USER GUIDE TO THE UNC PROCESS AND THREE UTILITY PROGRAMS FOR COMPUTATION OF NONLINEAR CONFIDENCE AND PREDICTION INTERVALS USING MODFLOW-2000

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PREFACE

This report introduces and documents the Uncertainty (UNC) Process, which is a new Process in MODFLOW-2000 that can be used to compute regression-based 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 report also documents three programs, RESAN2-2k, BEALE2-2k, and CORFAC-2k that are valuable for the evaluation of results from the Parameter-Estimation Process and for the preparation of input values for the UNC Process. The performance of the programs has been tested in a variety of applications; however, there may be 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 user guide by using the address on the back of the report title page. Updates might occasionally be made both to the user guide and to the programs. Users can check for updates on the Internet at URL http://water.usgs.gov/software/ground_water.html/.

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USER GUIDE TO THE UNC PROCESS AND THREE UTILITY PROGRAMS FOR COMPUTATION OF NONLINEAR CONFIDENCE AND PREDICTION INTERVALS USING MODFLOW-2000

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Abstract

This report introduces and documents the Uncertainty (UNC) Process, a new Process in MODFLOW-2000 that calculates uncertainty measures for model parameters and for predictions produced by the model. Uncertainty measures can be computed by various methods, but when regression is applied to calibrate a model (for example when using the Parameter-Estimation Process of MODFLOW-2000) it is advantageous to also use regression-based methods to quantify uncertainty. For this reason the UNC Process computes (1) confidence intervals for parameters of the Parameter-Estimation Process and (2) confidence and prediction intervals for most types of functions that can be computed by a MODFLOW-2000 model calibrated by the Parameter-Estimation Process. The types of functions for which the Process works include hydraulic heads, hydraulic head differences, head-dependent flows computed by 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), and for differences between flows computed by any of the mentioned flow packages. The UNC Process does not allow computation of intervals for the difference between flows computed by two different flow packages.

The report also documents three programs, RESAN2-2k, BEALE2-2k, and CORFAC-2k, which are valuable for the evaluation of results from the Parameter-Estimation Process and for the preparation of input values for the UNC Process. RESAN2-2k and BEALE2-2k are significant updates of the residual analysis and modified Beale's measure programs first published by Cooley and Naff (1990) and later modified for use with MODFLOWP (Hill, 1994) and MODFLOW-2000 (Hill and others, 2000). CORFAC-2k is a new program that computes correction factors to be used by UNC.

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Chapter 1. INTRODUCTION

Ground-water models almost never perfectly represent real systems or fit the data used for their calibration. This results in uncertainties in both estimates of parameters and predictions of model-related variables. The uncertainty of estimated parameters and predicted variables can be quantified by using either confidence or prediction intervals. However, computation of such intervals is not straightforward because model-computed hydraulic heads and quantities such as flows that are functions of hydraulic heads generally are nonlinear functions of the model parameters.

Vecchia and Cooley (1987) and Clark (1987) independently derived similar methodologies that can be used for the computation of confidence and prediction intervals for both the estimated parameters and the output from a nonlinear regression model with normally distributed observation errors. Vecchia and Cooley (1987) showed that the same computer program can be used both to estimate the parameters by nonlinear regression and to compute confidence limits from which the desired confidence intervals are obtained. Computation of each confidence limit is a separate optimization problem in which the limit is obtained as an extreme value on the edge of the parameter likelihood region. Beven and Binley (1992) and Brooks and others (1994) presented methods that are similar in intent to the method of Vecchia and Cooley (1987). For brevity we will term confidence intervals computed using the nonlinear regression model as nonlinear confidence intervals.

The nonlinear regression model can be linearized using a first-order Taylor series expansion. Confidence intervals computed using the linearized model are the standard ones found in most regression texts (for example, Seber and Wild, 1989, chapter 5) and are termed here linear confidence intervals. Hill (1994) presented two computer codes, BCINT and YCINT, that can be used to compute linear confidence intervals for parameters and linear confidence and prediction intervals for hydraulic heads and flows from MODFLOWP. Hill and others (2000) developed YCINT-2000 as a modification of YCINT to be used with MODFLOW-2000 to compute confidence and prediction intervals for hydraulic heads and flows; linear confidence intervals for the parameters are computed by MODFLOW-2000 at the end of the Parameter-Estimation Process.

Synthetic case studies (Cooley and Vecchia, 1987; Vecchia and Cooley, 1987; Hill, 1989; and Cooley, 1993a, b) show the following. Corresponding linear and nonlinear confidence intervals often are offset, and the nonlinear intervals generally are larger (Hill, 1989; Cooley, 1993b); the variability in sizes of nonlinear confidence intervals generally is larger than the variability in sizes of corresponding linear confidence intervals (Hill, 1989; Cooley, 1993b); the differences between the sizes of corresponding nonlinear and linear confidence intervals increase as the sizes of the intervals increase (Cooley, 1993a); and use of prior information can have a significant effect on the sizes of confidence intervals (Cooley, 1993b). Field case studies (Christensen and Cooley, 1996; Christensen and others 1998; and Christensen and Cooley, 1999a) support the conclusions from the synthetic studies. However, the studies of Christensen and Cooley (1996; 1999a) show that linear confidence intervals sometimes are larger than the corresponding nonlinear intervals.

Donaldson and Schnabel (1987) and Cooley (1997) present synthetic case studies that investigate the coverage probability of nonlinear confidence intervals as well as of linear confidence intervals. In the studied cases the coverage probability of nonlinear confidence intervals is correct, whereas the coverage probability of corresponding linear confidence intervals often is incorrect.

Christensen and Cooley (1999b) tested the accuracy of 95 percent individual prediction intervals for hydraulic heads, streamflow gains, and effective transmissivities computed by ground-water models of two Danish aquifers. An individual prediction interval is for a random variable $Y_p = g(\boldsymbol{\beta}) + \varepsilon_p$, where $g(\boldsymbol{\beta})$ is a model-related variable (for example, hydraulic head, flux, or a model parameter), and ε_p is a normally distributed error that is a composite of small-scale model error and other errors including measurement errors. Small-scale model errors result from smaller-scale variability in geology and hydrology than those represented in the model. Such errors often are significant in ground-water modeling because the model commonly is constructed using model parameters that represent only important, or large-scale, geologic and hydrologic features. Christensen and Cooley (1999b) tested the accuracy of the prediction intervals by a cross-validation method and by comparing new field measurements, which were not used to develop or calibrate the models, to corresponding prediction intervals. They concluded that for the ground-water models of the two real aquifers the linear as well as the nonlinear individual prediction intervals appear to be accurate. However, their results indicate that for the predicted values of streamflow gains some of the nonlinear prediction intervals may be conservative without using a correction factor. In a somewhat similar study Hamilton and Wiens (1987) found that for a confidence interval the correction factor can be either larger or smaller than unity.

Inspired by the experiences from the previously mentioned studies, Cooley (2004) developed and tested a regression theory for modeling ground-water flow in heterogeneous systems. The theory addresses the small-scale model error that usually is present in ground-water models of heterogeneous systems where the model only uses average system characteristics having the same form as the drift. Important aspects of the theory are summarized and further tested by Christensen and Cooley (2003) and Cooley and Christensen (written communication, 2003). Cooley (2004) showed, among other things, that small-scale model error can result in significant correlations among the true errors of the regression model; that the model error often contributes bias in estimated model parameters, whereas predictions of hydraulic head often are unbiased; that the statistic used to compute a confidence or prediction interval often should be multiplied by a correction factor that depends on covariances and interrelations among all of the types of system characteristics that give rise to model parameters. The synthetic case studies by Cooley (2004), Christensen and Cooley (2003), and Cooley and Christensen (written communication, 2003) show that correction factors for confidence intervals can be very large, whereas the correction factors for prediction intervals appear to be relatively close to one.

The results of Cooley (1997), Christensen and Cooley (2003), Cooley and Christensen (written communication, 2003), and Cooley (2004) strongly indicate that linear confidence intervals for estimated parameters and predictions of ground-water flow models may be inaccurate in many cases, whereas corresponding nonlinear confidence intervals seem to be correct or nearly correct in at least the synthetic cases without small-scale model error. Nonlinear prediction intervals seem to be correct for the field cases. This motivated development of the Uncertainty (UNC) Process (or simply UNC for simplicity) that can be incorporated into MODFLOW-2000 (Harbaugh and others, 2000) and can be used to compute nonlinear confidence and prediction intervals for any model parameter and for most types of data that can be used as regression data by MODFLOW-2000 (hydraulic head, differences between hydraulic heads, head dependent flow, and differences between head-dependent flows). UNC implements the computation method of Vecchia and Cooley (1987) into MODFLOW-2000.

Use of UNC is intended to be straightforward and flexible. This is accomplished by minimizing the amount of extra input needed for the computation of intervals compared to the input needed by MODFLOW-2000 for parameter estimation. Options have been added to facilitate the search for a global extreme value within the likelihood region (corresponding to the upper or lower limit of a confidence or prediction interval), and so convergence problems resulting from parameter correlations can sometimes be avoided. Any number and any type of confidence or prediction intervals can be computed in the same run. The output from UNC is similar to the output from the Parameter-Estimation Process of MODFLOW-2000. However, the results from the computation of interval limits also can be summarized in a separate easy-to-overview output file.

The procedures used by the UNC Process to compute nonlinear confidence and prediction intervals assume the model errors to be random and normally distributed. Whether or not this is the case is indicated by residuals analysis. The work of Cooley (2004) and Cooley and Christensen (written communication, 2003) indicate that some deviation from these ideals can be tolerated. The graphical procedures by Cooley and Naff (1990, p. 167-171) together with the results produced by the RESAN2-2k program are valuable for the analysis. Intrinsic nonlinearity also is assumed to be small for the UNC Process. Whether or not this may be the case can be investigated by using the RESAN2-2k and BEALE2-2k programs and by analyzing weighted residuals computed by UNC.

Purpose and Scope

This report introduces and documents the UNC Process, which is a new Process in MODFLOW-2000 that calculates uncertainty measures for model parameters and for predictions produced by the model. Uncertainty measures can be computed by various methods, but when regression is applied to calibrate a model (for example, when using the Parameter-Estimation

Process of MODFLOW-2000), it is advantageous to also use regression-based methods to quantify uncertainty. For this reason the UNC Process computes (1) confidence intervals for parameters of the Parameter-Estimation Process and (2) confidence and prediction intervals for most types of functions that can be computed by a MODFLOW-2000 model calibrated by the Parameter-Estimation Process. The report also documents two programs, RESAN2-2k and BEALE2-2k, that are valuable for the evaluation of results from the Parameter-Estimation Process and a third program, CORFAC-2k, that computes correction factors, including approximations that require minimal geostatistical information, for UNC. The theory behind UNC and the RESAN2-2k, BEALE2-2k, and CORFAC-2k programs is summarized in chapter 2 and appendixes A and B. (For a thorough description the reader is referred to Cooley, 2004.) Guidance in application of, and input instructions for, the programs are given in chapters 3 to 6. Appendix C includes input and output files for an example problem. Source files for MODFLOW-2000 (including the programs documented in this report) are available at the Internet address listed in the preface of the report.

Users of this report need to be familiar with the Ground-Water Flow Process as well as the Observation, Sensitivity, and Parameter-Estimation Processes of MODFLOW-2000. The Ground-Water Flow Process is described by Harbaugh and others (2000), and the three other Processes are described by Hill and others (2000). The user also should be familiar with basic statistics and the application of nonlinear regression. The book by Cooley and Naff (1990) discusses these subjects with the focus on application in ground-water modeling.

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Chapter 2. THEORY

The modeling concepts and terminology described in the this section have been more thoroughly described by Cooley (2004) and Christensen and Cooley (2003).

A ground-water flow system can be characterised by hydrogeologic variables (termed system characteristics) such as hydraulic head, hydraulic conductivity, recharge, discharge, hydraulic heads and fluxes along internal and external boundaries, and point sources and sinks. In a model these system characteristics can be conceptualized as being discretely variable (in space and/or time) because discrete variation can be at as small a scale as desired (depending only on model discretization), allowing it to be virtually the same as continuous variation. All of these system characteristics can be assembled into an m-vector $\boldsymbol{\beta}$. Because $\boldsymbol{\beta}$ includes all scales of variation necessary to construct an accurate model, any model function of $\boldsymbol{\beta}$ is almost free of model error, assuming that the model accurately represents the physical processes.

Seen from a practical modeling perspective, vector $\boldsymbol{\beta}$ represents small-scale variability that cannot be explicitly represented in a model and larger scale variability (the drift) that can. In addition, vector $\boldsymbol{\beta}$ is unknown. Because $\boldsymbol{\beta}$ has much too large a dimension to be estimated from a small number of uncertain observations, the vector of model parameters to be estimated is reduced from one of large dimension, $\boldsymbol{\beta}$, to one of much smaller dimension, $\boldsymbol{\theta}_*$. The p-vector $\boldsymbol{\theta}_*$ represents the spatial and temporal average of $\boldsymbol{\beta}$ and has the same form as the drift $\overline{\boldsymbol{\theta}}$; it does not represent the small-scale variation. A model function $f(\boldsymbol{\beta})$, which contains large- and small-scale variation from $\boldsymbol{\beta}$, is represented in terms of $\boldsymbol{\theta}_*$ as $f(\boldsymbol{\gamma\theta}_*)$, where $\boldsymbol{\gamma}$ is an $m \times p$ interpolation or averaging matrix.

In ground-water modeling we are interested in estimating $\boldsymbol{\theta}_*$ rather than $\overline{\boldsymbol{\theta}}$ because $\boldsymbol{\theta}_*$ characterizes the actual realization $\boldsymbol{\beta}$. An estimate of $\boldsymbol{\theta}_*$, $\hat{\boldsymbol{\theta}}$, can be found by minimizing

$$S(\boldsymbol{\theta}) = \left(\boldsymbol{Y} - \boldsymbol{f}(\boldsymbol{\gamma\theta})\right)' \boldsymbol{\omega}\left(\boldsymbol{Y} - \boldsymbol{f}(\boldsymbol{\gamma\theta})\right), \tag{1}$$

where $\boldsymbol{Y}$ is an n-vector of observations (m>>n>p), $\boldsymbol{f}(\boldsymbol{\gamma\theta})$ is the corresponding n-vector of values simulated using general vector $\boldsymbol{\gamma\theta}$ instead of $\boldsymbol{\beta}$, $\boldsymbol{\omega}$ is an $n \times n$ weight matrix, and the prime indicates transpose.

Predictions can be made with the ground-water model. In practice, variables of interest $g(\boldsymbol{\beta})$ are predicted by $g(\boldsymbol{\gamma}\hat{\boldsymbol{\theta}})$.

Different types of observations, $\boldsymbol{Y}$, can be used in the Parameter Estimation Process. Cooley (2004) does not distinguish among the several possible types of observations such as hydraulic heads, measured streamflow gains and losses, measured spring and well discharges, and measured direct (often called "prior") information on model parameters. It is convenient to divide the types of information into two groups: (1) measured direct observations of parameters or linear combinations of them and (2) observations corresponding to model functions of the parameters such as hydraulic heads and fluxes. The various matrices and vectors pertaining to observations have a subscript d for the partition of direct information and a subscript m for the partition for model-function information. Corresponding to this notation, the number of direct observations is designated n_d and the number of model-function observations is designated n_m, for a total of $n_d+n_m=n$ observations. The matrices and vectors are used in the partitioned form in an equation only when the form of the result for each partition is different. The difference is caused by the forms of the observation second-moment matrix, $\boldsymbol{\Omega}\sigma_\varepsilon^2 = E(\boldsymbol{Y} - \boldsymbol{f}(\gamma\boldsymbol{\theta}_*))(\boldsymbol{Y} - \boldsymbol{f}(\gamma\boldsymbol{\theta}_*))'$, and the weight matrix, $\boldsymbol{\omega}$, used as an approximation for $\boldsymbol{\Omega}^{-1}$ in the weighted regression analysis. As in standard regression analysis, σ_ε^2 is a generally unknown scalar multiplier that is estimated by the regression. We assume that the partition of the observation second-moment matrix for the model functions depends on an unknown model error and often may not be known, but that the partition for the direct information would be well estimated using the same techniques used to acquire the direct information. We also assume that the two partitions are not correlated. (This is a standard assumption dating back to Theil (1963). Should it prove to be inaccurate in any application, the correction factors computed by CORFAC-2k will be somewhat in error. If $n_d \ll n_m$, the errors should be small.) Thus, the forms for $\boldsymbol{\Omega}$ and $\boldsymbol{\omega}$ are

$$\boldsymbol{\Omega} = \begin{bmatrix} \boldsymbol{\Omega}_m & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{\Omega}_d \end{bmatrix}, \tag{2}$$

where $\boldsymbol{0}$ is a matrix of zeros, and

$$\boldsymbol{\omega} = \begin{bmatrix} \boldsymbol{\omega}_m & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{\Omega}_d^{-1} \end{bmatrix}. \tag{3}$$

The partitioning also can be used for the $n \times n$ matrix $\boldsymbol{R}$ defined as

$$\boldsymbol{R} = \boldsymbol{\omega}^{1/2}\boldsymbol{Df}\left(\boldsymbol{Df}'\boldsymbol{\omega}\boldsymbol{Df}\right)^{-1}\boldsymbol{Df}'\boldsymbol{\omega}^{1/2} = \begin{bmatrix} \boldsymbol{R}_m & \boldsymbol{R}_{md} \\ \boldsymbol{R}_{dm} & \boldsymbol{R}_d \end{bmatrix} \tag{4}$$

in which $\boldsymbol{Df}$ is the $n \times p$ sensitivity matrix of derivatives of $\boldsymbol{f}$ with respect to $\boldsymbol{\theta}$,

$$\boldsymbol{Df} = \left[\frac{\partial f_i}{\partial \theta_j}\right] \tag{5}$$

theoretically evaluated at the drift set of parameters $\bar{\boldsymbol{\theta}} = E\left(\boldsymbol{\theta}_*\right)$, and

$$\left.\begin{aligned} \boldsymbol{R}_m &= \boldsymbol{\omega}_m^{1/2}\boldsymbol{Df}_m\left(\boldsymbol{Df'\omega Df}\right)^{-1}\boldsymbol{Df}_m'\boldsymbol{\omega}_m^{1/2} \\ \boldsymbol{R}_{md} &= \boldsymbol{\omega}_m^{1/2}\boldsymbol{Df}_m\left(\boldsymbol{Df'\omega Df}\right)^{-1}\boldsymbol{Df}_d'\boldsymbol{\omega}_d^{1/2} \\ \boldsymbol{R}_{dm} &= \boldsymbol{\omega}_d^{1/2}\boldsymbol{Df}_d\left(\boldsymbol{Df'\omega Df}\right)^{-1}\boldsymbol{Df}_m'\boldsymbol{\omega}_m^{1/2} \\ \boldsymbol{R}_d &= \boldsymbol{\omega}_d^{1/2}\boldsymbol{Df}_d\left(\boldsymbol{Df'\omega Df}\right)^{-1}\boldsymbol{Df}_d'\boldsymbol{\omega}_d^{1/2} \end{aligned}\right\}, \qquad (6)$$

where $\boldsymbol{f}_m$ and $\boldsymbol{f}_d$ are model-function and direct-information partitions of $\boldsymbol{f}$, and $\boldsymbol{D}(\ldots)$ is the derivative operator applied as in equation 5 to yield the $n_m \times p$ and the $n_d \times p$ matrices $\boldsymbol{Df}_m$ and $\boldsymbol{Df}_d$. Similar partitioning is used for the n-vector $\boldsymbol{Q}$, defined as

$$\boldsymbol{Q} = \boldsymbol{\omega}^{1/2}\boldsymbol{Df}\left(\boldsymbol{Df'\omega Df}\right)^{-1}\boldsymbol{D}g' = \begin{bmatrix} \boldsymbol{\omega}_m^{1/2}\boldsymbol{Df}_m\left(\boldsymbol{Df'\omega Df}\right)^{-1}\boldsymbol{D}g' \\ \boldsymbol{\omega}_d^{1/2}\boldsymbol{Df}_d\left(\boldsymbol{Df'\omega Df}\right)^{-1}\boldsymbol{D}g' \end{bmatrix} = \begin{bmatrix} \boldsymbol{Q}_m \\ \boldsymbol{Q}_d \end{bmatrix}, \qquad (7)$$

where $\boldsymbol{D}g' = \left[\partial g/\partial\theta_i\right]$ is the column p-vector of sensitivities of the prediction $g(\boldsymbol{\gamma\theta})$.

