ISENS>0) is adjusted incrementally during an outer iteration loop, while the other NPE-1 parameters are computed in an inner iteration loop using the Vecchia and Cooley (1987) algorithm. A confidence or prediction interval cannot be computed in this case for the NPE'th parameter. BDEL is the initial increment by which the NPE'th parameter is changed. The algorithm reduces BDEL when approaching the solution. TOLDSQ is a percentage of deviation from the critical value that is accepted for sufficient convergence of the incremental computation procedure.

When IMAN≠0 and incremental adjustment of one parameter is used, then weighted residuals at the confidence or prediction limit should not be computed, printed, and used to check for model intrinsic nonlinearity and model combined intrinsic nonlinearity. (The reason is that the sensitivity of the NPE'th parameter is not computed when IMAN≠0, and the weighted residuals can therefore not be computed correctly.) To avoid this UNC automatically sets IWRP=0 when IMAN≠0.

Checking for Intrinsic Nonlinearity Using Weighted Residuals Produced By the UNC Process

As described in chapter 2, a comparison of weighted residuals computed by UNC when computing a confidence or prediction limit with the weighted residuals from the unconstrained regression made by MODFLOW-2000 during the Parameter-Estimation Process will indicate whether or not model intrinsic nonlinearity and model combined intrinsic nonlinearity both are small. If the two sets of residuals are nearly equal, it indicates that the two types of intrinsic nonlinearity both are small. If the test on the contrary indicates that model intrinsic nonlinearity and model combined intrinsic nonlinearity may not be small, then the correction factor for the confidence or prediction interval computed by the CORFAC-2k may be inaccurate, which also would make the corresponding computed interval limits inaccurate.

The weighted residuals from the constrained regression are printed to a file when IWRP>0 is specified in the UNC input file described in the 'Input Instructions' section. The weighted residuals are printed to this file for all computed interval limits.

Hydraulic Heads and Head-Dependent Flows

An interval for a hydraulic head computed by the Vecchia and Cooley (1987) method depends on the sensitivity of the hydraulic head to each of the model parameters. An easy way to have MODFLOW-2000 compute these sensitivities is to append information about the hydraulic heads to the list of hydraulic head observations in item 3 of the input to the Head-Observation Package (Hill and others, 2000, p. 38), and to increase NH in item 1 by one. If the OBS and SEN processes are active, the sensitivities are calculated for all hydraulic heads specified in the Head-Observation Package input file. To indicate that the last hydraulic head was not used to estimate the model parameters, but is a head for which an interval is to be computed, the input value of a new fourth variable, NHI, of integer type is appended to item 1 of the Head-Observation Package input file. The input value of NHI in this case must be equal to 1. For the head information appended to item 3, STATISTIC and STAT-FLAG define the weight ω_p used to compute a hydraulic head prediction interval (see equations 17-21), but they are not used for computation of a confidence interval; HOBS is not used for either type of interval.

If intervals are to be computed for more than one hydraulic head, the corresponding information must be appended to item 3 (and, optionally, items 4 through 6), and NH and NHI (and, optionally, MOBS and MAXM) must be changed correspondingly. If intervals are to be computed for differences between hydraulic heads, then the information for the second head of a pair must follow immediately after the information for the first head of the pair. That is, the NH-NHI+1'th and NH-NHI+2'th heads of the input file constitute the first pair, the NH-NHI+3'th and NH-NHI+4'th heads of the input file constitute the second pair, and so on. For the prediction interval of a head difference the weight, ω_p, is computed by UNC as $\omega_p=(\omega_{p1}^{-1}+\omega_{p2}^{-1})^{-1}$, where ω_{p1} and ω_{p2} are the weights defined by STATISTIC and STAT-FLAG in item 3 for each of the heads in the difference, respectively.