The UNC Process described in 'The UNC Process' section can be used to compute confidence or prediction intervals for parameters ($\hat{\boldsymbol{\theta}}$) of the Parameter-Estimation Process, and for most types of predictions ($g(\boldsymbol{\gamma\theta}_*)$ or $g(\boldsymbol{\beta})+\varepsilon$ where ε is a random observation error) that can be computed by a MODFLOW-2000 model calibrated by the Parameter-Estimation Process. The programs RESAN2-2k, BEALE2-2k, and CORFAC-2k that also are described in this report are valuable in the evaluation of results from the Parameter-Estimation Process and in the preparation of input values for UNC.

The UNC Process

The purpose of UNC is to compute confidence and prediction intervals for variables of the form $g(\boldsymbol{\gamma\theta}_*)$. Both the model functions $f(\boldsymbol{\gamma\theta}_*)$ and predictions $g(\boldsymbol{\gamma\theta}_*)$ can be nonlinear, and the intervals can be individual, Scheffé type, or, with correction factors not given in this report, other simultaneous types (Hill, 1994, p. 26-33). Calculation procedures are the same for all types of confidence intervals and for all types of prediction intervals; only the critical values described after equation 8 are different. Extensive information on the theory, calculation procedures, and use of confidence and prediction intervals can be found in Graybill (1976, chapters 6-10), Seber and Wild (1989, chapter 5), Hill (1994, p. 26-37), Cooley and Vecchia (1987), Vecchia and Cooley (1987), Cooley (1997), Christensen and Cooley (1999a, b), Cooley and Naff (1990, chapter 5), and Cooley (2004). Cooley (2004) summarizes much of the information found in the other references.

Confidence Intervals

A confidence interval for $g(\boldsymbol{\gamma\theta}_*)$ is defined by two confidence limits, the maximum and minimum values of $g(\boldsymbol{\gamma\theta})$ over a likelihood region. The definition of the region depends on the type of confidence interval being computed. For example, for a Scheffé interval the likelihood region is the standard confidence region given in terms of $S(\hat{\boldsymbol{\theta}})$, and for an individual confidence interval the likelihood region is of the same form but has a smaller diameter (Cooley, 2004, p. 53). If we assume that the maximum and minimum values of $g(\boldsymbol{\gamma\theta})$ occur on the boundary of the likelihood region as they do for linear problems, then these extreme values can be found using the method of Lagrange multipliers (Vecchia and Cooley, 1987). Cooley (1999, p. 118) states that this assumption is almost non-restrictive; the assumption has never been violated in any of the calculations made by the authors of this report. Therefore, confidence and prediction intervals computed by the UNC Process are based on the method of Lagrange multipliers.

A $(1-\alpha)\times 100$ percent confidence interval is computed by finding extreme values (the confidence limits) of the Lagrange function

$$L(\boldsymbol{\theta},\lambda) = g(\boldsymbol{\gamma\theta}) + \frac{1}{2\lambda}\left(d_\alpha^2 - S(\boldsymbol{\theta}) + S(\hat{\boldsymbol{\theta}})\right), \tag{8}$$

where λ^{-1} is the Lagrange multiplier and d_α^2 is the critical value that depends on the type of confidence interval being computed. For an individual confidence interval $d_\alpha^2 = c_c t_{\alpha/2}^2\, S(\hat{\boldsymbol{\theta}})/(n-p)$ and for a Scheffé interval $d_\alpha^2 = c_r F_\alpha(p, n-p) S(\hat{\boldsymbol{\theta}})/(n-p)$. Here c_c and c_r are correction factors defined in 'The RESAN2-2k Program' section, $t_{\alpha/2}$ is the $(1-\alpha/2)\times 100$ percentile of the cumulative *t* distribution, $F_\alpha(p, n-p)$ is the upper α point of the *F* distribution with *p* and $n-p$ degrees of freedom, *p* is the number of model parameters, and *n* is the total number of observations used to estimate $\hat{\boldsymbol{\theta}}$. Theoretically, the equations to compute extreme values are obtained simply by taking the derivatives of $L(\boldsymbol{\theta},\lambda)$ with respect to $\boldsymbol{\theta}$ and λ^{-1}, then setting the results to zero. However, this yields a set of nonlinear equations to be solved whenever $g(\boldsymbol{\gamma\theta})$ or $\boldsymbol{f}(\boldsymbol{\gamma\theta})$ (or both) are nonlinear. Another method was developed by Vecchia and Cooley (1987) and involves linearizing the nonlinear functions $g(\boldsymbol{\gamma\theta})$ and (or) $\boldsymbol{f}(\boldsymbol{\gamma\theta})$ first, then taking the derivatives of $L(\boldsymbol{\theta},\lambda)$ and setting the results to zero. The resulting linear system of equations then can be written to yield an iterative solution to the nonlinear problem. The iterative solution is derived in appendix A; the solution $\boldsymbol{\theta}_{r+1}$ at iteration *r*+1 is given in terms of quantities computed at iteration *r* as

$$\lambda_{r+1} = \pm\left(\frac{d_\alpha^2 - S(\boldsymbol{\theta}_r) + S(\hat{\boldsymbol{\theta}}) + (\boldsymbol{Y} - \boldsymbol{f}(\boldsymbol{\gamma\theta}_r))'\boldsymbol{\omega}^{1/2}\boldsymbol{R}_r\boldsymbol{\omega}^{1/2}(\boldsymbol{Y} - \boldsymbol{f}(\boldsymbol{\gamma\theta}_r))}{\boldsymbol{Q}_r'\boldsymbol{Q}_r}\right)^{1/2} \tag{9}$$

and

$$\boldsymbol{\theta}_{r+1} = \boldsymbol{\theta}_r + \lambda_{r+1}(\boldsymbol{Df}_r'\boldsymbol{\omega}\boldsymbol{Df}_r)^{-1}\boldsymbol{D}g_r' + (\boldsymbol{Df}_r'\boldsymbol{\omega}\boldsymbol{Df}_r)^{-1}\boldsymbol{Df}_r'\boldsymbol{\omega}(\boldsymbol{Y} - \boldsymbol{f}(\boldsymbol{\gamma\theta}_r)), \tag{10}$$

where subscript *r* indicates evaluation using parameter set $\boldsymbol{\theta}_r$ and $\boldsymbol{\theta}_0$ is the initial, user supplied, set. Use of the positive sign in equation 9 yields the maximum and use of the negative sign yields the minimum. At convergence of the process $\boldsymbol{\theta}_r \approx \boldsymbol{\theta}_{r+1} \approx \tilde{\boldsymbol{\theta}}$, the set of parameters defining either limit $g(\boldsymbol{\gamma}\tilde{\boldsymbol{\theta}})$.

To control round-off errors resulting from large variations in magnitude of the elements of $\boldsymbol{Df}_r'\boldsymbol{\omega}\boldsymbol{Df}_r$ and to put equation 10 into a form for the Marquardt-like solution scheme developed by Vecchia and Cooley (1987), $\boldsymbol{Df}_r$, $\boldsymbol{D}g_r$, $\boldsymbol{\theta}_r$, and $\boldsymbol{\theta}_{r+1}$ need to be scaled. Let $\boldsymbol{A}_r$ be a diagonal matrix composed of the square roots of the inverses of the diagonal elements of $\boldsymbol{Df}_r'\boldsymbol{\omega}\boldsymbol{Df}_r$. Then let

$$\boldsymbol{S}_r = \boldsymbol{Df}_r\boldsymbol{A}_r\,, \tag{11}$$

$$\boldsymbol{Z}_r = \boldsymbol{A}_r\boldsymbol{D}g_r'\,, \tag{12}$$

and

$$\boldsymbol{d}_{r+1} = \boldsymbol{A}_r^{-1}\left(\boldsymbol{\theta}_{r+1} - \boldsymbol{\theta}_r\right). \tag{13}$$

With the above scaled matrix and vectors, equation 10 transforms to

$$\boldsymbol{d}_{r+1} = \lambda_{r+1}\left(\boldsymbol{S}_r'\boldsymbol{\omega}\boldsymbol{S}_r\right)^{-1}\boldsymbol{Z}_r + \left(\boldsymbol{S}_r'\boldsymbol{\omega}\boldsymbol{S}_r\right)^{-1}\boldsymbol{S}_r'\boldsymbol{\omega}\left(\boldsymbol{Y} - \boldsymbol{f}(\boldsymbol{\gamma}\boldsymbol{\theta}_r)\right). \tag{14}$$

Note that $\boldsymbol{Q}_r$ and $\boldsymbol{R}_r$ in equation 9 are invariant under the scaling used for equations 11 and 12, so can be written in terms of $\boldsymbol{S}_r$ and $\boldsymbol{Z}_r$.

Vecchia and Cooley (1987) found that a Marquardt-like modification (Seber and Wild, 1989, p. 624) of equation 14 often was effective for solving ill-conditioned problems. We have used numerous tests to confirm this finding. The modification is simply to add $\mu_{r+1}\boldsymbol{I}$ to $\boldsymbol{S}_r'\boldsymbol{\omega}\boldsymbol{S}_r$ in equation 14 to obtain

$$\boldsymbol{d}_{r+1} = \lambda_{r+1}\left(\boldsymbol{S}_r'\boldsymbol{\omega}\boldsymbol{S}_r + \mu_{r+1}\boldsymbol{I}\right)^{-1}\boldsymbol{Z}_r + \left(\boldsymbol{S}_r'\boldsymbol{\omega}\boldsymbol{S}_r + \mu_{r+1}\boldsymbol{I}\right)^{-1}\boldsymbol{S}_r'\boldsymbol{\omega}\left(\boldsymbol{Y} - \boldsymbol{f}(\boldsymbol{\gamma}\boldsymbol{\theta}_r)\right), \tag{15}$$

where μ_{r+1} is a parameter obtained using the algorithm given by Cooley and Naff (1990, p. 71-72).

Another modification involves damping of the parameter displacement vector $\boldsymbol{d}_{r+1}$. This often is necessary to achieve convergence because $\boldsymbol{d}_{r+1}$ is frequently too large (Cooley and Vecchia, 1987). Thus, parameter set $\boldsymbol{\theta}_{r+1}$ is computed using a damped form of equation 13:

$$\boldsymbol{\theta}_{r+1} = \rho_{r+1}\boldsymbol{A}_r\boldsymbol{d}_{r+1} + \boldsymbol{\theta}_r\,. \tag{16}$$

Damping parameter ρ_{r+1} is computed using the algorithm given by Cooley (1993c, p. 2-3) except that t_{r+1} used by that algorithm is defined in the present report as the value of $\delta_j^{r+1}/\theta_{sj}$ for which $\left|t_{r+1}\right| = \max_j \left|\delta_j^{r+1}/\theta_{sj}\right|$, where δ_j^{r+1} is an element of $\boldsymbol{A}_r\boldsymbol{d}_{r+1}$, θ_{sj} is an element of $\boldsymbol{\theta}_s$, and $\boldsymbol{\theta}_s$ is a user-supplied scaling vector. The scaling vector adjusts for differing sizes of elements of $\boldsymbol{\theta}$, so should reflect the user's best knowledge of $\boldsymbol{\theta}_*$, except that no element of $\boldsymbol{\theta}_s$ can be zero.

We consider the iteration scheme to have converged if either $|t_{r+1}|$ or $\left|S(\boldsymbol{\theta}_{r+1}) - S(\boldsymbol{\theta}_r)\right|/S(\boldsymbol{\theta}_r) + \left|S(\boldsymbol{\theta}_r) - S(\boldsymbol{\theta}_{r-1})\right|/S(\boldsymbol{\theta}_{r-1})$ is small enough. The convergence criteria for $|t_{r+1}|$ and $\left|S(\boldsymbol{\theta}_{r+1}) - S(\boldsymbol{\theta}_r)\right|/S(\boldsymbol{\theta}_r) + \left|S(\boldsymbol{\theta}_r) - S(\boldsymbol{\theta}_{r-1})\right|/S(\boldsymbol{\theta}_{r-1})$ are user supplied. Another test that overrides the above two also is used, if specified by the user. Sometimes $g(\boldsymbol{\gamma\theta}_{r+1})$ can stabilize even though one or more elements of $\boldsymbol{\theta}$ have not converged. To address this case the user can specify that the process has converged whenever $\left|2 \times (g(\boldsymbol{\gamma\theta}_{r+1}) - g(\boldsymbol{\gamma\theta}_r))/(g(\boldsymbol{\gamma\theta}_{r+1}) + g(\boldsymbol{\gamma\theta}_r))\right|$ is smaller than another user-supplied criterion. This criterion is not used when $\left|(g(\boldsymbol{\gamma\theta}_{r+1}) + g(\boldsymbol{\gamma\theta}_r))\right| < 10^{-12}$.

Weighted Residuals

Cooley (2004, p. 56-57) showed that weighted residuals from a regression constrained so that $g(\boldsymbol{\gamma}\tilde{\boldsymbol{\theta}}) = g(\boldsymbol{\gamma\theta}_*)$ (where $\tilde{\boldsymbol{\theta}}$ is the constrained regression estimate) can be defined as $(\boldsymbol{I} - \boldsymbol{QQ}'/\boldsymbol{Q}'\boldsymbol{Q})\boldsymbol{\omega}^{1/2}(\boldsymbol{Y} - \boldsymbol{f}(\boldsymbol{\gamma}\tilde{\boldsymbol{\theta}}))$ and are equal to weighted residuals $\boldsymbol{\omega}^{1/2}(\boldsymbol{Y} - \boldsymbol{f}(\boldsymbol{\gamma}\hat{\boldsymbol{\theta}}))$ from the unconstrained regression if model intrinsic nonlinearity and model combined intrinsic nonlinearity as defined by Cooley (2004, p. 35-36) both are small. Parameter set $\tilde{\boldsymbol{\theta}}$ can be the set computed for either confidence limit because minimization of $S(\boldsymbol{\theta})$, subject to the constraint $g(\boldsymbol{\gamma\theta}) = g(\boldsymbol{\gamma\theta}_*)$, is the same as finding an extreme value of $g(\boldsymbol{\gamma\theta})$, subject to the constraint $S(\boldsymbol{\theta}) - S(\hat{\boldsymbol{\theta}}) = d_\alpha^2$, if $g(\boldsymbol{\gamma\theta}_*)$ assumed for the constrained regression is the confidence limit for $g(\boldsymbol{\gamma\theta}_*)$ computed using d_α^2. Thus, the constrained weighted residuals for both confidence limits for $g(\boldsymbol{\gamma\theta}_*)$ are computed and printed if specified by the user. Vector $\boldsymbol{Q}$ is computed using the initial set of parameters $\boldsymbol{\theta}_0$ because if $\tilde{\boldsymbol{\theta}}$ were used, the term in $(\boldsymbol{I} - \boldsymbol{QQ}'/\boldsymbol{Q}'\boldsymbol{Q})\boldsymbol{\omega}^{1/2}(\boldsymbol{Y} - \boldsymbol{f}(\boldsymbol{\gamma}\tilde{\boldsymbol{\theta}}))$ expressing model combined intrinsic nonlinearity, that is $(\boldsymbol{R} - \boldsymbol{QQ}'/\boldsymbol{Q}'\boldsymbol{Q})\boldsymbol{\omega}^{1/2}(\boldsymbol{Y} - \boldsymbol{f}(\boldsymbol{\gamma}\tilde{\boldsymbol{\theta}}))$, always would be zero, as shown in appendix B.

Prediction Intervals

As for a confidence interval, a prediction interval for a predicted observation of g(**ß**), Y_p, is defined by two limits, the maximum and minimum values of $g(\boldsymbol{\gamma\theta}) + v$ over a likelihood region, where v is the predicted error (Cooley, 2004, p. 59-60). The form of the likelihood region is developed in Cooley (2004, p. 61) and the prediction limits are assumed to lie on the edge of the likelihood region so that the method of Lagrange multipliers can again be used to find the extreme values. To obtain the Lagrange function we assume that the weight matrix incorporating the prediction, $\boldsymbol{\omega}_a$ of Cooley (2004, p. 63), is block diagonal of the form

$$\boldsymbol{\omega}_a = \begin{bmatrix} \boldsymbol{\omega} & \boldsymbol{0} \\ \boldsymbol{0} & \omega_p \end{bmatrix} \tag{17}$$

as described by Cooley (2004, p. 63). In equation 17, ω_p is the weight for the prediction that is analogous to diagonal elements of $\boldsymbol{\omega}$. The form given by equation 17 not only simplifies calculations, but also does not require the user to estimate second moments between observations and the prediction, which often would be unknown. However, if such second moments actually exist so that the second-moment matrix that includes the prediction is of the form (Cooley, 2004, equation 5-87)

$$\boldsymbol{\Omega}_a = \begin{bmatrix} \boldsymbol{\Omega} & \boldsymbol{C} \\ \boldsymbol{C}' & b\hat{\omega}_p^{-1} \end{bmatrix}, \tag{18}$$

then a correction factor c_p, described in 'The RESAN2-2k Program' section, must be used. In equation 18, $\boldsymbol{C} = E(\boldsymbol{Y} - \boldsymbol{f}(\boldsymbol{\gamma\theta}_*))(Y_p - g(\boldsymbol{\gamma\theta}_*))/\sigma_\varepsilon^2$, $\hat{\omega}_p^{-1} = E(Y_p - g(\boldsymbol{\gamma\theta}_*))^2/\sigma_\varepsilon^2$, and $b = tr(\boldsymbol{\omega}^{1/2}\boldsymbol{\Omega}\boldsymbol{\omega}^{1/2})/n$, where $tr(\ldots)$ signifies matrix trace.

On the basis of the assumed structure of $\boldsymbol{\omega}_a$, Cooley (2004, p. 65) stated the Lagrange function as

$$L(\boldsymbol{\theta}, v, \lambda) = g(\boldsymbol{\gamma\theta}) + v + \frac{1}{2\lambda}\left(d_\alpha^2 - S(\boldsymbol{\theta}) - \omega_p v^2 + S(\hat{\boldsymbol{\theta}})\right), \tag{19}$$

where critical value d_α^2 is equal to $c_p t_{\alpha/2}^2 (n-p) S(\hat{\boldsymbol{\theta}})/(n-p)$ for an individual prediction interval. As explained by Cooley (2004, p. 65), sometimes the second moment of $Y_p - g(\boldsymbol{\gamma\theta}_*)$, $E(Y_p - g(\boldsymbol{\gamma\theta}_*))^2$, can be estimated more easily than $\hat{\omega}_p$ for use in equation 19. In this case, the term $E(Y_p - g(\boldsymbol{\gamma\theta}_*))^{-2} s^2$ can replace the general weight ω_p in equation 19.

Iterative solution of the extreme value problem based on equation 19 is derived in appendix A using the same method as used for equation 8. The solution is given as

$$\lambda_{r+1} = \pm\left(\frac{d_\alpha^2 - S(\boldsymbol{\theta}_r) + S(\hat{\boldsymbol{\theta}}) + (\boldsymbol{Y} - \boldsymbol{f}(\boldsymbol{\gamma\theta}_r))'\boldsymbol{\omega}^{1/2}\boldsymbol{R}_r\boldsymbol{\omega}^{1/2}(\boldsymbol{Y} - \boldsymbol{f}(\boldsymbol{\gamma\theta}_r))}{\boldsymbol{Q}_r'\boldsymbol{Q}_r + \omega_p^{-1}}\right)^{1/2}, \tag{20}$$

$$v_{r+1} = \omega_p^{-1}\lambda_{r+1}, \tag{21}$$

and equation 10. All of the developments following equation 10 for a confidence interval are used for a prediction interval.

The RESAN2-2k Program

The purpose of analyzing residuals is to test whether or not the assumptions made for nonlinear regression and uncertainty analysis seem to be violated (Cooley and Naff, 1990, p. 167). RESAN2-2k focuses on detection of model and system types of intrinsic nonlinearity as defined by Cooley (2004, p. 35-36), as well as the traditional graphical examination of residuals plots for lack of model fit and testing of residuals for indications of non-normality. More on the purposes, theory, and methods of residuals analysis is given in Draper and Smith (1998, chapters 2, 7, and 8), Cooley and Naff (1990, chapter 5), Hill (1992, p. 56-66, 88-89), Hill (1994), Cooley (2004), and references cited in these works.

A Test for Model Intrinsic Nonlinearity

Model intrinsic nonlinearity causes confidence regions, confidence intervals, and prediction intervals to be too small unless they are corrected with a correction factor. Cooley (2004, section 5) showed that (1) the size of a confidence region is proportional to $c_r F_\alpha(p, n-p)$, where c_r is the correction factor; (2) the size of a Scheffé interval is proportional to $\left(c_r F_\alpha(p, n-p)\right)^{1/2}$; (3) the size of an individual confidence interval is proportional to $\left(c_c t^2_{\alpha/2}(n-p)\right)^{1/2}$, where c_c is the correction factor; and (4) the size of an individual prediction interval is proportional to $\left(c_p t^2_{\alpha/2}(n-p)\right)^{1/2}$, where c_p is the correction factor. The correction factors are defined by

$$c_r = \frac{\sigma^2_\varepsilon + \left(\gamma_{wr}\sigma^2_\beta + \gamma_{Ir}\sigma^4_\varepsilon\right)/p}{\sigma^2_\varepsilon + \left(\hat{\gamma}_w\sigma^2_\beta + \hat{\gamma}_I\sigma^4_\varepsilon\right)/(n-p)}, \tag{22}$$

$$c_c = \frac{\sigma^2_\varepsilon + \gamma_{wc}\sigma^2_\beta + \gamma_{Ic}\sigma^4_\varepsilon}{\sigma^2_\varepsilon + \left(\hat{\gamma}_w\sigma^2_\beta + \hat{\gamma}_I\sigma^4_\varepsilon\right)/(n-p)}, \tag{23}$$

and, for the form of prediction interval computed by UNC,

$$c_p = \frac{\sigma^2_\varepsilon + \gamma_{wa}\sigma^2_\beta + \gamma_{Ia}\sigma^4_\varepsilon}{\sigma^2_\varepsilon + \left(\hat{\gamma}_w\sigma^2_\beta + \hat{\gamma}_I\sigma^4_\varepsilon\right)/(n-p)}. \tag{24}$$

Variables contained in equations 22-24 are defined as follows: σ^2_β is a scalar multiplier for the variance of the vector of system characteristics, $\boldsymbol{\beta}$, defined by $Var(\boldsymbol{\beta}) = \boldsymbol{V}_\beta\sigma^2_\beta$; σ^2_ε is a scalar multiplier for the variance of the observation-error vector, $\boldsymbol{\varepsilon}$, of order *n*, defined by $Var(\boldsymbol{\varepsilon}) = \boldsymbol{V}_\varepsilon\sigma^2_\varepsilon$; and $\hat{\gamma}_w\sigma^2_\beta, \hat{\gamma}_I\sigma^4_\varepsilon, \gamma_{wr}\sigma^2_\beta, \gamma_{Ir}\sigma^4_\varepsilon, \gamma_{wc}\sigma^2_\beta, \gamma_{Ic}\sigma^4_\varepsilon, \gamma_{wa}\sigma^2_\beta,$ and $\gamma_{Ia}\sigma^4_\varepsilon$ are component correction factors defined by Cooley (2004, section 5). (The subscripts *r* and *c* were added in the present report.)

The factors examined by RESAN2-2k, $\hat{\gamma}_I\sigma^4_\varepsilon$ and $\gamma_{Ir}\sigma^4_\varepsilon$, measure the importance of model intrinsic nonlinearity. Cooley (2004, p. 50) showed that $\gamma_{Ir}\sigma^4_\varepsilon = -\hat{\gamma}_I\sigma^4_\varepsilon$. Thus, only $\hat{\gamma}_I\sigma^4_\varepsilon$ needs to be computed, and this factor is expressed by Cooley (2004, equation 6-3) as

$$
\begin{aligned}
&\hat{\gamma}_I \sigma_\varepsilon^4 = 2E\left(\boldsymbol{f}(\gamma\boldsymbol{\theta}_*) - \boldsymbol{f}_0(\gamma\boldsymbol{\theta}_*) - \boldsymbol{f}\left(\gamma\hat{\boldsymbol{\theta}}\right) + \boldsymbol{f}_0\left(\gamma\hat{\boldsymbol{\theta}}\right)\right)' \boldsymbol{\omega}^{1/2}(\boldsymbol{I}-\boldsymbol{R})\boldsymbol{\omega}^{1/2}(\boldsymbol{Y} - \boldsymbol{f}(\gamma\boldsymbol{\theta}_*)) \\
&+ E\left(\boldsymbol{f}(\gamma\boldsymbol{\theta}_*) - \boldsymbol{f}_0(\gamma\boldsymbol{\theta}_*) - \boldsymbol{f}\left(\gamma\hat{\boldsymbol{\theta}}\right) + \boldsymbol{f}_0\left(\gamma\hat{\boldsymbol{\theta}}\right)\right)' \boldsymbol{\omega}^{1/2}(\boldsymbol{I}-\boldsymbol{R})\boldsymbol{\omega}^{1/2} \cdot \\
&\left(\boldsymbol{f}(\gamma\boldsymbol{\theta}_*) - \boldsymbol{f}_0(\gamma\boldsymbol{\theta}_*) - \boldsymbol{f}\left(\gamma\hat{\boldsymbol{\theta}}\right) + \boldsymbol{f}_0\left(\gamma\hat{\boldsymbol{\theta}}\right)\right) + E\left(\boldsymbol{Y} - \boldsymbol{f}\left(\gamma\hat{\boldsymbol{\theta}}\right)\right)' \boldsymbol{\omega}^{1/2}\boldsymbol{R}\boldsymbol{\omega}^{1/2}\left(\boldsymbol{Y} - \boldsymbol{f}\left(\gamma\hat{\boldsymbol{\theta}}\right)\right) \\
&= 2E\left(\boldsymbol{f}_m(\gamma\boldsymbol{\theta}_*) - \boldsymbol{f}_{0m}(\gamma\boldsymbol{\theta}_*) - \boldsymbol{f}_m\left(\gamma\hat{\boldsymbol{\theta}}\right) + \boldsymbol{f}_{0m}\left(\gamma\hat{\boldsymbol{\theta}}\right)\right)' \boldsymbol{\omega}_m^{1/2} \cdot \\
&\left((\boldsymbol{I}_m - \boldsymbol{R}_m)\boldsymbol{\omega}_m^{1/2}(\boldsymbol{Y}_m - \boldsymbol{f}_m(\gamma\boldsymbol{\theta}_*)) - \boldsymbol{R}_{md}\boldsymbol{\omega}_d^{1/2}(\boldsymbol{Y}_d - \boldsymbol{f}_d(\gamma\boldsymbol{\theta}_*))\right) \\
&+ E\left(\boldsymbol{f}_m(\gamma\boldsymbol{\theta}_*) - \boldsymbol{f}_{0m}(\gamma\boldsymbol{\theta}_*) - \boldsymbol{f}_m\left(\gamma\hat{\boldsymbol{\theta}}\right) + \boldsymbol{f}_{0m}\left(\gamma\hat{\boldsymbol{\theta}}\right)\right)' \boldsymbol{\omega}_m^{1/2}(\boldsymbol{I}_m - \boldsymbol{R}_m)\boldsymbol{\omega}_m^{1/2} \cdot \\
&\left(\boldsymbol{f}_m(\gamma\boldsymbol{\theta}_*) - \boldsymbol{f}_{0m}(\gamma\boldsymbol{\theta}_*) - \boldsymbol{f}_m\left(\gamma\hat{\boldsymbol{\theta}}\right) + \boldsymbol{f}_{0m}\left(\gamma\hat{\boldsymbol{\theta}}\right)\right) + E\left(\boldsymbol{Y} - \boldsymbol{f}\left(\gamma\hat{\boldsymbol{\theta}}\right)\right)' \boldsymbol{\omega}^{1/2}\boldsymbol{R}\boldsymbol{\omega}^{1/2}\left(\boldsymbol{Y} - \boldsymbol{f}\left(\gamma\hat{\boldsymbol{\theta}}\right)\right),
\end{aligned}
\tag{25}
$$

where $\boldsymbol{f}_0(\gamma\boldsymbol{\theta}_*)$ is the linear-model approximation of $\boldsymbol{f}(\gamma\boldsymbol{\theta}_*)$ defined in Cooley (2004, equation 5-104 and text preceding equation 6-2), $\boldsymbol{f}_0\left(\gamma\hat{\boldsymbol{\theta}}\right)$ is the linear-model approximation of $\boldsymbol{f}\left(\gamma\hat{\boldsymbol{\theta}}\right)$ defined in Cooley (2004, equation 5-104 and text preceding equation 6-2), and $\boldsymbol{I}$ is the identity matrix.

The last term of equation 25 is the expected value of the product of row vector $(\boldsymbol{Y} - \boldsymbol{f}(\gamma\hat{\boldsymbol{\theta}}))'\boldsymbol{\omega}^{1/2}\boldsymbol{R}$ and its transpose. If ***Df*** in ***R*** is evaluated using $\hat{\boldsymbol{\theta}}$, then $\boldsymbol{R}\boldsymbol{\omega}^{1/2}(\boldsymbol{Y} - \boldsymbol{f}(\gamma\hat{\boldsymbol{\theta}}))$ is always $\boldsymbol{0}$ (Cooley, 2004, p. 39). Also, if model intrinsic nonlinearity is absent, then ***R*** is constant (that is, the same for any set $\boldsymbol{\theta}$) (Cooley, 2004, p. 39). Thus, a test for the importance of intrinsic nonlinearity in the denominators of the correction factors is to compare the estimate of the last term of equation 25, $(\boldsymbol{Y} - \boldsymbol{f}(\gamma\hat{\boldsymbol{\theta}}))'\boldsymbol{\omega}^{1/2}\boldsymbol{R}\boldsymbol{\omega}^{1/2}(\boldsymbol{Y} - \boldsymbol{f}(\gamma\hat{\boldsymbol{\theta}}))$, where ***R*** is not computed using $\hat{\boldsymbol{\theta}}$, with another appropriate term in equations 22-24. This term is obtained from equation 5-16 of Cooley (2004, p. 48), which shows that model intrinsic nonlinearity is negligible in the denominator of the correction factors if $\left|\hat{\gamma}_I\sigma_\varepsilon^4\right| << (n-p)\sigma_\varepsilon^2 + \hat{\gamma}_w\sigma_\beta^2 = b(n-ap)\sigma_\varepsilon^2$, where *a* and *b* are factors that equal 1 if $b\boldsymbol{\omega}^{-1} = \boldsymbol{\Omega}$, the inverse of the correct weight matrix for the Gauss-Markov method of weighted regression to find $\hat{\boldsymbol{\theta}}$ (Cooley, 2004, section 4). Specifically,

$$
a = tr\left(\boldsymbol{R}(\boldsymbol{\omega}/b)^{1/2}\boldsymbol{\Omega}(\boldsymbol{\omega}/b)^{1/2}\right)/p = \left(tr\left(\boldsymbol{R}_m(\boldsymbol{\omega}_m/b)^{1/2}\boldsymbol{\Omega}_m(\boldsymbol{\omega}_m/b)^{1/2}\right) + tr(\boldsymbol{R}_d)/b\right)/p \tag{26}
$$

and

$$
b = tr\left(\boldsymbol{\omega}^{1/2}\boldsymbol{\Omega}\boldsymbol{\omega}^{1/2}\right)/n = \left(tr\left(\boldsymbol{\omega}_m^{1/2}\boldsymbol{\Omega}_m\boldsymbol{\omega}_m^{1/2}\right) + n_d\right)/n\,. \tag{27}
$$

Because $b\sigma_\varepsilon^2$ is estimated by s^2 defined by (Cooley, 2004, p. 50) as

$$
s^2 = \frac{S\left(\hat{\boldsymbol{\theta}}\right)}{n-ap}, \tag{28}
$$

$b(n-ap)\sigma_\varepsilon^2$ is estimated by $S\left(\hat{\boldsymbol{\theta}}\right)$, where

$$S(\hat{\boldsymbol{\theta}}) = \left(\boldsymbol{Y} - \boldsymbol{f}(\gamma\hat{\boldsymbol{\theta}})\right)' \boldsymbol{\omega} \left(\boldsymbol{Y} - \boldsymbol{f}(\gamma\hat{\boldsymbol{\theta}})\right). \tag{29}$$

Thus, the test is that $(\boldsymbol{Y} - \boldsymbol{f}(\gamma\hat{\boldsymbol{\theta}}))'\boldsymbol{\omega}^{1/2}\boldsymbol{R}\boldsymbol{\omega}^{1/2}(\boldsymbol{Y} - \boldsymbol{f}(\gamma\hat{\boldsymbol{\theta}}))$ should be much smaller than $S(\hat{\boldsymbol{\theta}})$ if $\boldsymbol{R}$ is computed using some reasonable set of parameters $\boldsymbol{\theta}$ not equal to $\hat{\boldsymbol{\theta}}$. A set of direct observations or initial estimates for $\boldsymbol{\theta}_*$ should work. If desired, vector $\boldsymbol{R}\boldsymbol{\omega}^{1/2}\left(\boldsymbol{Y} - \boldsymbol{f}(\gamma\hat{\boldsymbol{\theta}})\right)$ can be examined to determine where in observation space the model intrinsic nonlinearity is large.

Because $\gamma_{Ir}\sigma_\varepsilon^4 = -\hat{\gamma}_I\sigma_\varepsilon^4$, the test also can be used to assess the importance of model intrinsic nonlinearity in the numerator of c_r, except that the test criterion should be changed. From Cooley (2004, p. 48) model intrinsic nonlinearity is negligible in the numerator of c_r when $\left|\gamma_{Ir}\sigma_\varepsilon^4\right| << p\sigma_\varepsilon^2 + \gamma_w\sigma_\beta^2 = bap\sigma_\varepsilon^2$. The term $bap\sigma_\varepsilon^2$ is estimated by $aps^2 = apS(\hat{\boldsymbol{\theta}})/(n - ap)$, so the test is that $(\boldsymbol{Y} - \boldsymbol{f}(\gamma\hat{\boldsymbol{\theta}}))'\boldsymbol{\omega}^{1/2}\boldsymbol{R}\boldsymbol{\omega}^{1/2}(\boldsymbol{Y} - \boldsymbol{f}(\gamma\hat{\boldsymbol{\theta}}))$ should be much smaller than $apS(\hat{\boldsymbol{\theta}})/(n - ap)$. When a is unknown, the more conservative criterion $pS(\hat{\boldsymbol{\theta}})/(n - p)$ should be used.

A Test for Model and System Types of Intrinsic Nonlinearity

Cooley (2004, p. 38-39) showed that both the mean weighted residual $\sum_i \boldsymbol{\omega}_i^{1/2}(\boldsymbol{Y} - \boldsymbol{f}(\gamma\hat{\boldsymbol{\theta}}))/n$ (where $\boldsymbol{\omega}_i^{1/2}$ is row i of $\boldsymbol{\omega}^{1/2}$) and the slope of the plot of weighted residuals $\boldsymbol{\omega}_i^{1/2}(\boldsymbol{Y} - \boldsymbol{f}(\gamma\hat{\boldsymbol{\theta}}))$ in relation to weighted model functions $\boldsymbol{\omega}_i^{1/2}\boldsymbol{f}(\gamma\hat{\boldsymbol{\theta}})$ should be small if the model $\boldsymbol{f}(\gamma\hat{\boldsymbol{\theta}})$ is adequate and both model and system types of intrinsic nonlinearity are small. Formal t tests could be used to determine the significance of these measures, but graphical examination as performed by Cooley (2004, section 7) on test problems and comparisons with synthetic residual sets as described next should be adequate to detect significant model and system types of intrinsic nonlinearity as well as significant model inadequacy as described in the references cited at the beginning of this section.

A Test for Normality of the Weighted Residuals

Examination of the probability plot of weighted residuals $\boldsymbol{\omega}_i^{1/2}\left(\boldsymbol{Y} - \boldsymbol{f}(\gamma\hat{\boldsymbol{\theta}})\right)$ will sometimes reveal obvious departures from normality. However, as discussed by Cooley and Naff (1990, p. 168-170), departures from a standard normal distribution are expected for weighted residuals because they always are correlated and heteroscedastic. Under ideal conditions of no model or system intrinsic nonlinearity and zero-mean normal distributions of $\boldsymbol{\beta}$ and $\boldsymbol{\varepsilon}$, Cooley (2004, p. 38) showed that the weighted residuals have the normal distribution

$$\boldsymbol{\omega}^{1/2}\left(\boldsymbol{Y} - \boldsymbol{f}(\gamma\hat{\boldsymbol{\theta}})\right) \sim N\left(\boldsymbol{0}, (\boldsymbol{I} - \boldsymbol{R})(\boldsymbol{\omega}/b)^{1/2}\boldsymbol{\Omega}(\boldsymbol{\omega}/b)^{1/2}(\boldsymbol{I} - \boldsymbol{R})b\sigma_\varepsilon^2\right). \tag{30}$$

If Gauss-Markov estimation is used so that $b\boldsymbol{\omega}^{-1} = \boldsymbol{\Omega}$, then equation 30 becomes

$$\boldsymbol{\omega}^{1/2}\left(\boldsymbol{Y} - \boldsymbol{f}(\gamma\hat{\boldsymbol{\theta}})\right) \sim N\left(\boldsymbol{0}, (\boldsymbol{I} - \boldsymbol{R})b\sigma_\varepsilon^2\right), \tag{31}$$

which is of the form of the distribution of standard linear-regression weighted residuals.

The weighted residual distribution can be graphically compared with synthetic weighted residual distributions generated according to equation 30 (or 31) as described by Cooley and Naff (1990, p. 168-171) to determine whether or not the weighted residuals appear to have the specified normal distribution. However, a more precise test also can be used. To make the test, first synthetic weighted residuals are generated from equation 30 or 31 (with the estimate s^2 replacing $b\sigma_\varepsilon^2$) as follows.

1. Standard normal deviates are generated from $\boldsymbol{u} \sim N\left(\boldsymbol{0}, \boldsymbol{I}s^2\right)$. Vector $\boldsymbol{u}_T$ is initialized as $\boldsymbol{u}_T = \boldsymbol{u}$.
2. If specified in the input, $\boldsymbol{u}$ is modified to be the synthetic, weighted, true error vector $\boldsymbol{u}_T = \boldsymbol{Lu}$, where $\boldsymbol{L}$ is the lower triangular Cholesky factor of $(\boldsymbol{\omega}/b)^{1/2}\boldsymbol{\Omega}(\boldsymbol{\omega}/b)^{1/2}$. (See Kitanidis (1997, p. 237-238).)
3. Vector $\boldsymbol{u}_T$ is modified according to equation 30 (or 31) to give $\boldsymbol{d}^k = (\boldsymbol{I} - \boldsymbol{R})\boldsymbol{u}_T$, the set of synthetic, weighted residuals for realization *k*.
4. Steps 1-3 are repeated for a large number of realizations, *M*.

Note that skipping step 2 yields synthetic weighted residuals distributed according to equation 31 (with the estimate s^2 replacing $b\sigma_\varepsilon^2$). This step would be skipped if Gauss-Markov estimation were used or if $\boldsymbol{\Omega}$ were unknown, in which case $b\sigma_\varepsilon^2$ would have to be estimated by $S(\hat{\boldsymbol{\theta}})/(n-p)$ or *a* in the estimate s^2 would have to be approximated using equation 76 in ‘The CORFAC-2k Program’ section of this report.

Next, the following quantities are computed:

$$\bar{\boldsymbol{d}} = \sum_k \boldsymbol{d}^k / M, \tag{32}$$

the mean *n*-vector over all *M* realizations,

$$\boldsymbol{s} = \left[\sum_k d_i^k d_i^k\right], \tag{33}$$

the vector of sum of squared values of d_i^k over all realizations, and

$$\boldsymbol{v} = \left[\sqrt{\left(s_i - M\bar{d}_i\bar{d}_i\right)/(M-1)}\right], \tag{34}$$

the sample standard deviation *n*-vector.