If intervals are to be computed for flows (or differences between flows) of one of the head-dependent flow packages, information about these flows is appended similarly to the corresponding flow-observation input file. For example, for an interval for a General-Head Boundary (GHB) flow, the General-Head Boundary Flow Observation input file is modified by increasing NQTGB in item 1 by one, and either a new cell group is created by increasing NQGB in item 1 by one and appending new items 3, 4, and 5, or the last group is enlarged by increasing NQOBGB of the last group's item 3 by one and appending a record of information to the corresponding item 4. If IOWTQGB in item 2 is greater than 0, then the variance-covariance matrix (WTQ) specified in item 7 must be expanded by a line and a column. Because only the diagonal value is used to compute the weight, ω_p, for the added flow (and only for a prediction interval), all off-diagonal values can be set equal to 0. Finally, to indicate that the last input value of flow is not used in the regression but is used for the computation of a confidence or prediction interval, an input value of a new fourth variable, NGHBI, of integer type must be appended to item 1 of the General-Head Boundary Flow Observation input file. The input value of NGHBI for only one GHB flow interval must be equal to 1. If more than one GHB flow interval is to be computed, or if intervals are to be computed for differences between GHB flows, then information must be appended to and changed in the General-Head Boundary Flow Observation input file in a manner similar to that explained for the hydraulic head intervals.

For intervals for head-dependent flows computed by other packages, flow information is appended, values of variables are changed, and input of a fourth variable to item 1 (indicating the number of appended flows that are to be used for computation of confidence or prediction intervals) are appended similarly for the flow observation input file of each of the flow packages. The total number of head-dependent flows used to define variables for which a confidence or prediction interval is computed equals NQI = NGHBI + NDRNI + NRIVI + NSTRI + NCHDI + NDRTI, where NGHBI, NDRNI, NRIVI, NSTRI, NCHDI, and NDRTI are the numbers of appended flows defined in the GHB, DRN, RIV, STR, CHD, and DRT Flow Observation input files, respectively.

Input Instructions

Computation of an upper or lower confidence or prediction limit is similar to the iterative solution of the nonlinear regression problem solved by the Parameter Estimation (PES) Process of MODFLOW-2000. The solution algorithm for interval limits therefore requires input values for variables also used by the solution algorithm of the PES Process. This includes MAX-ITER, MAX-CHANGE, IOSTAR, CSA and information about prior information (Hill and others, 2000, p. 78-83). UNC uses the values for these variables specified in the PES file. Other values important to the solution algorithm of UNC are read from the UNC input file described in the following section.

Instructions for the UNC Input File

Input in addition to that just explained is read from a file that is specified with file type “UNC” in the MODFLOW-2000 name file. Meanings of the following variables are given in the ‘Explanation of Variables in UNC Input File’ section.

0. `[#Text]`
   Item 0 is optional and can include as many lines as desired. Each line needs to begin with the “#” character in the first column.
1. `IACT NPI IDIF ISGN ITYP NIB IOIN IDSQ ITPR IMAN IWRP IBS` (free format)
2. `TOLP TOLS TOLY` (free format)
   If IMAN is not equal to 0, then read item 3.
3. `BDEL TOLDSQ` (free format)
4. `DSQ(1), ... , DSQ(ndsq)` (list directed input)
   If IDSQ is equal to 0 then ndsq = 1. Otherwise ndsq = NHI + NQI + NPI when intervals are for heads and flows, or ndsq = NHI/2 + NQI/2 + NPI when intervals are for head and flow differences. (NHI and NQI are defined in the ‘Hydraulic Heads and Head-Dependent Flows’ section.)
   Read NPI repetitions of item 5.
5. `PARNAM VAR` (list directed input)
   Read NIB repetitions of item 6.
6. `B2(1), B2(2), B2(3), ... , B2(NPLIST)` (list directed input)
   NPLIST is the number of named parameters listed in the Sensitivity Process input file (Hill and others, 2000, p. 72).

If IBS>0 read item 7.

7. `BS(1), BS(2), BS(3), ... , BS(NPLIST)` (list directed input)

If IACT=1 read items 8 and 9.

8. `CFR (free format)`

9. `CFI(1), ... , CFI(ncfi)` (list directed input)

Variable ncfi = NHI + NQI + NPI when intervals are for heads and flows, or ncfi = NHI/2 + NQI/2 + NPI when intervals are for head and flow differences.