A normal probability plot of vectors $\bar{\boldsymbol{d}} \pm 2\boldsymbol{v}$ gives a band within which the weighted residuals usually might be expected to lie (Cooley, 2004, section 7). Even though $\bar{d}_i \pm 2v_i$ defines an approximate 95 percent individual confidence interval, interpretation of the plot is limited because each interval is an individual one so that all intervals in the band cannot be interpreted simultaneously. A better test for normality is obtained as follows as a generalization of a test given by Shapiro and Francia (1972) and used by Hill (1992, p. 63). First, the grand mean is computed:

$$\bar{\bar{d}} = \sum_i \bar{d}_i / n, \tag{35}$$

Next the square of the correlation between synthetic weighted residuals for each realization k and the means over all realizations is obtained:

$$c^k = \frac{\left(\sum_i \left(d_i^k - \sum_j d_j^k / n\right)\left(\bar{d}_i - \bar{\bar{d}}\right)\right)^2}{\sum_i \left(d_i^k - \sum_j d_j^k / n\right)^2 \sum_i \left(\bar{d}_i - \bar{\bar{d}}\right)^2}. \tag{36}$$

Then, all values of c^k are ordered from smallest to largest.

By definition, the probability that c^k has some specified value c_s or a smaller value is

$$P = \sum_k I\left(c_s \le c^k\right) / M, \tag{37}$$

where $I\left(c_s \le c^k\right)$ is the indicator function $I = 0$ when $c_s > c^k$ and $I = 1$ when $c_s \le c^k$. Therefore, a 95 percentile is given by $c_s = c^{k_1}$, where $k_1 = \text{int}(0.95M)$ and $\text{int}(\cdots)$ indicates truncation to the nearest integer. Similar 90 and 99 percentiles also can be computed. These percentiles should be compared to c_d, the square of the correlation between weighted residuals $\hat{\boldsymbol{e}}_i = \boldsymbol{\omega}_i^{1/2}\left(\boldsymbol{Y} - \boldsymbol{f}\left(\boldsymbol{y}\hat{\boldsymbol{\theta}}\right)\right)$ and the means $\bar{d}_i$, which is

$$c_d = \frac{\left(\sum_i \left(\hat{e}_i - \sum_j \hat{e}_j / n\right)\left(\bar{d}_i - \bar{\bar{d}}\right)\right)^2}{\sum_i \left(\hat{e}_i - \sum_j \hat{e}_j / n\right)^2 \sum_i \left(\bar{d}_i - \bar{\bar{d}}\right)^2}. \tag{38}$$

The comparison will tell if the weighted residuals are significantly different from the specified normal distribution at some predetermined level of significance equal to 100 minus the selected percentile. Also, by letting $c_s = c_d$, the probability P of c_d or a smaller value can be obtained, which is a more direct test.

The BEALE2-2k Program

The purpose of BEALE2-2k is to compute measures of total model nonlinearity, model intrinsic nonlinearity, and model combined intrinsic nonlinearity in the vicinity of $\hat{\boldsymbol{\theta}}$. These measures relate to component correction factors $\hat{\gamma}_I\sigma_\varepsilon^4, \gamma_{Ir}\sigma_\varepsilon^4,\ \gamma_{Ic}\sigma_\varepsilon^4,$ and $\gamma_{Ia}\sigma_\varepsilon^4$ that compose correction factors c_r, c_c, and c_p.

A Measure of Average Total Model Nonlinearity

Total model nonlinearity is the sum of model intrinsic nonlinearity and parameter effects nonlinearity, the latter of which is nonlinearity that can be eliminated by some generally unknown transformation of parameters $\boldsymbol{\varphi}(\boldsymbol{\theta})$ (Draper and Smith, 1998, p. 528-529). In effect, intrinsic nonlinearity is the smallest possible total model nonlinearity for any transformation of parameters. The measure of total nonlinearity was developed to determine when linear theory can be used to compute confidence regions (Beale, 1960; Guttman and Meeter, 1965; Cooley and Naff, 1990, p. 187-188).

Cooley and Naff (1990, p. 187-188) defined a measure of average total nonlinearity as a combination of measures developed by Beale (1960) and Linssen (1975). For reasons discussed by Cooley (2004, p. 85) the measure used in this report was altered slightly from the one defined by Cooley and Naff (1990). It is defined as the average weighted sum of squared discrepancies between nonlinear and linear model values on the edge of the linear probability region having diameter $apb\sigma_\varepsilon^2$ and centered on the drift set of parameters $\bar{\boldsymbol{\theta}}$. Therefore, the measure of average total model nonlinearity is calculated using estimates as (Cooley, 2004, p. 87)

$$\begin{aligned}\hat{N} &= \frac{1}{aps^2}\sum_{l=1}^{2p}\left(\boldsymbol{f}(\gamma\boldsymbol{\theta}_l)-\boldsymbol{f}_0(\gamma\boldsymbol{\theta}_l)\right)'\boldsymbol{\omega}\left(\boldsymbol{f}(\gamma\boldsymbol{\theta}_l)-\boldsymbol{f}_0(\gamma\boldsymbol{\theta}_l)\right)\Big/(2p)\\ &= \frac{1}{aps^2}\sum_{l=1}^{2p}\left(\boldsymbol{f}_m(\gamma\boldsymbol{\theta}_l)-\boldsymbol{f}_{0m}(\gamma\boldsymbol{\theta}_l)\right)'\boldsymbol{\omega}_m\left(\boldsymbol{f}_m(\gamma\boldsymbol{\theta}_l)-\boldsymbol{f}_{0m}(\gamma\boldsymbol{\theta}_l)\right)\Big/(2p),\end{aligned} \tag{39}$$

where $\boldsymbol{f}_0(\cdots)$ and $\boldsymbol{f}_{0m}(\cdots)$ indicate linear model values, and the sets $\boldsymbol{\theta}_l, l=1,2,\cdots,2p,$ are calculated as given by Cooley and Naff (1990, p. 189):

$$\boldsymbol{\theta}_l = \hat{\boldsymbol{\theta}} + \lambda\left(\boldsymbol{D}\hat{\boldsymbol{f}}'\boldsymbol{\omega}\boldsymbol{D}\hat{\boldsymbol{f}}\right)^{-1}\boldsymbol{l}', \tag{40}$$

in which

$$\lambda = \pm\left(\frac{aps^2}{\boldsymbol{l}\left(\boldsymbol{D}\hat{\boldsymbol{f}}'\boldsymbol{\omega}\boldsymbol{D}\hat{\boldsymbol{f}}\right)^{-1}\boldsymbol{l}'}\right)^{1/2} \tag{41}$$

and $\boldsymbol{l}$ is the row p-vector

$$\boldsymbol{l} = [0 \; 0 \; \cdots \; 1 \; \cdots \; 0], \tag{42}$$

with the 1 being in column l. Sensitivity matrix $\boldsymbol{D\hat{f}}$ is evaluated at $\hat{\boldsymbol{\theta}}$. Note that the diameter of the linear confidence region aps^2 can be written in terms of c_r as evaluated in CORFAC-2k (which assumes no model intrinsic nonlinearity) as

$$aps^2 = \frac{apS(\hat{\boldsymbol{\theta}})}{n-ap} = \frac{(n-p)a}{n-ap} p \frac{S(\hat{\boldsymbol{\theta}})}{n-p} = c_r p \frac{S(\hat{\boldsymbol{\theta}})}{n-p}. \tag{43}$$

If $\boldsymbol{\Omega}$ is unknown so that a cannot be calculated using equation 26, then a may be estimated using equation 76 derived in ‘The CORFAC-2k Program’ section.

By analogy with the standard criteria for ranking nonlinearity first given by Beale (1960, p. 60) and later augmented by Cooley and Naff (1990, p. 189), we consider the model to be highly nonlinear if $\hat{N} > 1$ so that the numerator of $\hat{N}$ is greater than the diameter aps^2 of the confidence region; nonlinear if $1 \geq \hat{N} > 0.09$; moderately nonlinear if $0.09 \geq \hat{N} > 0.01$; and essentially linear if $\hat{N} \leq 0.01$. Linear theory for computing confidence regions seems to produce good approximate results when $\hat{N} \leq 0.09$ (Cooley and Naff, 1990, p. 189).

A Measure of Average Model Intrinsic Nonlinearity

Average model intrinsic nonlinearity is assessed by the measure $\hat{N}_{\min}$ modified by Cooley (2004, p. 85) from forms given earlier by Beale (1960) and Linssen (1975). As for the measure of total nonlinearity, this measure is defined in terms of the linear probability region centered on $\bar{\boldsymbol{\theta}}$ and having diameter $apb\sigma_\varepsilon^2$. It is calculated using the same estimates and linear confidence region as used for $\hat{N}$. Therefore, the model intrinsic nonlinearity measure is calculated as (Cooley, 2004, p. 85)

$$\begin{aligned}
\hat{N}_{\min} &= \frac{1}{aps^2} \sum_{l=1}^{2p} \left(\boldsymbol{f}(\gamma\boldsymbol{\theta}_l) - \boldsymbol{f}_0(\gamma\boldsymbol{\theta}_l) - \boldsymbol{D\hat{f}\psi}_l \right)' \boldsymbol{\omega} \left(\boldsymbol{f}(\gamma\boldsymbol{\theta}_l) - \boldsymbol{f}_0(\gamma\boldsymbol{\theta}_l) - \boldsymbol{D\hat{f}\psi}_l \right) \Big/ (2p) \\
&= \frac{1}{aps^2} \sum_{i=1}^{2p} \Big(\left(\boldsymbol{f}_m(\gamma\boldsymbol{\theta}_l) - \boldsymbol{f}_{0m}(\gamma\boldsymbol{\theta}_l) - \boldsymbol{D\hat{f}}_m\boldsymbol{\psi}_l \right)' \boldsymbol{\omega}_m \left(\boldsymbol{f}_m(\gamma\boldsymbol{\theta}_l) - \boldsymbol{f}_{0m}(\gamma\boldsymbol{\theta}_l) - \boldsymbol{D\hat{f}}_m\boldsymbol{\psi}_l \right) \\
&\quad + \left(\boldsymbol{D\hat{f}}_d\boldsymbol{\psi}_l \right)' \boldsymbol{\omega}_d \, \boldsymbol{D\hat{f}}_d\boldsymbol{\psi}_l \Big) \Big/ (2p),
\end{aligned} \tag{44}$$

where $\boldsymbol{\theta}_l$ is computed using equations 40-42, and

$$\begin{aligned}
\boldsymbol{\psi}_l &= \left(\boldsymbol{D\hat{f}}'\boldsymbol{\omega}\boldsymbol{D\hat{f}} \right)^{-1} \boldsymbol{D\hat{f}}'\boldsymbol{\omega} \left(\boldsymbol{f}(\gamma\boldsymbol{\theta}_l) - \boldsymbol{f}_0(\gamma\boldsymbol{\theta}_l) \right) \\
&= \left(\boldsymbol{D\hat{f}}'\boldsymbol{\omega}\boldsymbol{D\hat{f}} \right)^{-1} \boldsymbol{D\hat{f}}_m'\boldsymbol{\omega}_m \left(\boldsymbol{f}_m(\gamma\boldsymbol{\theta}_l) - \boldsymbol{f}_{0m}(\gamma\boldsymbol{\theta}_l) \right).
\end{aligned} \tag{45}$$

The measure $aps^2\hat{N}_{\min}$ is similar to the second expected value in $\hat{\gamma}_I\sigma_\varepsilon^4$ given by equation 25. Hence, the measure provides another test of the importance of model intrinsic nonlinearity in c_r, c_c, and c_p in addition to the test using the term $(\boldsymbol{Y}-\boldsymbol{f}(\boldsymbol{\gamma}\hat{\boldsymbol{\theta}}))'\boldsymbol{\omega}^{1/2}\boldsymbol{R}\boldsymbol{\omega}^{1/2}(\boldsymbol{Y}-\boldsymbol{f}(\boldsymbol{\gamma}\hat{\boldsymbol{\theta}}))$ given after equation 29. By analogy with the former test, $aps^2\hat{N}_{\min}$ should be much smaller than $S(\hat{\boldsymbol{\theta}})$ when applied as a test of the size of $\hat{\gamma}_I\sigma_\varepsilon^4$ and should be much smaller than aps^2 when applied as a test of the size of $\gamma_{Ir}\sigma_\varepsilon^4$. Therefore, the test criterion for $\hat{\gamma}_I\sigma_\varepsilon^4$ is that $\hat{N}_{\min}$ should be much smaller than $(n\text{–}ap)/(ap)$, and the test criterion for $\gamma_{Ir}\sigma_\varepsilon^4$ is that $\hat{N}_{\min}$ should be much smaller than 1. The ranking used to classify nonlinearity for $\hat{N}$ also can be used for $\hat{N}_{\min}$ because $\hat{N}_{\min}$ is just the smallest possible value for $\hat{N}$.

A Measure of Model Combined Intrinsic Nonlinearity for Confidence Intervals

Model combined intrinsic nonlinearity affects c_c because $\gamma_{Ic}\sigma_\varepsilon^4$ is a component of this correction factor. Cooley (2004, equation 6-20) expressed the component correction factor $\gamma_{Ic}\sigma_\varepsilon^4$ as

$$
\begin{aligned}
\gamma_{Ic}\sigma_\varepsilon^4 = 2E\Bigg(&\Big(\boldsymbol{f}(\boldsymbol{\gamma\theta}_*)-\boldsymbol{f}_0(\boldsymbol{\gamma\theta}_*)-\boldsymbol{f}(\boldsymbol{\gamma}\tilde{\boldsymbol{\theta}})+\boldsymbol{f}_0(\boldsymbol{\gamma}\tilde{\boldsymbol{\theta}})\Big)'\boldsymbol{\omega}^{1/2} \\
&-\Big(g(\boldsymbol{\gamma\theta}_*)-g_0(\boldsymbol{\gamma\theta}_*)-g(\boldsymbol{\gamma}\tilde{\boldsymbol{\theta}})+g_0(\boldsymbol{\gamma}\tilde{\boldsymbol{\theta}})\Big)\frac{\boldsymbol{Q}'}{\boldsymbol{Q}'\boldsymbol{Q}}\Bigg)\left(\boldsymbol{I}-\boldsymbol{R}+\frac{\boldsymbol{QQ}'}{\boldsymbol{Q}'\boldsymbol{Q}}\right)\boldsymbol{\omega}^{1/2}\big(\boldsymbol{Y}-\boldsymbol{f}(\boldsymbol{\gamma\theta}_*)\big) \\
&+E\Bigg(\Big(\boldsymbol{f}(\boldsymbol{\gamma\theta}_*)-\boldsymbol{f}_0(\boldsymbol{\gamma\theta}_*)-\boldsymbol{f}(\boldsymbol{\gamma}\tilde{\boldsymbol{\theta}})+\boldsymbol{f}_0(\boldsymbol{\gamma}\tilde{\boldsymbol{\theta}})\Big)'\boldsymbol{\omega}^{1/2} \\
&-\Big(g(\boldsymbol{\gamma\theta}_*)-g_0(\boldsymbol{\gamma\theta}_*)-g(\boldsymbol{\gamma}\tilde{\boldsymbol{\theta}})+g_0(\boldsymbol{\gamma}\tilde{\boldsymbol{\theta}})\Big)\frac{\boldsymbol{Q}'}{\boldsymbol{Q}'\boldsymbol{Q}}\Bigg)\left(\boldsymbol{I}-\boldsymbol{R}+\frac{\boldsymbol{QQ}'}{\boldsymbol{Q}'\boldsymbol{Q}}\right)\cdot \\
&\left(\boldsymbol{\omega}^{1/2}\Big(\boldsymbol{f}(\boldsymbol{\gamma\theta}_*)-\boldsymbol{f}_0(\boldsymbol{\gamma\theta}_*)-\boldsymbol{f}(\boldsymbol{\gamma}\tilde{\boldsymbol{\theta}})+\boldsymbol{f}_0(\boldsymbol{\gamma}\tilde{\boldsymbol{\theta}})\Big)-\frac{\boldsymbol{Q}}{\boldsymbol{Q}'\boldsymbol{Q}}\Big(g(\boldsymbol{\gamma\theta}_*)-g_0(\boldsymbol{\gamma\theta}_*)-g(\boldsymbol{\gamma}\tilde{\boldsymbol{\theta}})+g_0(\boldsymbol{\gamma}\tilde{\boldsymbol{\theta}})\Big)\right) \\
&+E\left(\Big(\boldsymbol{Y}-\boldsymbol{f}(\boldsymbol{\gamma}\tilde{\boldsymbol{\theta}})\Big)'\boldsymbol{\omega}^{1/2}\left(\boldsymbol{R}-\frac{\boldsymbol{QQ}'}{\boldsymbol{Q}'\boldsymbol{Q}}\right)\boldsymbol{\omega}^{1/2}\Big(\boldsymbol{Y}-\boldsymbol{f}(\boldsymbol{\gamma}\tilde{\boldsymbol{\theta}})\Big)\right)-\hat{\gamma}_I\sigma_\varepsilon^4,
\end{aligned}
\tag{46}
$$

where $g(\boldsymbol{\gamma\theta})$, with $\boldsymbol{\theta}=\boldsymbol{\theta}_*$ or $\tilde{\boldsymbol{\theta}}$, is a model prediction for which a confidence interval is to be computed, $g_0(\boldsymbol{\gamma\theta})$ is the linearized approximation of it analogous to $\boldsymbol{f}_0(\boldsymbol{\gamma\theta})$, and $\tilde{\boldsymbol{\theta}}$ is the weighted regression estimate of $\boldsymbol{\theta}_*$ that is constrained so that $g(\boldsymbol{\gamma\theta}_*)=g(\boldsymbol{\gamma}\tilde{\boldsymbol{\theta}})$.

Cooley (2004, p. 86-87) developed a measure of model combined intrinsic nonlinearity, $\hat{M}_{\min}$, similar to the second expected value in equation 46. As for $\hat{N}_{\min}$, the measure is defined in terms of a likelihood region centered on $\bar{\boldsymbol{\theta}}$, but this time having diameter $\xi b\sigma_\varepsilon^2$, where

$$
\xi=\boldsymbol{Q}'(\boldsymbol{\omega}/b)^{1/2}\boldsymbol{\Omega}(\boldsymbol{\omega}/b)^{1/2}\boldsymbol{Q}/\boldsymbol{Q}'\boldsymbol{Q}=\Big(\boldsymbol{Q}_m'(\boldsymbol{\omega}_m/b)^{1/2}\boldsymbol{\Omega}_m(\boldsymbol{\omega}_m/b)^{1/2}\boldsymbol{Q}_m+\boldsymbol{Q}_d'\boldsymbol{Q}_d/b\Big)\Big/\boldsymbol{Q}'\boldsymbol{Q}\,. \tag{47}
$$

Thus, it is calculated using estimates as

$$\begin{aligned}\hat{M}_{\min} &= \frac{1}{\xi s^2}\sum_{l=1}^{2}\left(\boldsymbol{f}(\gamma\boldsymbol{\theta}_l)-\boldsymbol{f}_0(\gamma\boldsymbol{\theta}_l)-\boldsymbol{D}\hat{\boldsymbol{f}}\boldsymbol{\psi}_l\right)'\boldsymbol{\omega}\left(\boldsymbol{f}(\gamma\boldsymbol{\theta}_l)-\boldsymbol{f}_0(\gamma\boldsymbol{\theta}_l)-\boldsymbol{D}\hat{\boldsymbol{f}}\boldsymbol{\psi}_l\right)\Big/2\\ &= \frac{1}{\xi s^2}\sum_{l=1}^{2}\Big(\left(\boldsymbol{f}_m(\gamma\boldsymbol{\theta}_l)-\boldsymbol{f}_{0m}(\gamma\boldsymbol{\theta}_l)-\boldsymbol{D}\hat{\boldsymbol{f}}_m\boldsymbol{\psi}_l\right)'\boldsymbol{\omega}_m\left(\boldsymbol{f}_m(\gamma\boldsymbol{\theta}_l)-\boldsymbol{f}_{0m}(\gamma\boldsymbol{\theta}_l)-\boldsymbol{D}\hat{\boldsymbol{f}}_m\boldsymbol{\psi}_l\right)\\ &+\left(\boldsymbol{D}\hat{\boldsymbol{f}}_d\boldsymbol{\psi}_l\right)'\boldsymbol{\omega}_d\,\boldsymbol{D}\hat{\boldsymbol{f}}_d\boldsymbol{\psi}_l\Big)\Big/2,\end{aligned} \tag{48}$$

where $\boldsymbol{\theta}_l$ is given by Cooley (2004, p. 87) as

$$\boldsymbol{\theta}_l = \hat{\boldsymbol{\theta}} \pm \left(\frac{\xi s^2}{\hat{\boldsymbol{Q}}'\hat{\boldsymbol{Q}}}\right)^{1/2}\left(\boldsymbol{D}\hat{\boldsymbol{f}}'\boldsymbol{\omega}\boldsymbol{D}\hat{\boldsymbol{f}}\right)^{-1}\boldsymbol{D}\hat{g}', \tag{49}$$

in which the carets over $\boldsymbol{f}$, g, and $\boldsymbol{Q}$ indicate evaluation using $\boldsymbol{\theta}=\hat{\boldsymbol{\theta}}$,

$$\boldsymbol{\psi}_l = \boldsymbol{\psi}_l^0 + \frac{\left(\boldsymbol{D}\hat{\boldsymbol{f}}'\boldsymbol{\omega}\boldsymbol{D}\hat{\boldsymbol{f}}\right)^{-1}\boldsymbol{D}\hat{g}'}{\hat{\boldsymbol{Q}}'\hat{\boldsymbol{Q}}}\left(g(\gamma\boldsymbol{\theta}_l)-g_0(\gamma\boldsymbol{\theta}_l)\right) \tag{50}$$

and

$$\begin{aligned}\boldsymbol{\psi}_l^0 &= -\left(\frac{\left(\boldsymbol{D}\hat{\boldsymbol{f}}'\boldsymbol{\omega}\boldsymbol{D}\hat{\boldsymbol{f}}\right)^{-1}\boldsymbol{D}\hat{g}'\hat{\boldsymbol{Q}}'}{\hat{\boldsymbol{Q}}'\hat{\boldsymbol{Q}}}-\left(\boldsymbol{D}\hat{\boldsymbol{f}}'\boldsymbol{\omega}\boldsymbol{D}\hat{\boldsymbol{f}}\right)^{-1}\boldsymbol{D}\hat{\boldsymbol{f}}'\boldsymbol{\omega}^{1/2}\right)\boldsymbol{\omega}^{1/2}\left(\boldsymbol{f}(\gamma\boldsymbol{\theta}_l)-\boldsymbol{f}_0(\gamma\boldsymbol{\theta}_l)\right)\\ &= -\left(\frac{\left(\boldsymbol{D}\hat{\boldsymbol{f}}'\boldsymbol{\omega}\boldsymbol{D}\hat{\boldsymbol{f}}\right)^{-1}\boldsymbol{D}\hat{g}'\hat{\boldsymbol{Q}}_m'}{\hat{\boldsymbol{Q}}'\hat{\boldsymbol{Q}}}-\left(\boldsymbol{D}\hat{\boldsymbol{f}}'\boldsymbol{\omega}\boldsymbol{D}\hat{\boldsymbol{f}}\right)^{-1}\boldsymbol{D}\hat{\boldsymbol{f}}_m'\boldsymbol{\omega}_m^{1/2}\right)\boldsymbol{\omega}_m^{1/2}\left(\boldsymbol{f}_m(\gamma\boldsymbol{\theta}_l)-\boldsymbol{f}_{0m}(\gamma\boldsymbol{\theta}_l)\right).\end{aligned} \tag{51}$$

Note that the diameter of the linear likelihood region ξs^2 can be written in terms of c_c as evaluated in CORFAC-2k (which assumes no model combined intrinsic nonlinearity) as

$$\xi s^2 = \frac{\boldsymbol{Q}'(\boldsymbol{\omega}/b)^{1/2}\,\boldsymbol{\Omega}(\boldsymbol{\omega}/b)^{1/2}\,\boldsymbol{Q}}{\boldsymbol{Q}'\boldsymbol{Q}}\,\frac{S(\hat{\boldsymbol{\theta}})}{n-ap} = \frac{(n-p)\boldsymbol{Q}'(\boldsymbol{\omega}/b)^{1/2}\,\boldsymbol{\Omega}(\boldsymbol{\omega}/b)^{1/2}\,\boldsymbol{Q}}{\boldsymbol{Q}'\boldsymbol{Q}(n-ap)}\,\frac{S(\hat{\boldsymbol{\theta}})}{n-p} = c_c\,\frac{S(\hat{\boldsymbol{\theta}})}{n-p}. \tag{52}$$

If $\boldsymbol{\Omega}$ is unknown so that c_c cannot be exactly computed, then the approximate bound for c_c given by equation 83 derived in the sub-section titled 'The CORFAC-2k Program' can be used. In all cases, $\boldsymbol{Q}$ is replaced with $\hat{\boldsymbol{Q}}$ to make the calculations.

Note that $\gamma_{Ic}\sigma_\varepsilon^4$ as defined by equation 46 contains $\hat{\gamma}_I\sigma_\varepsilon^4$. A measure similar to the sum $(\gamma_{Ic}+\hat{\gamma}_I)\sigma_\varepsilon^4$ uses two components in addition to $\hat{M}_{\min}$. These are (Cooley, 2004, p. 86)

$$\hat{B}_U = \frac{1}{\xi s^2}\sum_{l=1}^{2}\left(g(\gamma\boldsymbol{\theta}_l) - g_0(\gamma\boldsymbol{\theta}_l)\right)^2 \Big/ \left(2\hat{\boldsymbol{Q}}'\hat{\boldsymbol{Q}}\right) \tag{53}$$

and

$$\begin{aligned}\hat{B}_L &= \frac{1}{\xi s^2}\sum_{l=1}^{2}\left(\boldsymbol{f}(\gamma\boldsymbol{\theta}_l) - \boldsymbol{f}_0(\gamma\boldsymbol{\theta}_l) - \boldsymbol{D}\hat{\boldsymbol{f}}\boldsymbol{\psi}_l^0\right)' \boldsymbol{\omega}\left(\boldsymbol{f}(\gamma\boldsymbol{\theta}_l) - \boldsymbol{f}_0(\gamma\boldsymbol{\theta}_l) - \boldsymbol{D}\hat{\boldsymbol{f}}\boldsymbol{\psi}_l^0\right)\Big/2 \\ &= \frac{1}{\xi s^2}\sum_{l=1}^{2}\left(\left(\boldsymbol{f}_m(\gamma\boldsymbol{\theta}_l) - \boldsymbol{f}_{0m}(\gamma\boldsymbol{\theta}_l) - \boldsymbol{D}\hat{\boldsymbol{f}}_m\boldsymbol{\psi}_l^0\right)' \boldsymbol{\omega}_m\left(\boldsymbol{f}_m(\gamma\boldsymbol{\theta}_l) - \boldsymbol{f}_{0m}(\gamma\boldsymbol{\theta}_l) - \boldsymbol{D}\hat{\boldsymbol{f}}_m\boldsymbol{\psi}_l^0\right)\right. \\ &\left. + \left(\boldsymbol{D}\hat{\boldsymbol{f}}_d\boldsymbol{\psi}_l^0\right)'\boldsymbol{\omega}_d\boldsymbol{D}\hat{\boldsymbol{f}}_d\boldsymbol{\psi}_l^0\right)\Big/2.\end{aligned} \tag{54}$$

The measure of model combined intrinsic nonlinearity related to the sum is given by the maximum in absolute value of $\hat{M}_{\min} + 2\hat{B}_U$ and $\hat{M}_{\min} - 2\hat{B}_L$ (Cooley, 2004, p. 87).

From Cooley (2004, equation 5-49), model combined intrinsic nonlinearity is negligible in the correction factor c_c if $\left|\gamma_{Ic}\sigma_\varepsilon^4\right| << \sigma_\varepsilon^2 + \gamma_{wc}\sigma_\beta^2 = \boldsymbol{Q}'(\boldsymbol{\omega}/b)^{1/2}\boldsymbol{\Omega}(\boldsymbol{\omega}/b)^{1/2}\boldsymbol{Q}b\sigma_\varepsilon^2 / \boldsymbol{Q}'\boldsymbol{Q} = \xi b\sigma_\varepsilon^2$. Thus, $(\gamma_{Ic} + \hat{\gamma}_I)\sigma_\varepsilon^4 / (\xi b\sigma_\varepsilon^2)$ should be much greater than $(\xi b\sigma_\varepsilon^2 + apb\sigma_\varepsilon^2)/(\xi b\sigma_\varepsilon^2) = (\xi + ap)/\xi$, which has a value greater than 1, so that, as a conservative test criterion, $\hat{M}_{\min} + 2\hat{B}_U$ and $\left|\hat{M}_{\min} - 2\hat{B}_L\right|$ should both be much less than 1. It is likely that the same ranking used to classify nonlinearity for $\hat{N}$ also can be used to classify model intrinsic nonlinearity for its measure, although this ranking might be conservative in the present instance.

Cooley (2004, p. 66) showed that when model intrinsic nonlinearity and model combined intrinsic nonlinearity both are small, standard linear confidence intervals are accurate approximations of nonlinear intervals. Thus, because $\hat{M}_{\min}$ measures the magnitude of these two sources of nonlinearity, $\hat{M}_{\min}$ can be used to indicate when standard linear confidence intervals can be used. On the basis of preliminary results given by Cooley (2004, section 7), linear confidence intervals should be good approximations when $\hat{M}_{\min} \leq 0.01$.

A Measure of Model Combined Intrinsic Nonlinearity for Prediction Intervals

The development and measure of model combined intrinsic nonlinearity for prediction intervals is analogous to the development and measure for confidence intervals. The measure for prediction intervals was not explicitly derived by Cooley (2004) but follows from the equations derived for confidence intervals with some added terms obtained from equations 6-50 - 6-55 of Cooley (2004, p. 84-85). For the prediction intervals calculated by UNC, the diameter of the likelihood region analogous to ξs^2 is $\xi_a s^2$, where ξ_a is defined using equation 7-12 from Cooley (2004, p. 113) as

$$\xi_a = \frac{\boldsymbol{Q}'(\boldsymbol{\omega}/b)^{1/2}\boldsymbol{\Omega}(\boldsymbol{\omega}/b)^{1/2}\boldsymbol{Q} - 2\omega_p^{-1/2}(\omega_p/b)^{1/2}\boldsymbol{C}'(\boldsymbol{\omega}/b)^{1/2}\boldsymbol{Q} + \hat{\omega}_p^{-1}}{\boldsymbol{Q}'\boldsymbol{Q} + \omega_p^{-1}}$$
$$= \frac{\boldsymbol{Q}_m'(\boldsymbol{\omega}_m/b)^{1/2}\boldsymbol{\Omega}_m(\boldsymbol{\omega}_m/b)^{1/2}\boldsymbol{Q}_m + \boldsymbol{Q}_d'\boldsymbol{Q}_d/b - 2\omega_p^{-1/2}(\omega_p/b)^{1/2}\boldsymbol{C}_m'(\boldsymbol{\omega}_m/b)^{1/2}\boldsymbol{Q}_m + \hat{\omega}_p^{-1}}{\boldsymbol{Q}'\boldsymbol{Q} + \omega_p^{-1}}. \tag{55}$$

We assume in this report that errors $Y_p - g(\gamma\boldsymbol{\theta}_*)$ in predictions are not correlated with errors $\boldsymbol{Y}_d - \boldsymbol{f}_d(\gamma\boldsymbol{\theta}_*)$ in direct information so that $\boldsymbol{C}_d = \boldsymbol{0}$. The three measures analogous to equations 48, 53, and 54 are

$$\hat{M}^a_{\min} = \frac{1}{\xi_a s^2}\sum_{l=1}^{2}\Big(\big(\boldsymbol{f}(\gamma\boldsymbol{\theta}_l) - \boldsymbol{f}_0(\gamma\boldsymbol{\theta}_l) - \boldsymbol{D}\hat{\boldsymbol{f}}\boldsymbol{\psi}_{al}\big)'\boldsymbol{\omega}\big(\boldsymbol{f}(\gamma\boldsymbol{\theta}_l) - \boldsymbol{f}_0(\gamma\boldsymbol{\theta}_l) - \boldsymbol{D}\hat{\boldsymbol{f}}\boldsymbol{\psi}_{al}\big)$$
$$+ \psi_{pl}\omega_p\psi_{pl}\Big)/2$$
$$= \frac{1}{\xi_a s^2}\sum_{l=1}^{2}\Big(\big(\boldsymbol{f}_m(\gamma\boldsymbol{\theta}_l) - \boldsymbol{f}_{0m}(\gamma\boldsymbol{\theta}_l) - \boldsymbol{D}\hat{\boldsymbol{f}}_m\boldsymbol{\psi}_{al}\big)'\boldsymbol{\omega}_m\big(\boldsymbol{f}_m(\gamma\boldsymbol{\theta}_l) - \boldsymbol{f}_{0m}(\gamma\boldsymbol{\theta}_l) - \boldsymbol{D}\hat{\boldsymbol{f}}_m\boldsymbol{\psi}_{al}\big) \tag{56}$$
$$+ \big(\boldsymbol{D}\hat{\boldsymbol{f}}_d\boldsymbol{\psi}_{al}\big)'\boldsymbol{\omega}_d\boldsymbol{D}\hat{\boldsymbol{f}}_d\boldsymbol{\psi}_{al} + \psi_{pl}\omega_p\psi_{pl}\Big)/2,$$

$$\hat{B}^a_U = \frac{1}{\xi_a s^2}\sum_{l=1}^{2}\big(g(\gamma\boldsymbol{\theta}_l) - g_0(\gamma\boldsymbol{\theta}_l)\big)^2\Big/\Big(2\big(\hat{\boldsymbol{Q}}'\hat{\boldsymbol{Q}} + \omega_p^{-1}\big)\Big), \tag{57}$$

and

$$\hat{B}^a_L = \frac{1}{\xi_a s^2}\sum_{l=1}^{2}\Big(\big(\boldsymbol{f}(\gamma\boldsymbol{\theta}_l) - \boldsymbol{f}_0(\gamma\boldsymbol{\theta}_l) - \boldsymbol{D}\hat{\boldsymbol{f}}\boldsymbol{\psi}^0_{al}\big)'\boldsymbol{\omega}\big(\boldsymbol{f}(\gamma\boldsymbol{\theta}_l) - \boldsymbol{f}_0(\gamma\boldsymbol{\theta}_l) - \boldsymbol{D}\hat{\boldsymbol{f}}\boldsymbol{\psi}^0_{al}\big) + \psi^0_{pl}\omega_p\psi^0_{pl}\Big)/2$$
$$= \frac{1}{\xi_a s^2}\sum_{l=1}^{2}\Big(\big(\boldsymbol{f}_m(\gamma\boldsymbol{\theta}_l) - \boldsymbol{f}_{0m}(\gamma\boldsymbol{\theta}_l) - \boldsymbol{D}\hat{\boldsymbol{f}}_m\boldsymbol{\psi}^0_{al}\big)'\boldsymbol{\omega}_m\big(\boldsymbol{f}_m(\gamma\boldsymbol{\theta}_l) - \boldsymbol{f}_{0m}(\gamma\boldsymbol{\theta}_l) - \boldsymbol{D}\hat{\boldsymbol{f}}_m\boldsymbol{\psi}^0_{al}\big) \tag{58}$$
$$+ \big(\boldsymbol{D}\hat{\boldsymbol{f}}_d\boldsymbol{\psi}^0_{al}\big)'\boldsymbol{\omega}_d\boldsymbol{D}\hat{\boldsymbol{f}}_d\boldsymbol{\psi}^0_{al} + \psi^0_{pl}\omega_p\psi^0_{pl}\Big)/2,$$

where $\boldsymbol{\theta}_l$ is obtained from equation H-12 in Cooley (2004, p. 205) as

$$\boldsymbol{\theta}_l = \hat{\boldsymbol{\theta}} \pm \left(\frac{\xi_a s^2}{\hat{\boldsymbol{Q}}'\hat{\boldsymbol{Q}} + \omega_p^{-1}}\right)^{1/2}\big(\boldsymbol{D}\hat{\boldsymbol{f}}'\boldsymbol{\omega}\boldsymbol{D}\hat{\boldsymbol{f}}\big)^{-1}\boldsymbol{D}\hat{g}', \tag{59}$$

and remaining variables are obtained straightforwardly from equations 6-51 - 6-55 in Cooley (2004, p. 84-85) as

$$\boldsymbol{\psi}_{al} = \boldsymbol{\psi}_{al}^{0} + \frac{\left(\boldsymbol{D}\hat{\boldsymbol{f}}'\boldsymbol{\omega}\boldsymbol{D}\hat{\boldsymbol{f}}\right)^{-1}\boldsymbol{D}\hat{g}'}{\hat{\boldsymbol{Q}}'\hat{\boldsymbol{Q}} + \omega_p^{-1}}\left(g(\gamma\boldsymbol{\theta}_l) - g_0(\gamma\boldsymbol{\theta}_l)\right), \tag{60}$$

$$\begin{aligned}\boldsymbol{\psi}_{al}^{0} &= -\left(\frac{\left(\boldsymbol{D}\hat{\boldsymbol{f}}'\boldsymbol{\omega}\boldsymbol{D}\hat{\boldsymbol{f}}\right)^{-1}\boldsymbol{D}\hat{g}'\hat{\boldsymbol{Q}}'}{\hat{\boldsymbol{Q}}'\hat{\boldsymbol{Q}} + \omega_p^{-1}} - \left(\boldsymbol{D}\hat{\boldsymbol{f}}'\boldsymbol{\omega}\boldsymbol{D}\hat{\boldsymbol{f}}\right)^{-1}\boldsymbol{D}\hat{\boldsymbol{f}}'\boldsymbol{\omega}^{1/2}\right)\boldsymbol{\omega}^{1/2}\left(\boldsymbol{f}(\gamma\boldsymbol{\theta}_l) - \boldsymbol{f}_0(\gamma\boldsymbol{\theta}_l)\right) \\ &= -\left(\frac{\left(\boldsymbol{D}\hat{\boldsymbol{f}}'\boldsymbol{\omega}\boldsymbol{D}\hat{\boldsymbol{f}}\right)^{-1}\boldsymbol{D}\hat{g}'\hat{\boldsymbol{Q}}_m'}{\hat{\boldsymbol{Q}}'\hat{\boldsymbol{Q}} + \omega_p^{-1}} - \left(\boldsymbol{D}\hat{\boldsymbol{f}}'\boldsymbol{\omega}\boldsymbol{D}\hat{\boldsymbol{f}}\right)^{-1}\boldsymbol{D}\hat{\boldsymbol{f}}_m'\boldsymbol{\omega}_m^{1/2}\right)\boldsymbol{\omega}_m^{1/2}\left(\boldsymbol{f}_m(\gamma\boldsymbol{\theta}_l) - \boldsymbol{f}_{0m}(\gamma\boldsymbol{\theta}_l)\right),\end{aligned} \tag{61}$$

$$\psi_{pl} = \psi_{pl}^{0} - \frac{\omega_p^{-1}}{\hat{\boldsymbol{Q}}'\hat{\boldsymbol{Q}} + \omega_p^{-1}}\left(g(\gamma\boldsymbol{\theta}_l) - g_0(\gamma\boldsymbol{\theta}_l)\right), \tag{62}$$

$$\begin{aligned}\psi_{pl}^{0} &= \frac{\omega_p^{-1}}{\hat{\boldsymbol{Q}}'\hat{\boldsymbol{Q}} + \omega_p^{-1}}\hat{\boldsymbol{Q}}'\boldsymbol{\omega}^{1/2}\left(\boldsymbol{f}(\gamma\boldsymbol{\theta}_l) - \boldsymbol{f}_0(\gamma\boldsymbol{\theta}_l)\right) \\ &= \frac{\omega_p^{-1}}{\hat{\boldsymbol{Q}}'\hat{\boldsymbol{Q}} + \omega_p^{-1}}\hat{\boldsymbol{Q}}_m'\boldsymbol{\omega}_m^{1/2}\left(\boldsymbol{f}_m(\gamma\boldsymbol{\theta}_l) - \boldsymbol{f}_{0m}(\gamma\boldsymbol{\theta}_l)\right).\end{aligned} \tag{63}$$

The criteria for assessing the importance of model combined intrinsic nonlinearity in c_p are completely analogous to the criteria pertaining to c_c; equations 5-93 and 7-12 of Cooley (2004) replace equation 5-49 of Cooley (2004) in the development. Thus, $\hat{M}_{\min}^{a} + 2\hat{B}_U^{a}$ and $\left|\hat{M}_{\min}^{a} - 2\hat{B}_L^{a}\right|$ should be much less than 1, and the ranking used to classify nonlinearity for $\hat{N}$ can again be used to classify model combined nonlinearity for its measures.