Example UNC Input File

```
# Example UNC file
#
 0 4 0 0 1 2 61 0 1 1 0 1 ITEM 1: IACT NPI IDIF ISGN ITYP NIB IOIN
IDSQ ITPR IMAN IWRP IBS
0.01 0.001 0.0            ITEM 2: TOLP TOLS TOLY
 0.1  0.05                ITEM 3: BDEL TOLDSQ
 42.4383                  ITEM 4: DSQ
 RCH_ZONE_1  0.0          ITEMS 5: PARNAM VAR
 RIVERS      0.0
 SS_1        0.0
 VERT_K_CB   0.0
-1.  34.  50.  0.001  0.001  0.4E-3  0.2E-6  0.6E-4  0.5E-4 ITEM 6: B2
-.9  24.  40.  0.002  0.001  0.6E-3  0.3E-6  0.5E-4  0.6E-4 ITEM 6: B2
-1.  34.  50.  0.001  0.001  0.4E-3  0.2E-6  0.6E-4  0.5E-4 ITEM 7: BS
```

In this example RCH_ZONE_1, RIVERS, SS_1, and VERT_K_CB are parameter names that need to be defined in Ground-Water Flow Process input files and need to be listed with ISENS>0 in the Sensitivity Process input file (Hill and others, 2000, p. 72-75). The program matches parameter names among the various input files in a case-insensitive manner. Because IMAN is 1, the last parameter listed with ISENS>0 in the Sensitivity Process input file (not shown here) is incrementally adjusted during the calculation of confidence intervals for RCH_ZONE_1, RIVERS, SS_1, and VERT_K_CB. The incrementally adjusted parameter must therefore not be identical to RCH_ZONE_1, RIVERS, SS_1, and VERT_K_CB as indicated above. (In the example it is thus assumed that more parameters than RCH_ZONE_1, RIVERS, SS_1, and VERT_K_CB have been estimated.)

Explanation of Variables in UNC Input File

Text-----is a character string (maximum of 79 characters) that starts in column 2. Any characters can be included in the text. The “#” character needs to be in column 1. Text is printed when the file is read and provides an opportunity for the user to include information about the model both in the input file and in the associated output file.

IACT---is a flag controlling the action of UNC. For IACT=0 confidence or prediction intervals are computed. For IACT=1 the _b1 and _b3 files for the BEALE2-2k program are generated. For IACT=2 the _b2 and _b4 files for the BEALE2-2k program are generated. For IACT=3 the input file for the CORFAC-2k program is generated.

NPI-----is the number of intervals computed for estimated parameters (NPI≤NPE, where NPE is the number of parameters listed with ISENS>0 in the Sensitivity Process input file).

IDIF----is a flag that controls whether the computed intervals pertaining to heads and flows are for differences of heads and differences of flows (IDIF=1), or for heads and flows (IDIF≠1).

ISGN---is a flag that controls whether only lower limits (ISGN<0), or only upper limits (ISGN>0), or both lower and upper limits (ISGN=0) are computed for the intervals.

ITYP---is a flag that controls whether confidence intervals (ITYP≠2) or prediction intervals (ITYP=2) are computed.

NIB-----is the number of sets of parameter values (B2) to be read and used as starting parameter values for the computation of each limit of all confidence or prediction intervals.

IOIN----is the unit number of an output file defined in the MODFLOW-2000 name file to be used for summary output of computed confidence or prediction limits. No other output should be directed to this file. If IOIN<2, no output summary is written; output is written only in the GLOBAL and/or LIST output files of MODFLOW-2000 (Harbaugh and others, 2000, p. 6-7).

IDSQ---is a flag that controls whether the same critical value is to be used for the computation of all confidence or prediction intervals (IDSQ=0), or if individual critical values are to be read and used for calculation of each confidence or prediction interval (IDSQ≠0).

ITPR----is a flag that controls the printing of information from iterations to the screen and to the LIST output file. If ITPR = 1 data from each iteration is printed; otherwise it is not.

IMAN---is a flag that controls when the intervals are computed by an approximate procedure where one parameter is computed by incremental adjustment in an outer iteration loop, while the other parameters are computed in an inner iteration loop by the Vecchia and Cooley (1987) algorithm. The incrementally adjusted parameter is the last parameter listed with ISENS>1 in the Sensitivity-Process input file (Hill and others, 2000, p. 72-75). The approximate procedure is used when IMAN≠0.

IWRP---is a flag that controls the printing of weighted residuals. If IWRP>0, they are printed in an output file defined in the MODFLOW-2000 name file with the unit number being equal to IWRP. If IMAN≠0, IWRP is automatically set equal to 0, and the weighted residuals will not be printed. When IWRP>0 then a scratch file with the unit number equal to IWRP+1 is generated automatically by the program. Other files used by the program must not use this unit number.

IBS------is a flag that controls setting the scaling values used in each iteration to compute the damping parameter used in equation 16. If IBSC≠0, the scaling vector, BS, is read as item 6 of the UNC input file, otherwise BS is set equal to the starting parameter values given as B in item 3 of the Sensitivity Process input file (Hill and others, 2000, p. 72-75).

TOLP----is the convergence criterion for the fractional parameter change. Convergence is achieved when $|t_{r+1}| = \max_j \left|\delta_j^{r+1} / BS_j\right| <$ TOLP, where δ_j^{r+1} is the computed change for parameter j and BS_j is the scaling value for the parameter.

TOLS----is the convergence criterion for the change of the objective function over two iterations. Convergence is achieved when $|S(\boldsymbol{\theta}_{r+1}) - S(\boldsymbol{\theta}_r)|/S(\boldsymbol{\theta}_r) + |S(\boldsymbol{\theta}_r) - S(\boldsymbol{\theta}_{r-1})|/S(\boldsymbol{\theta}_{r-1}) <$ TOLS. A value of one tenth of TOLP has often been found to work well.

TOLY---is the convergence criterion for the change of the value of the computed confidence or prediction limit. Convergence is achieved when $|2 \times (g(\gamma\boldsymbol{\theta}_{r+1}) - g(\gamma\boldsymbol{\theta}_r))/(g(\gamma\boldsymbol{\theta}_{r+1}) + g(\gamma\boldsymbol{\theta}_r))| <$ TOLY. This criterion is not applied to check for convergence of incremental parameter adjustment when IMAN≠0.

BDEL---is the initial increment by which the NPE'th parameter is changed when IMAN≠0. The algorithm reduces BDEL when approaching the solution.

TOLDSQ—is a percentage of deviation from the critical value that is accepted for sufficient convergence of the incremental computation procedure.

DSQ-----is the critical value (equal to $D_{1-\alpha}^2$ in equation 86) that determines the size of the likelihood region on the edge of which it is assumed that parameter sets producing maximum and minimum limits of a confidence or prediction interval are found.

PARNAM—is a set of parameter names. The names also must be specified in the Sensitivity Process input file and have values of ISENS>0.

VAR-----is a value that defines the weight, $\hat{\omega}_p$ = VAR^{-1}, which is used to compute the prediction interval for the parameter (see equations 80-84). VAR is not used for the computation of a confidence interval, but a value must still be specified (for example 0). If the parameter was log-transformed during the Parameter-Estimation Process, VAR must be specified for the $\log_{10}$-transformed parameter value.

B2-------is a set of parameter values used as starting values for the computation of confidence and prediction intervals. The specified values must not be log-transformed because this is done internally when necessary. If more sets (as specified by NIB) are read, then each interval is computed NIB times, each time using a different set of B2 as starting parameter values. If NIB=0, then B2 is automatically set equal to values given as B in item 3 of the Sensitivity Process input file (Hill and others, 2000, p. 72-75).

BS-------is the scaling vector used in the computation of the damping parameter used in equation 16. The scaling vector adjusts for differing sizes of elements of the parameter vector (defined as item 3 of the Sensitivity Process input file; Hill and others, 2000, p. 72-75) and should reflect the user's best knowledge of the parameter values. For a log-transformed parameter (with LN>0 in item 3 of the Sensitivity Process input file), the scaling value is log-transformed internally by UNC. If the (possibly log-transformed) scaling value equals zero, then UNC automatically sets the scaling value equal to 1.

CFR-----is the correction factor for the confidence region used to generate the _b1 and _b2 input files for the BEALE2-2k program when IACT equals 1. These input files are used by BEALE2-2k to compute measures of total model nonlinearity and model intrinsic nonlinearity. If $\text{CFR} = F_\alpha(p, n-p)$, then the generated _b1 and _b2 files will be identical to the corresponding files generated by MODFLOW-2000 for BEALE-2000.

CFI------are correction factors for confidence intervals used to generate the _b3 and _b4 input files for the BEALE2-2k program when IACT equals 1. These input files are used by BEALE2-2k to compute model combined intrinsic nonlinearity measures.