The measure $\hat{M}_{\min}^{a}$ can be used in the same way as $\hat{M}_{\min}$ was used for confidence intervals to indicate when standard linear prediction intervals should be accurate approximations of nonlinear ones. Thus, linear prediction intervals should be good approximations of nonlinear ones when $\hat{M}_{\min}^{a} \leq 0.01$.

The CORFAC-2k Program

The purpose of CORFAC-2k is to compute correction factors c_r, c_c, and c_p, together with components of them, assuming that model intrinsic nonlinearity and model combined intrinsic nonlinearity are negligible. The component correction factors $\hat{\gamma}_w\sigma_\beta^2$, $\gamma_{wr}\sigma_\beta^2$, $\gamma_{wc}\sigma_\beta^2$, and $\gamma_{wa}\sigma_\beta^2$ are equal to zero when weight matrix $\boldsymbol{\omega}$ is equal to the inverse of the matrix $\boldsymbol{\Omega}$. When $\boldsymbol{\Omega}$ is unknown, approximations and bounds are developed for the correction factors.

Calculation of the Correction Factors When $\boldsymbol{\Omega}$ Is Known

Component correction factor $\hat{\gamma}_w\sigma_\beta^2$ is defined using equations 5-10 and F-133 of Cooley (2004) as

$$\hat{\gamma}_w\sigma_\beta^2 = \left(\left(b-1\right)n - \left(ba-1\right)p\right)\sigma_\varepsilon^2, \tag{64}$$

and $\gamma_{wr}\sigma_\beta^2$ is defined using equations 5-12 and F-135 of Cooley (2004) as

$$\gamma_{wr}\sigma_\beta^2 = \left(ba-1\right)p\sigma_\varepsilon^2, \tag{65}$$

where a and b are given by equations 26 and 27 and $a \geq 1$ (Cooley, 2004, p. 52). Note that if $b \geq 1$, then $\hat{\gamma}_w\sigma_\beta^2 \leq 0$, and if $b = 1$, then $\hat{\gamma}_w\sigma_\beta^2 = -\gamma_{wr}\sigma_\beta^2$. Correction factor c_r is obtained by combining equations 64 and 65 according to equation 22, assuming $\hat{\gamma}_I\sigma_\varepsilon^4$ and $\gamma_{Ir}\sigma_\varepsilon^4$ are both zero, to get

$$c_r = \frac{\left(n-p\right)a}{n-ap}. \tag{66}$$

Note from equations 26 and 27 that if $\boldsymbol{\omega}$ is proportional to, but not equal to, $\boldsymbol{\Omega}^{-1}$, then $a = 1$, but $b \neq 1$ and component correction factors from equations 64 and 65 are both nonzero. However, b cancels when obtaining equation 66 so that $\boldsymbol{\omega}$ only has to be proportional to $\boldsymbol{\Omega}^{-1}$ for c_r to be equal to 1. Also note that at least when model intrinsic nonlinearity is negligible, $c_r \geq 1$, so that uncorrected confidence regions and uncorrected Scheffé intervals would be too small unless $\boldsymbol{\omega} \propto \boldsymbol{\Omega}^{-1}$. To compute c_r, a and thus $\boldsymbol{\Omega}$ have to be known.

Component correction factor $\gamma_{wc}\sigma_\beta^2$ is defined using equation F-146 of Cooley (2004, p. 187) and equation 47 as

$$\gamma_{wc}\sigma_\beta^2 = (b\xi - 1)\sigma_\varepsilon^2. \tag{67}$$

Variable ξ given by equation 52 is not necessarily greater than 1, so $\gamma_{wc}\sigma_\beta^2$ is not necessarily greater than zero. Correction factor c_c is obtained by combining equations 64 and 67 according to equation 23, assuming $\hat{\gamma}_I\sigma_\varepsilon^4$ and $\gamma_{Ic}\sigma_\varepsilon^4$ are both zero, to get

$$c_c = \frac{\left(n-p\right)\xi}{n-ap}, \tag{68}$$

where again $\boldsymbol{\omega}$ only has to be proportional to $\boldsymbol{\Omega}$ for c_c to equal 1. Matrix $\boldsymbol{\Omega}$ has to be known in order to compute c_c.

Finally, component correction factor $\gamma_{wa}\sigma_\beta^2$ is defined using equation 5-93 of Cooley (2004, p. 63) and equation 55 as

$$\gamma_{wa}\sigma_\beta^2 = \left(b\xi_a - 1\right)\sigma_\varepsilon^2. \tag{69}$$

As for equation 67, ξ_a is not necessarily greater than 1, so $\gamma_{wa}\sigma_\beta^2$ is not necessarily greater than zero. Correction factor c_p is obtained by combining equations 64 and 69 according to equation 24, assuming $\hat{\gamma}_I\sigma_\varepsilon^4$ and $\gamma_{Ia}\sigma_\varepsilon^4$ are both zero, to get

$$c_p = \frac{(n-p)\xi_a}{n-ap}, \tag{70}$$

which behaves like c_c does. However, c_p can differ from 1 even when $\boldsymbol{\omega}$ is equal to $\boldsymbol{\Omega}^{-1}$ because of the term involving $\boldsymbol{C}$ in equation 55.

Approximate Calculation of the Correction Factors When $\boldsymbol{\Omega}$ Is Unknown

When $\boldsymbol{\Omega}_m$ is unknown, a, ξ, and ξ_a must be approximated. To obtain the approximations, we set $\boldsymbol{\omega}_m$ equal to the diagonal weight matrix $\hat{\boldsymbol{\omega}}_m$ composed of the inverses of the diagonals of $\boldsymbol{\Omega}_m$, we let $\boldsymbol{\omega}_d = \hat{\boldsymbol{\omega}}_d = \boldsymbol{\Omega}_d^{-1}$, and we set ω_p equal to $\hat{\omega}_p$. (Usually, $\hat{\boldsymbol{\omega}}_m$ will only be an approximation of the inverse of the diagonals of $\boldsymbol{\Omega}_m$. This is discussed briefly later in this section.) Then we make use of approximations from equations 5-20, 5-56, and 5-117 of Cooley (2004). To approximate a we use equation 5-20 in equation 5-10 of Cooley (2004), noting that b=1 and $\boldsymbol{\omega}_d = \boldsymbol{\Omega}_d^{-1}$ so that equation 5-20 need only be applied to the model function partition. Therefore,

$$tr\left(\left(\boldsymbol{I}_m - \hat{\boldsymbol{R}}_m\right)\left((1-c)\boldsymbol{I}_m + c\boldsymbol{1}_m\right)\right) + tr\left(\boldsymbol{I}_d - \hat{\boldsymbol{R}}_d\right) = (1-c)t_m + cs_m + t_d = n - ap, \tag{71}$$

where c is an effective correlation, $\boldsymbol{1}_m$ is an $n_m \times n_m$ matrix of 1's, partitions of $\hat{\boldsymbol{R}}$ are partitions of $\boldsymbol{R}$ computed using $\hat{\boldsymbol{\omega}}$, and the traces are evaluated as

$$t_m = tr\left(\left(\boldsymbol{I}_m - \hat{\boldsymbol{R}}_m\right)\boldsymbol{I}_m\right) = \sum_{i=1}^{n_m}\left(1 - \hat{r}_{ii}\right) = n_m - \sum_{i=1}^{n_m}\hat{r}_{ii}, \tag{72}$$

$$s_m = tr\left(\left(\boldsymbol{I}_m - \hat{\boldsymbol{R}}_m\right)\boldsymbol{1}_m\right) = \sum_{i=1}^{n_m}\sum_{j=1}^{n_m}\left(\delta_{ij} - \hat{r}_{ij}\right) = n_m - \sum_{i=1}^{n_m}\sum_{j=1}^{n_m}\hat{r}_{ij}, \tag{73}$$

$$t_d = tr\left(\boldsymbol{I}_d - \hat{\boldsymbol{R}}_d\right) = \sum_{i=n_m+1}^{n}\left(1 - \hat{r}_{ii}\right) = n_d - \sum_{i=n_m+1}^{n}\hat{r}_{ii}. \tag{74}$$

In equations 72-74, $\hat{r}_{ij}$ is an element of $\hat{\boldsymbol{R}}$ and δ_{ij} is the Kronecker delta ($\delta_{ij} = 1$ when $i = j$ and $\delta_{ij} = 0$ when $i \neq j$).

Equation 71 can be solved for c by making use of the fact that $t_m + t_d = n - p$. The result is

$$c = \frac{(a-1)p}{t_m - s_m}, \tag{75}$$

which can serve as a definition of *c*. Note that if $t_m > s_m, c \geq 0$. The condition $t_m > s_m$ has always been found to hold. If *c* is presumed known, then equation 75 can be solved for *a* to get

$$a = \frac{c}{p}(t_m - s_m) + 1, \tag{76}$$

which has a lower bound of *a*=1 when *c*=0 and an upper bound of $1 + (t_m - s_m)/p$ when *c*=1. By assuming a reasonable upper limit for *c*, c_e, an approximate upper limit for *a* can be computed using equation 76.

The variable ξ can be bounded using equation 5-56 from Cooley (2004, p. 56). However, a more refined approximation can be obtained as follows. From equation 5-56 from Cooley (2004) and the fact that the approximation need not be applied for the direct information,

$$\xi = \left(\hat{\boldsymbol{Q}}_m' \hat{\boldsymbol{\omega}}_m^{1/2} \boldsymbol{\Omega}_m \hat{\boldsymbol{\omega}}_m^{1/2} \hat{\boldsymbol{Q}}_m + \hat{\boldsymbol{Q}}_d' \hat{\boldsymbol{Q}}_d\right) / \hat{\boldsymbol{Q}}' \hat{\boldsymbol{Q}} \leq \left(V_{mx} + \hat{\boldsymbol{Q}}_d' \hat{\boldsymbol{Q}}_d\right) / \hat{\boldsymbol{Q}}' \hat{\boldsymbol{Q}}, \tag{77}$$

where

$$V_{mx} = \max_s \left(\sum_{i(s)} Q_{mi} \right)^2 \tag{78}$$

and the notation indicates the maximum of either the squared sum of positive values of the Q_{mi}'s or the squared sum of negative values of the Q_{mi}'s (Cooley, 2004, p. 55-56). Also, if $\boldsymbol{\Omega}_m$ is diagonal so that $\hat{\boldsymbol{\omega}}_m^{1/2} \boldsymbol{\Omega}_m \hat{\boldsymbol{\omega}}_m^{1/2} = \boldsymbol{I}_m$, then $\hat{\boldsymbol{Q}}_m' \hat{\boldsymbol{\omega}}_m^{1/2} \boldsymbol{\Omega}_m \hat{\boldsymbol{\omega}}_m^{1/2} \hat{\boldsymbol{Q}}_m = \hat{\boldsymbol{Q}}_m' \hat{\boldsymbol{Q}}_m$ so that $\xi = 1$. Therefore, a value of $c_e \leq 1$ always exists so that

$$\xi \leq \left((1 - c_e) \hat{\boldsymbol{Q}}_m' \hat{\boldsymbol{Q}}_m + c_e V_{mx} + \hat{\boldsymbol{Q}}_d' \hat{\boldsymbol{Q}}_d\right) / \hat{\boldsymbol{Q}}' \hat{\boldsymbol{Q}}. \tag{79}$$

It is almost certain that equation 79 with c_e<1 would produce a closer bound than equation 77.

Finally, ξ_a is bounded using equation 5-117 of Cooley (2004, p. 68) and a development completely analogous to the one used to obtain equation 79 to obtain

$$\xi_a \leq \left((1 - c_e)\left(\hat{\boldsymbol{Q}}_m' \hat{\boldsymbol{Q}}_m + \hat{\omega}_p^{-1}\right) + c_e V_{mxa} + \hat{\boldsymbol{Q}}_d' \hat{\boldsymbol{Q}}_d\right) / \left(\hat{\boldsymbol{Q}}' \hat{\boldsymbol{Q}} + \hat{\omega}_p^{-1}\right), \tag{80}$$

where V_{mxa} is evaluated using equation 78 as

$$\left.\begin{aligned} &V_{mxa} = V_{mx} \quad \text{for} \sum_{i(s)} Q_{mi} \text{ as a sum of positive values} \\ &V_{mxa} = V_{mx} + 2\hat{\omega}_p^{-1/2} V_{mx}^{1/2} + \hat{\omega}_p^{-1} \quad \text{for} \sum_{i(s)} Q_{mi} \text{ as a sum of negative values} \end{aligned}\right\}. \tag{81}$$

Correction factors c_r, c_c, and c_p are approximated by letting $c = c_e$ and using equations 71, 76, 79, and 80 to get

$$c_r \approx \frac{n-p}{p} \frac{c_e(t_m - s_m) + p}{(1-c_e)t_m + c_e s_m + t_d}, \tag{82}$$

$$c_c \approx \frac{n-p}{\hat{\boldsymbol{Q}}'\hat{\boldsymbol{Q}}} \frac{(1-c_e)\hat{\boldsymbol{Q}}'_m \hat{\boldsymbol{Q}}_m + c_e V_{mx} + \hat{\boldsymbol{Q}}'_d \hat{\boldsymbol{Q}}_d}{(1-c_e)t_m + c_e s_m + t_d}, \tag{83}$$

and

$$c_p \approx \frac{n-p}{\hat{\boldsymbol{Q}}'\hat{\boldsymbol{Q}} + \hat{\omega}_p^{-1}} \frac{(1-c_e)\left(\hat{\boldsymbol{Q}}'_m \hat{\boldsymbol{Q}}_m + \hat{\omega}_p^{-1}\right) + c_e V_{mxa} + \hat{\boldsymbol{Q}}'_d \hat{\boldsymbol{Q}}_d}{(1-c_e)t_m + c_e s_m + t_d}. \tag{84}$$

Note that if c_e=0 is correct, then c_r=1, c_c=1, and c_p=1, which also are correct. If c_e=1, then c_r, c_c, and c_p, attain their maximum values, which could be very large because the denominators could be very small. For the correction factors examined thus far in tests by the authors of this report, c_e=0.8 has yielded bounds for all values of c_c and c_p. This value of c_e also has yielded bounds for most values of c_r and has yielded good approximations of c_r for the remainder.

For field problems $\hat{\boldsymbol{\omega}}_m$ will only be an approximation of the matrix of inverses of the diagonal elements of $\boldsymbol{\Omega}_m$. The results of example 2 of Cooley (2004, section 7) suggest that a reasonable estimate of $\hat{\boldsymbol{\omega}}_m$ yields very little error in the correction factors. Further work by the senior author suggests that use of the approximation for $\hat{\boldsymbol{\omega}}_m$ obtained for the Tude aa case studied by Christensen and Cooley (1999b) also yields very little error. It appears that careful hydrogeologic work can yield a satisfactory estimate for $\hat{\boldsymbol{\omega}}_m$.

Approximate Calculation of the Correction Factors When $\boldsymbol{\Omega}$ Is Partly Known

In order to make the approximations in equations 71, 76, 79, and 80, we assumed the matrix $\hat{\boldsymbol{\omega}}_m^{1/2} \boldsymbol{\Omega}_m \hat{\boldsymbol{\omega}}_m^{1/2}$ to be similar to a correlation matrix so that all elements have magnitudes ≤1 (Cooley, 2004, p. 48-49). This implies that $\hat{\boldsymbol{\omega}}_m$ is diagonal with elements equal to the inverses of the diagonal elements of $\boldsymbol{\Omega}_m$. Matrix $\boldsymbol{\Omega}_m$ has the form $\boldsymbol{V}_{\varepsilon m} + \boldsymbol{V}_m$, where $\boldsymbol{V}_{\varepsilon m}$ is the diagonal block in $\boldsymbol{V}_\varepsilon$ for model functions and $\boldsymbol{V}_m = E(\boldsymbol{f}_m(\boldsymbol{\beta}) - \boldsymbol{f}_m(\boldsymbol{\gamma\theta}_*))(\boldsymbol{f}_m(\boldsymbol{\beta}) - \boldsymbol{f}_m(\boldsymbol{\gamma\theta}_*))' / \sigma_\varepsilon^2$, which is the model-error second-moment matrix for model functions divided by σ_ε^2 (Cooley, 2004, p. 18-19). Observations such as streamflow gains and losses may have measurement errors that have known correlation so that $\boldsymbol{V}_{\varepsilon m}$ is not diagonal. In this case, assuming $\hat{\boldsymbol{\omega}}_m$ to be diagonal would result in a loss of information. If $\boldsymbol{V}_{\varepsilon m}$ is known, then to preserve this information $\hat{\boldsymbol{\omega}}_m$ should be written in the form

$$\hat{\boldsymbol{\omega}}_m = (\boldsymbol{V}_{\varepsilon m} + \boldsymbol{D}_m)^{-1}, \tag{85}$$

which gives $\hat{\boldsymbol{\omega}}_m^{1/2} \boldsymbol{\Omega}_m \hat{\boldsymbol{\omega}}_m^{1/2}$ the form $\boldsymbol{C}_m = (\boldsymbol{V}_{\varepsilon m} + \boldsymbol{D}_m)^{-1/2} (\boldsymbol{V}_{\varepsilon m} + \boldsymbol{V}_m)(\boldsymbol{V}_{\varepsilon m} + \boldsymbol{D}_m)^{-1/2}$, where $\boldsymbol{D}_m$ is the diagonal matrix of diagonal elements of $\boldsymbol{V}_m$. Unless $\boldsymbol{V}_{\varepsilon m}$ is diagonal, $\boldsymbol{C}_m$ does not have a correlation-like form. However, as $\boldsymbol{V}_{\varepsilon m}$ approaches $\boldsymbol{0}$, $\boldsymbol{C}_m$ approaches the matrix $\boldsymbol{D}_m^{-1/2} \boldsymbol{V}_m \boldsymbol{D}_m^{-1/2}$, which is similar to a correlation matrix; as $\boldsymbol{V}_m$ approaches $\boldsymbol{0}$, $\boldsymbol{C}_m$ approaches $\boldsymbol{I}$, the identity matrix; and if $\boldsymbol{V}_{\varepsilon m}$ is diagonal, $\boldsymbol{C}_m$ has the standard form. Thus, $\boldsymbol{C}_m$ has the form assumed for the approximations in the limits. We assume that elements of $\boldsymbol{C}_m$ have magnitudes ≤1 (at least in final effect) for all matrices $\boldsymbol{V}_{\varepsilon m}$, so that equations 82, 83, and 84 can be used to compute correction factors when $\hat{\boldsymbol{\omega}}_m$ is defined by equation 85. (This assumption held in tests made during development of the computer code for this report.) Note, however, that as in the standard case where $\hat{\boldsymbol{\omega}}_m$ is diagonal, $\boldsymbol{D}_m$ is approximate because $\boldsymbol{V}_m$ is unknown.

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, $c_c t^2_{\alpha/2}$ should be used instead of $t^2_{\alpha/2}$; 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, $c_p t^2_{\alpha/2}$ should be used instead of $t^2_{\alpha/2}$.)

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 $|t_{r+1}| = \max_j |\delta_j^{r+1} / BS_j| <$ 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, $\hat{\omega}_p = \text{VAR}^{-1}$, 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.

Chapter 4. USER GUIDE TO RESAN2-2k

RESAN2-2k performs two functions. The first function is to test residuals for indications of non-normality. This purpose is shared by earlier codes like RESAN (Cooley and Naff, 1990) and RESAN-2000 (Hill and others, 2000), but the analysis is somewhat different and more precise when using RESAN2-2k. The second function is to compute measures that can be used to detect model and system types of intrinsic nonlinearity.

Testing Weighted Residuals for Indications of Non-Normality

Like earlier versions of the residuals analysis program, RESAN2-2k generates sets of synthetic weighted residuals having the distribution given by equation 30 or 31. A normal probability plot of the actual weighted residuals distribution together with the synthetic sets will give a preliminary idea as to whether or not the weighted residuals appear to have the specified normal distribution, as described by Cooley and Naff (1990, p. 168-171). If a large number of synthetic sets of weighted residuals are generated, then the mean values, $\bar{\boldsymbol{d}}$ (equation 32), and standard deviation, $\boldsymbol{v}$ (equation 34), over all realizations can be computed for the synthetic weighted residuals. The necessary number to obtain stable results is usually from several hundred to several thousand. A normal probability plot of $\bar{\boldsymbol{d}} \pm 2\boldsymbol{v}$ gives a band within which the weighted residuals might usually be expected to lie. Figure 1 shows an example of a normal probability plot with weighted residuals plotted together with the corresponding band given by $\bar{\boldsymbol{d}} \pm 2\boldsymbol{v}$ computed from 1,000 realizations. The results used to produce this kind of plot are all written by RESAN2-2k to a file with extension _md.

RESAN2-2k computes a measure of the correlation, c_d (equation 38), between weighted residuals and the means of the synthetic residuals, and it computes the probability P that c_d or a smaller value can be obtained. The larger the probability P, the larger is the probability that the weighted residuals have the theoretical distribution given by equation 30 or 31. RESAN2-2k also computes and prints 99, 95, and 90 percent confidence limits for the correlation. These measures are written by RESAN2-2k to the file with extension #nr, where they are listed the following way:

```
CORRELATION (CED) --------------- = 0.98984
PROBABILITY OF CORRELATION (PROB) = 0.71300
99% CONFIDENCE LIMIT (CL99) ----- = 0.99624
95% CONFIDENCE LIMIT (CL95) ----- = 0.99423
90% CONFIDENCE LIMIT (CL90) ----- = 0.99304
```

CED corresponds to c_d, PROB corresponds to P, CL99 corresponds to the 99 percent confidence limit, CL95 corresponds to the 95 percent confidence limit, and CL90 corresponds to the 90 percent confidence limit.

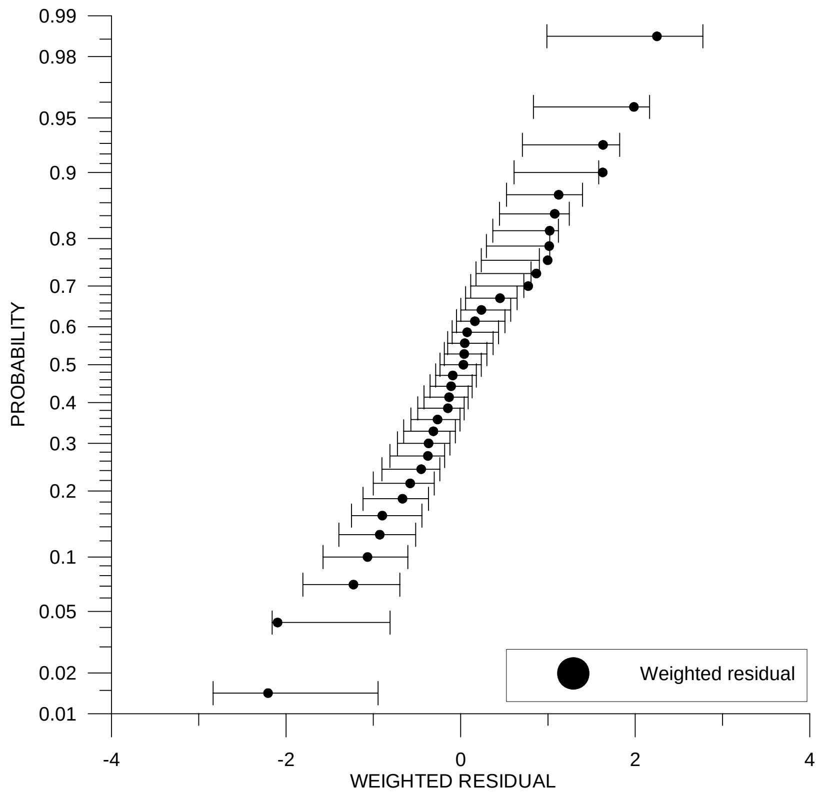

Figure 1. Ordered weighted residuals plotted with $\bar{\boldsymbol{d}} \pm 2\boldsymbol{v}$ confidence band (approximate 95 percent confidence intervals).

Testing for Intrinsic Nonlinearity

As described in chapter 2, RESAN2-2k computes three measures that can be used to detect model intrinsic nonlinearity: the mean weighted residual, the slope of weighted residuals in relation to weighted model functions, and $(\boldsymbol{Y} - \boldsymbol{f}(\gamma\hat{\boldsymbol{\theta}}))'\boldsymbol{\omega}^{1/2}\boldsymbol{R}\boldsymbol{\omega}^{1/2}(\boldsymbol{Y} - \boldsymbol{f}(\gamma\hat{\boldsymbol{\theta}}))$. If the first two measures are small (close to zero), and if the third measure is much smaller than $S(\hat{\boldsymbol{\theta}})$ (the weighted sum of squared residuals computed using the optimum parameter set, $\hat{\boldsymbol{\theta}}$), then the model intrinsic nonlinearity probably is small. In the RESAN2-2k output file with extension #nr, the measures are listed as

```
MEAN WEIGHTED RESIDUAL (EM) --------- = 0.99903E-01
SLOPE OF WEIGHTED RESIDUAL PLOT (SLP) = 0.56149E-05
INTRINSIC NONLINEARITY MEASURE (QINT) = 0.56149E-05 (SHOULD BE<<36.506)
```

EM and SLP are both close to 0, and QINT is much smaller than 36.506, which is the weighted sum of squared residuals at the optimum in this example. The three measures thus all indicate that model intrinsic nonlinearity is small.

Input Instructions

RESAN2-2k needs two input files that can be generated by MODFLOW-2000, the _rs file and the _ws file (Hill and others, 2000, tables 5 and 8). The first file is the input file also used by the RESAN-2000 program of Hill and others (2000). The content of the second file is weighted simulated functions and weighted residuals. To generate the files MODFLOW-2000 must be run in the Sensitivty Analysis or Parameter-Estimation mode, and OUTNAM in the Observation Process input file must be specified as a string other than "NONE." It is important that the two files be generated in two different steps using MODFLOW-2000:

1. The _rs file must be generated using a parameter set other than the optimal, $\hat{\boldsymbol{\theta}}$.
2. The _ws file must be generated using the optimal parameter set, $\hat{\boldsymbol{\theta}}$.

Before running RESAN2-2k the following changes must be made to the _rs file. First, NSETS in item 1 defines the number of sets of synthetic weighted residuals generated to test for normality of the weighted residuals. NSETS must be set to a value of several hundred or a few thousand. Second, values of additional input variables used by RESAN2-2k (but not by RESAN-2000) can be added to item 1 as described in the 'Content of the _rs Input File Needed by RESAN2-2k' section if special features of the program are wanted. Third, depending on the value of two of the variables added to item 1, it may be necessary to append two new arrays, ET and V, to the file. The content of the input files is described in the 'Content of the _rs Input File Needed by RESAN2-2k' and the 'Content of the _ws Input File Needed by RESAN2-2k' sections.

Output

The RESAN2-2k program produces two files with extensions #nr and _md. The #nr file contains input values and summarizes the results from testing for nonlinearity and from testing weighted residuals for indications of non-normality. The summary of results is described in the 'Testing Weighted Residuals for Indications of Non-Normality' and the 'Testing for Intrinsic Nonlinearity' sections. The _md file contains results that can be used to produce a probability plot of ordered weighted residuals together with the ordered means of simulated weighted residuals and a confidence band (for example, fig. 1). The content of the columns in the file is: (1) ordered weighted residuals; (2) ordered means of simulated weighted residuals; (3) standard deviations of simulated weighted residuals; (4) two times the standard deviations of simulated weighted residuals; (5) frequency/probability; probability plot position; (6) observation name; and (7) plot symbol identifier.

Content of the _rs Input File Needed by RESAN2-2k

RESAN2-2k reads the following from the _rs file. Explanations of the variables follow this list.

1. `NPAR NOBS NH NQT MPR IPR NSETS NRAN VAR STDV IPCF IPRN IERT ICOV`
   (format: 7I5, I10, F25.0, F10.0, 4I5)
2. `PARNAM(NPAR)` (format: 6(A10,1X))
3. `COV(NPAR,NPAR)` (format: 16F25.0)
4. `WT(NH)` (format: 16F15.0)
5. `WQ(NQT,NQT)` (format: 16F15.0)
6. `X(NPAR,NOBS)` (format: 16F15.0)
7. `PRM(NP,I), WP(I), I=1,MPR` (format: 8F15.0)
8. `NIPR(IPR)` (format: 16I5)
9. `WTPS(IPR,IPR)` (format: 8F15.0)
   If IERT is greater than zero, read item 10.
10. `ET(NOBS)` (free format)
    If ICOV is greater than zero, read item 11.
11. `V(NOBS,NOBS)` (free format)

The variables have the following explanations.

NPAR---is the number of estimated parameters.

NOBS---is the number of model function observations used for estimation. NOBS must thus be equal to NH+NQT.

NH-------is the number of head observations.

NQT-----is the number of observations other than heads.

MPR-----is the number of prior information equations

IPR------is the number of prior information observations with a full weight matrix.

NSETS—is the number of sets of synthetic weighted residuals generated to test for normality of the weighted residuals. NSETS must be increased from 4 (the default value set by MODFLOW-2000) to a value of several hundred or a few thousand.

NRAN---is the seed for the random number generator.

VAR-----is the calculated error variance, $\hat{s}^2 = S(\hat{\boldsymbol{\theta}})/(n-p)$.

STDV---is the theoretical error variance, $b\sigma_\varepsilon^2$, used to generate synthetic weighted residuals distributed as given by equation 30. If a value of 0 is specified, RESAN2-2k automatically sets it equal to $\hat{s}^2$, the calculated error variance from the least squares estimation, before the synthetic weighted residuals are generated.

IPCF-----is a flag. If IPCF is greater than zero, the program prints the ***I–R*** matrix.

IPRN----is a printing flag. Weighted simulated residuals are printed when IPRN is greater than zero.

IERT----is a flag. If IERT is greater than zero, the program reads the ET array described below.

ICOV----is a flag. If ICOV is greater than zero, the program reads the V array described below.

PARNAM—is the parameter name list.

COV-----is the parameter covariance matrix.

WT------are the square roots of weights for heads.

WQ------is the square root of the full weight matrix for observations other than heads.

X---------is the sensitivity matrix for all parameters and observations. (For log-transformed parameters the sensitivities are with respect to natural log-transformed parameters, not with respect to $\log_{10}$-transformed parameters.)

PRM----are coefficients for the prior information equations.

WP------are weights for prior information equations.

NIPR----is the number list for parameters with prior information observations that have a full weight matrix.

WTPS---is the square root of the full weight matrix for correlated prior information. (For log-transformed parameters the weights are for natural log-transformed parameters, not for $\log_{10}$-transformed parameters.)

ET-------are the expected values of the true errors for the model function observations, $E\left(\boldsymbol{Y}_m - \boldsymbol{f}_m(\boldsymbol{\gamma\theta}_*)\right)$, which are used to generate the synthetic, weighted, true error vectors used to test weighted residuals for normality. If IERT=0, then ET is not read but is assumed to be all zeros.

V------ is the matrix $\boldsymbol{\Omega}_m = E\left(\boldsymbol{Y}_m - \boldsymbol{f}_m(\boldsymbol{\gamma\theta}_*)\right)\left(\boldsymbol{Y}_m - \boldsymbol{f}_m(\boldsymbol{\gamma\theta}_*)\right)' / \sigma_\varepsilon^2$ for model function observations that is used to generate the synthetic, weighted, true error vectors from equation 30. If ICOV=0, then V is not read and equation 31 is used instead of equation 30.

Content of the _ws Input File Needed By RESAN2-2k

RESAN2-2k reads the following items from the _ws file NTOT times, where NTOT= NOBS+MPR+IPR. That is, the items are read once for each observation that was used to estimate the model parameters.

1. `F E ISYM DID` (format: 2(G15.7,1X),I5,2X,A)

The variables have the following explanations.

F---------is the weighted simulated equivalent to the observation.

E---------is the corresponding weighted residual.

ISYM---is a plot symbol identifier (an integer value).

DID-----is the observation name.

Chapter 5. USER GUIDE TO BEALE2-2k

BEALE2-2k computes measures of total model nonlinearity, model intrinsic nonlinearity, and model combined intrinsic nonlinearity. The measures can be used as a guide for whether confidence or prediction intervals can be computed using linearized approximations (for example, using YCINT-2000 of Hill and others, 2000), or if nonlinear intervals should be computed using MODFLOW-2000 with UNC. The measures also indicate whether correction factors computed by CORFAC-2k may be inaccurate because of model intrinsic nonlinearity or model combined intrinsic nonlinearity. BEALE2-2k extends the capabilities of BEALE (Cooley and Naff, 1990) and BEALE-2000 (Hill and others, 2000) to include the measures of model intrinsic nonlinearity and model combined intrinsic nonlinearity in addition to the measure of total nonlinearity, which was all that was computed in BEALE and BEALE-2000. BEALE2-2k also redefines the measure of total model nonlineariy slightly to make it more directly useful for evaluating the accuracy of a linearized confidence region (Cooley, 2004, p. 85-87).

Total model nonlinearity is quantified by calculating $\hat{N}$ (equation 39), which is called BNT in the BEALE2-2k output file. The model is considered to be highly nonlinear if $\hat{N} > 1$, nonlinear if $1 \geq \hat{N} > 0.09$, moderately nonlinear if $0.09 \geq \hat{N} > 0.01$, and essentially linear if $\hat{N} \leq 0.01$. Linear theory for computing confidence regions seems to produce good approximate results when $\hat{N} \leq 0.09$ (Cooley and Naff, 1990, p. 189).

Model intrinsic nonlinearity is quantified by calculating $\hat{N}_{\min}$ (equation 44), which is called BNI in the BEALE2-2k output file. The same criteria as used to rank values of $\hat{N}$ are used for $\hat{N}_{\min}$. In particular, if $\hat{N}_{\min} \leq 0.09$, then the model intrinsic nonlinearity is so small that correction factors for confidence regions, confidence intervals, and prediction intervals are probably not significantly dependent on such nonlinearity.

Model combined intrinsic nonlinearity is computed either for confidence intervals or for prediction intervals. For a confidence interval this is quantified by $\hat{M}_{\min}$ (equation 48), $\hat{B}_U$ (equation 53), and $\hat{B}_L$ (equation 54). In the output file these variables are called BMI, BMF0, and BMG0, respectively. If the larger of $\hat{M}_{\min} + 2\hat{B}_U$ and $\left|\hat{M}_{\min} - 2\hat{B}_L\right|$ (that is, BMI+2BMF0 and the absolute value of BMI-2BMG0) is less than 0.09, then model combined intrinsic nonlinearity probably does not contribute significantly to the correction factor for the confidence interval although, as indicated in chapter 2, this criterion is apt to be conservative. The larger of $\hat{M}_{\min} + 2\hat{B}_U$ and $\left|\hat{M}_{\min} - 2\hat{B}_L\right|$ is called BMIMAX in the output file. A standard linear confidence interval should be a good approximation if $\hat{M}_{\min} \leq 0.01$ (Cooley, 2004, section 7).

For a prediction interval BMI, BMF0, and BMG0 in the output file correspond to $\hat{M}^a_{\min}$ (equation 56), $\hat{B}^a_U$ (equation 57), and $\hat{B}^a_L$ (equation 58), respectively. If the larger of $\hat{M}^a_{\min} + 2\hat{B}^a_U$ and $\left|\hat{M}^a_{\min} - 2\hat{B}^a_L\right|$ (that is, BMI+2BMF0 and the absolute value of BMI-2BMG0) is less than 0.09, then model combined intrinsic nonlinearity probably does not contribute significantly to the correction factor for the prediction interval although again this criterion is apt to be conservative.

A standard linear prediction interval should be a good approximation if $\hat{M}^{a}_{\min} \leq 0.01$ (Cooley, 2004, section 7).

Input Instructions

The nonlinearity measures are calculated by BEALE2-2k using four input files that can be generated by MODFLOW-2000 using UNC. The generated files have the extensions _b1, _b2, _b3, and _b4, and they are generated in two steps like the _b1 and _b2 files needed by BEALE-2000 (Hill and others, 2000, p. 92). Actually, the _b1 and _b2 files needed by BEALE2-2k are almost identical to the _b1 and _b2 files needed by BEALE-2000 (Hill and others, 2000, tables 12 and 13), and they can be read and used by BEALE-2000. To generate the four files, MODFLOW-2000 must be run in the Uncertainty Process mode. OUTNAM in the Observation Process input file must be specified as a string other than "NONE."

First generate the _b1 and _b3 files as follows:

1. In the Uncertainty Process input file, set IACT=1 in item 1 and specify CFR and CFI in items 8 and 9, respectively.
2. Substitute the final calibrated parameter values from the _b file into the Sensitivity Process input file.
3. Execute MODFLOW-2000. This run will generate the _b1 and _b3 files.

Next, generate the _b2 and _b4 files and execute BEALE2-2k as follows:

4. In the Uncertainty Process input file, set IACT=2.
5. Execute MODFLOW-2000. This run will generate the _b2 and _b4 files.
6. Finally, execute BEALE2-2k, which directs output to a file with extension #be. It will overwrite a possible output file already produced by BEALE-2000.

The content of the four input files is described in the four sections following the next section, 'Output from BEALE2-2k.'

Output from BEALE2-2k

The BEALE2-2k program produces an output file with the extension #be. This file will overwrite a possible output file with the same name already produced by BEALE-2000 (Hill and others, 2000). The #be file contains input values and computed measures of total model nonlinearity, model intrinsic nonlinearity, and model combined intrinsic nonlinearity. The measures of total model nonlinearity and model intrinsic nonlinearity are listed in the file as

```
TOTAL NONLINEARITY (BNT).......... = 0.70303E-01
INTRINSIC NONLINEARITY (BNI)...... = 0.26567E-04
```

The measures of model combined intrinsic nonlinearity for confidence (or prediction) intervals are listed (here for 7 intervals) as

```
  COMBINED INTRINSIC NONLINEARITY
 INTERVAL NO.       BMI           INTERVAL NO.       BMI
 1  G1            0.91136E-01     5  G5            0.92165E-01
 2  G2            0.13976E-04     6  G6            0.89142E-01
 3  G3            0.80532E-01     7    HK_1        0.37137E-01
 4  G4            0.92049E-01     8    HK_2        0.22188E-01

   COMBINED INTRINSIC NONLINEARITY AS IF F WERE LINEAR
  INTERVAL NO.      BMF0           INTERVAL NO.      BMF0
 1  G1            0.12232E-01     5  G5            0.12491E-01
 2  G2            0.37404E-02     6  G6            0.11832E-01
 3  G3            0.99148E-02     7    HK_1        0.58584E-12
 4  G4            0.12468E-01     8    HK_2        0.59462E-10

   COMBINED INTRINSIC NONLINEARITY AS IF G WERE LINEAR
  INTERVAL NO.      BMG0           INTERVAL NO.      BMG0
 1  G1            0.36826E-01     5  G5            0.37051E-01
 2  G2            0.40559E-02     6  G6            0.36261E-01
 3  G3            0.34126E-01     7    HK_1        0.37137E-01
 4  G4            0.37003E-01     8    HK_2        0.22186E-01

        COMBINED INTRINSIC NONLINEARITY - MAX. SUM
  INTERVAL NO.      BMIMAX         INTERVAL NO.      BMIMAX
 1  G1            0.11560         5  G5            0.11715
 2  G2            0.80979E-02     6  G6            0.11280
 3  G3            0.10036         7    HK_1        0.37137E-01
 4  G4            0.11699         8    HK_2        0.22188E-01
```

The various measures and their uses are explained in the beginning of this chapter.

Content of the _b1 Input File Needed By BEALE2-2k

The _b1 file contains the following items.

1. NPE NOBS NQ MPR IPR VAR CR (format: 5I10,2F14.0)
2. PARNAM(NPE) (format: 6(A10,1X))
3. BOPT(NPE) (format: 6F13.0)

4. `OBSNAM(NOBS)` (format: 6(A12,1X))
5. `H(NOBS)` (format: 6F13.0)
6. `HOBS(NOBS)` (format: 6F13.0)
7. `WH(NH)` (NH=NOBS-NQ) (format: 8F15.0)
8. `WQ(NQ,NQ)` (format: 8F15.0)
9. `X(NPE,NOBS)` (format: 6F13.0)
10. `PRM(NPE+1,J), WP(J), J=1,MPR` (format: 8F15.0)
11. `NIPR(IPR)` (format: 8I10)
12. `BPRI(IPR)` (format: 6F13.0)
13. `WTP(IPR,IPR)` (format: 6F13.0)
14. `LN(NPE)` (format: 8I10)
15. A line with the text: `THE PARAMETER SETS FOLLOW`
    Read 2×NPE repetitions of item 16.
16. `B(NPE)` (format: 8F13.0)

The explanation of variables follows:

NPE-----is the number of estimated parameters.

NOBS---is the number of observations used for estimation.

NQ-------is the number observations other than heads.

MPR-----is the number of prior information equations.

IPR-------is the number of prior information observations with a full weight matrix.

VAR------is the calculated error variance, $\hat{s}^2 = S(\hat{\theta})/(n-p)$.

CR--------is the correction factor for the confidence region (computed using CORFAC-2k).

PARNAM—is the parameter name list.

BOPT----are the optimized parameter values.

OBSNAM—are the observation names.

H---------are the simulated equivalents of the observations using the optimized parameter values.

HOBS---are the observed values of hydraulic heads and head dependent flows (not used by BEALE2-2k).

WH------are the weights for hydraulic heads.

WQ------is the weight matrix for the observations other than heads.

X---------is the sensitivity matrix for all parameters and observations. (For log-transformed parameters the sensitivities are with respect to natural log-transformed parameters, not with respect to $\log_{10}$-transformed parameters.)

PRM----are coefficients for the prior information equations.

WP------are weights for prior information equations.

NIPR----is the number list for parameters with prior information observations that have a full weight matrix.

BPRI----are the prior information observations (not used by BEALE2-2k).

WTP-----is the full weight matrix for correlated prior information observations. (For log-transformed parameters the weights are for natural log-transformed parameters, not for $\log_{10}$-transformed parameters.)

LN-------flag indicating whether each parameter is log-transformed. The parameter is log-transformed if LN≠0.

B---------is a set of parameter values used to calculate measures of total model nonlinearity and model intrinsic nonlinearity.

Content of the _b2 Input File Needed By BEALE2-2k

The following two items are repeated 2 × NPE times.

```
1.    B(NPE)                    (format: 8F13.0)
2.    F(NOBS)                   (format: 6F13.0)
```

These variables are:

B---------are parameter values for one of the 2 × NPE sets of parameter values used to calculate measures of total model nonlinearity and model intrinsic nonlinearity.

F---------are simulated equivalents of the observations, calculated using the preceding set of parameter values.

Content of the _b3 Input File Needed By BEALE2-2k

The _b3 file contains the following items.

```
1.   NOINT NHI NQI NPI ITYP IDIF    (format: 6I10)
2.   GNAM(NOINT)                    (format: 6(A12,1X))
3.   GOPT(NOINT)                    (format: 6F13.0)
4.   WG(NOINT)                      (format: 8F15.0)
5.   Z(NPE,NOINT)                   (format: 6F13.0)
6.   CC(NOINT)                      (format: 6(1X,F13.0))
```

The variables are defined as:

NOINT—is the number of intervals for which model combined intrinsic nonlinearity measure is calculated.

NHI------is the number of intervals for hydraulic heads.

NQI------is the number of intervals for head dependent flows.

NPI------is the number of intervals for parameters.

ITYP----is a flag for the type of interval: ITYP=1 is for confidence intervals; ITYP=2 is for prediction intervals.

IDIF-----is a flag. When IDIF=1 it indicates in the output that intervals pertaining to heads and head dependent flows are for differences of heads or flows. When IDIF=0 it indicates that the intervals pertain to heads and head dependent flows.

GNAM—is the name of each prediction for which model combined intrinsic nonlinearity measure is calculated.

GOPT---is the predicted value using the optimized parameter values.

WG------are weights for the predictions corresponding to ω_p. Values must always be specified for WG whenever NOINT is greater than 0, but WG is only used in calculations pertaining to prediction intervals. For prediction intervals for log-transformed parameters WG must be specified for the natural log-transforms of the parameters, not for the $\log_{10}$-transforms.

Z---------is the sensitivity matrix for all parameters and predictions. (For log-transformed parameters the sensitivities are with respect to natural log-transformed parameters, not with respect to $\log_{10}$-transformed parameters.)

CC-------are correction factors for each of the confidence or prediction intervals.

Content of the _b4 Input File Needed By BEALE2-2k

The following two items are repeated 2 × NOINT times.

1.	B(NPE)	(format: 8F13.0)
2.	F(NOBS)	(format: 6F13.0)
3.	G	(free format)

The variables are defined as:

B---------are parameter values for one of the 2 × NOINT sets of parameter values used to calculate measures of model combined intrinsic nonlinearity for confidence or prediction intervals.

F---------are simulated equivalents of the observations, calculated using the preceding set of parameter values.

G---------is simulated equivalent of the prediction, calculated using the preceding set of parameter values.

The first two repetitions of items 1 and 3 are used by BEALE2-2k to compute a measure of model combined intrinsic nonlinearity for the first confidence interval. For these repetitions G is the simulated value of the first prediction. The third and fourth repetitions of items 1 and 3 are used to compute the same kind of measure for the second confidence interval, and G is the simulated value of the second prediction. This logic is continued for the remaining repetitions.

Chapter 6. USER GUIDE TO CORFAC-2k

The purpose of CORFAC-2k is to compute correction factors for confidence regions, confidence intervals, and prediction intervals. In the development of the procedures implemented in CORFAC-2k, Cooley (2004, section 5) assumed that the model intrinsic nonlinearity and model combined intrinsic nonlinearity are negligible. As described in previous chapters, the validity of this assumption can be investigated using BEALE2-2k and RESAN2-2k, and by analyzing weighted residuals computed by the UNC Process.

The correction factors are to be used to calculate the critical value ($D^2_{1-\alpha}$, equation 86) needed by UNC for the calculation of confidence and prediction intervals, and by BEALE2-2k for computation of nonlinearity measures. CORFAC-2k is used first to compute correction factors, and then BEALE2-2k, RESAN2-2k, and weighted residuals computed by UNC are used to analyze for model intrinsic nonlinearity and model combined intrinsic nonlinearity. If this indicates that model intrinsic nonlinearity and/or model combined intrinsic nonlinearity are not small then the correction factors computed by CORFAC-2k, and thus the confidence or prediction intervals computed by UNC, may be inaccurate.

When the true error covariance structure, $\boldsymbol{\Omega}$, is known, c_r is computed from equation 66, c_c is computed from equation 68, and c_p is computed from equation 70. In the output file these correction factors are called CR, CC, and CP, respectively.

When $\boldsymbol{\Omega}$ is unknown, the approximate bound for c_r is computed from equation 82, the approximate bound for c_c is computed from equation 83, and the approximate bound for c_p is computed from equation 84. In the output file these approximations are called CRB, CCB, and CPB, respectively. CRB, CCB and CPB also are written in the output file when $\boldsymbol{\Omega}$ is known.

Input Instructions

The correction factors are calculated by CORFAC-2k using an input file with the extension _cf that can be generated by MODFLOW-2000 using the UNC Process. To generate the file, MODFLOW-2000 must be run in the Uncertainty-Process mode (with IACT=3), and OUTNAM in the Observation Process input file must be specified as a string other than "NONE." Before running MODFLOW-2000, the final calibrated parameter values must be substituted from the _b file into the Sensitivity Process input file. The content of the input file is described in detail in the 'Content of the _cf Input File Needed By CORFAC-2k' section.

If the effective correlation c_e and/or $\boldsymbol{\Omega}$ is known, it is necessary to manually make the following changes to the _cf file produced by MODFLOW-2000 before running CORFAC-2k:

1. Change the value for the effective correlation, EC, from -1 (which is the value always written by MODFLOW-2000) to a value in the range from 0.0 to 1.0. If the value for EC is specified to be less than 0.0 or larger than 1.0, then CORFAC-2k automatically changes the value to 0.8.

2. Set ITRN to a value larger than 0 if $\boldsymbol{\Omega}$ is known, and append V, VP and CP to the file. VP and CP are only needed if correction factors are to be computed for prediction intervals.

Output From CORFAC-2k

The CORFAC-2k program produces an output file with the extension #cf. When $\boldsymbol{\Omega}$ is known, the output for a confidence region has the form

```
CORRECTION FACTOR FOR N-P (A) ---- =  6.0528
SCALING FACTOR (B) --------------- =  1.0000
EFFECTIVE CORRELATION (C) -------- = 0.77891
(N-P)/(N-A*P) VALUE (FAC) -------- =  4.1308
CORRECTION FACTOR (CR) ----------- =  25.003

APPROXIMATE N-A*P VALUE (DFB) ---- =  4.4313
APPROX. (N-P)/(N-A*P) VALUE (FACB) =  4.5134
APPROXIMATE BOUND FOR CR (CRB) --- =  27.936
```

where the number of observations, n, used for parameter estimation is called N; the number of estimated parameters, p, is called P; a computed from equation 26 is called A; b computed from equation 27 is called B; c computed from equation 75 is called C; c_r computed from equation 66 is called CR; $n - ap$ computed from equation 71 using the input value c_e (EC in input file) for c is called DFB; and c_b approximated from equation 82 is called CRB. If $\boldsymbol{\Omega}$ is unknown, then only DFB, FACB, and CRB are printed.

For each confidence interval the output is

```
CORRECTION FACTOR XI FOR C. I. ------ =  2.9713
CORRECTION FACTOR (CC) -------------- =  12.274

ESTIMATED VARIANCE OF PREDICTION (VE) = 0.39250
BOUND FOR XI USING POS. VALUES (XIPB) =  4.8727
BOUND FOR XI USING NEG. VALUES (XINB) = 0.38389E-01
APPROXIMATE BOUND FOR CC (CCB) ------ =  18.497
```

where ξ computed from equation 47 is called XI; c_c computed from equation 68 is called CC; VE is computed as $\text{VE} = \boldsymbol{Q'Q}\, S(\hat{\theta})/(n - p)$; XIPB is the squared sum of positive values of the Q_{mi}'s used in equation 78; XINB is the squared sum of negative values of the Q_{mi}'s used in equation 78; and c_c approximated from equation 83 is called CCB. If $\boldsymbol{\Omega}$ is unknown, then only VE, XIPB, XINB, and CCB are printed.

For a prediction interval the output is

```
CORRECTION FACTOR XI FOR P. I. ------ = 0.26079
CORRECTION FACTOR (CP) -------------- =  1.0773

ESTIMATED VARIANCE OF PREDICTION (VE) = 0.15901
BOUND FOR XI USING POS. VALUES (XIPB) = 0.77966
BOUND FOR XI USING NEG. VALUES (XINB) = 0.93736
APPROXIMATE BOUND FOR CP (CPB) ------ =  4.2872
```

where ξ_a computed from equation 55 is called XI, c_p computed from equation 70 is called CP; VE is again computed as $\mathrm{VE} = \boldsymbol{Q'Q}\, S(\hat{\theta}) / (n - p)$; XIPB is the squared sum of positive values of the Q_{mi}'s used in equation 81; XINB is the squared sum of negative values of the Q_{mi}'s used in equation 81; and c_p approximated from equation 84 is called CPB. If $\boldsymbol{\Omega}$ is unknown, only VE, XIPB, XINB, and CPB are printed.

Content of the _cf Input File Needed By CORFAC-2k

The _cf file contains the following items.

1. NPE NOBS NQ MPR IPR VAR EC ITRN (format: 5I10,2F14.0,I10)
2. PARNAM(NPE) (format: 6(A10,1X))
3. OBSNAM(NOBS) (format: 6(A12,1X))
4. WH(NH)(NH=NOBS-NQ) (format: 8F15.0)
5. WQ(NQ,NQ) (format: 8F15.0)
6. X(NPE,NOBS) (format: 6F13.0)
7. PRM(NPE,J), WP(J), J=1,MPR (format: 8F15.0)
8. NIPR(IPR) (format: 8I10)
9. WTP(IPR,IPR) (format: 6F13.0)
10. NOINT NHI NQI NPI ITYP IDIF (format: 6I10)
11. GNAM(NOINT) (format: 6(A12,1X))
12. WG(NOINT) (format: 8F15.0)
13. Z(NPE,NOINT) (format: 6F13.0)

    If ITRN is greater than zero, read the following item.

14. V(NOBS,NOBS) (free format)

    If ITRN is greater than zero and ITYP is greater then 1, read the following item NOINT times.

15. VP CP(NOBS) (free format)

The variables are defined as:

.

NPE-----is the number of estimated parameters.

NOBS---is the number of observations used for estimation.

NQ-------is the number observations other than hydraulic heads.

MPR-----is the number of prior information equations.

IPR-------is the number of prior information observations with a full weight matrix.

VAR------is the calculated error variance, $\hat{s}^2$.

EC--------is the effective correlation, c_e.

ITRN----is a flag that when specified to be greater than zero directs CORFAC-2k to read and use V, VE, and CP (defined below).

PARNAM—are the parameter names.

OBSNAM—are the observation names.

WH-----are the square root of the weights for hydraulic heads.

WQ-----is the square root of the full weight matrix for the observations other than heads.

X--------is the sensitivity matrix for all parameters and observations. (For log-transformed parameters the sensitivities are with respect to natural log-transformed parameters, not with respect to $\log_{10}$-transformed parameters.)

PRM----are coefficients for the prior information equations.

WP------are the square root of weights for prior information equations.

NIPR----is the number list for parameters with prior information observations that have a full weight matrix.

WTP----is the square root of the full weight matrix for correlated prior information. (For log-transformed parameters the weights are for natural log-transformed parameters, not for $\log_{10}$-transformed parameters.)

NOINT—is the number of intervals for which a correction factor is calculated.

NHI-----is the number of intervals for hydraulic heads.

NQI-----is the number of intervals for head-dependent flows.

NPI-----is the number of intervals for parameters.

ITYP---is a flag for the type of interval: ITYP=1 is for confidence intervals; ITYP=2 is for prediction intervals.

IDIF-----is a flag. When IDIF=1 it indicates in the output that intervals pertaining to heads and head-dependent flows are for differences of heads or flows. When IDIF=0 it indicates that the intervals pertain to heads and head-dependent flows.

GNAM—is the name of each prediction for which an interval correction factor is calculated.

WG------are the square roots of the weights for the predictions corresponding to ω_p. Values must always be specified for WG whenever NOINT is greater than 0, but WG is only used in calculations pertaining to prediction intervals. For prediction intervals for log-transformed parameters WG must be specified for the natural log-transforms of the parameters, not for the $\log_{10}$-transforms.

Z---------is the sensitivity matrix for all parameters and predictions. (For log-transformed parameters the sensitivities are with respect to natural log-transformed parameters, not with respect to $\log_{10}$-transformed parameters.)

V---------is equal to $\boldsymbol{\Omega}_m = E\left(\boldsymbol{Y}_m - \boldsymbol{f}_m(\gamma\boldsymbol{\theta}_*)\right)\left(\boldsymbol{Y}_m - \boldsymbol{f}_m(\gamma\boldsymbol{\theta}_*)\right)' / \sigma_\varepsilon^2$.

VP-------is equal to $\hat{\omega}_p^{-1} = E\left(Y_p - g(\gamma\boldsymbol{\theta}_*)\right)^2 / \sigma_\varepsilon^2$.

CP-------is equal to $\boldsymbol{C} = E\left(\boldsymbol{Y}_m - \boldsymbol{f}_m(\gamma\boldsymbol{\theta}_*)\right)\left(Y_p - g(\gamma\boldsymbol{\theta}_*)\right)' / \sigma_\varepsilon^2$.

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APPENDIX A. SOLUTIONS FOR EXTREME VALUES

Confidence Intervals

In this section we derive equations for extreme values of $g(\gamma\boldsymbol{\theta})$ for a linearized form of $L(\boldsymbol{\theta},\lambda)$ given by equation 8. These equations become iteration equations to solve the nonlinear problem.

First, we linearize $g(\gamma\boldsymbol{\theta})$ and $\boldsymbol{f}(\gamma\boldsymbol{\theta})$ using a truncated Taylor series around parameter set $\boldsymbol{\theta}_r$ obtained at the rth iteration:

$$g(\gamma\boldsymbol{\theta}) \approx g(\gamma\boldsymbol{\theta}_r) + \boldsymbol{D}g_r(\boldsymbol{\theta}-\boldsymbol{\theta}_r), \tag{A-1}$$

$$\boldsymbol{f}(\gamma\boldsymbol{\theta}) \approx \boldsymbol{f}(\gamma\boldsymbol{\theta}_r) + \boldsymbol{Df}_r(\boldsymbol{\theta}-\boldsymbol{\theta}_r), \tag{A-2}$$

where subscript r indicates evaluation using $\boldsymbol{\theta}_r$. Second, we take derivatives of $L(\boldsymbol{\theta},\lambda)$ written using equations A-1 and A-2 and set the results to zero to obtain

$$\boldsymbol{Df}_r'\boldsymbol{\omega}\boldsymbol{Df}_r(\boldsymbol{\theta}-\boldsymbol{\theta}_r) = \lambda\boldsymbol{D}g' + \boldsymbol{Df}_r'\boldsymbol{\omega}(\boldsymbol{Y}-\boldsymbol{f}(\gamma\boldsymbol{\theta}_r)), \tag{A-3}$$

$$d_\alpha^2 = S(\boldsymbol{\theta}) - S(\hat{\boldsymbol{\theta}}). \tag{A-4}$$

Third, we write $S(\boldsymbol{\theta})$ using equation A-2, then substitute $\boldsymbol{\theta}-\boldsymbol{\theta}_r$ from equation A-3 into the result to get

$$\begin{aligned} S(\boldsymbol{\theta}) &= S(\boldsymbol{\theta}_r) - 2(\boldsymbol{\theta}-\boldsymbol{\theta}_r)'\boldsymbol{Df}_r'\boldsymbol{\omega}(\boldsymbol{Y}-\boldsymbol{f}_r(\gamma\boldsymbol{\theta}_r)) + (\boldsymbol{\theta}-\boldsymbol{\theta}_r)'\boldsymbol{Df}_r'\boldsymbol{\omega}\boldsymbol{Df}_r(\boldsymbol{\theta}-\boldsymbol{\theta}_r) \\ &= S(\boldsymbol{\theta}_r) - 2(\lambda\boldsymbol{D}g_r' + \boldsymbol{Df}_r'\boldsymbol{\omega}(\boldsymbol{Y}-\boldsymbol{f}_r(\gamma\boldsymbol{\theta}_r)))'(\boldsymbol{Df}_r'\boldsymbol{\omega}\boldsymbol{Df}_r)^{-1}\boldsymbol{Df}_r'\boldsymbol{\omega}(\boldsymbol{Y}-\boldsymbol{f}_r(\gamma\boldsymbol{\theta}_r)) \\ &\quad + (\lambda\boldsymbol{D}g_r' + \boldsymbol{Df}_r'\boldsymbol{\omega}(\boldsymbol{Y}-\boldsymbol{f}_r(\gamma\boldsymbol{\theta}_r)))'(\boldsymbol{Df}_r'\boldsymbol{\omega}\boldsymbol{Df}_r)^{-1}(\lambda\boldsymbol{D}g_r' + \boldsymbol{Df}_r'\boldsymbol{\omega}(\boldsymbol{Y}-\boldsymbol{f}_r(\gamma\boldsymbol{\theta}_r))) \\ &= S(\boldsymbol{\theta}_r) + \lambda^2\boldsymbol{D}g_r(\boldsymbol{Df}_r'\boldsymbol{\omega}\boldsymbol{Df}_r)^{-1}\boldsymbol{D}g_r' - (\boldsymbol{Y}-\boldsymbol{f}_r(\gamma\boldsymbol{\theta}_r))'\boldsymbol{\omega}\boldsymbol{Df}_r(\boldsymbol{Df}_r'\boldsymbol{\omega}\boldsymbol{Df}_r)^{-1}\boldsymbol{Df}_r'\boldsymbol{\omega}(\boldsymbol{Y}-\boldsymbol{f}_r(\gamma\boldsymbol{\theta}_r)) \\ &= S(\boldsymbol{\theta}_r) + \lambda^2\boldsymbol{Q}_r'\boldsymbol{Q}_r - (\boldsymbol{Y}-\boldsymbol{f}_r(\gamma\boldsymbol{\theta}_r))'\boldsymbol{\omega}^{1/2}\boldsymbol{R}_r\boldsymbol{\omega}^{1/2}(\boldsymbol{Y}-\boldsymbol{f}_r(\gamma\boldsymbol{\theta}_r)). \end{aligned} \tag{A-5}$$

Fourth, we put equation A-5 into equation A-4 and solve for λ to get

$$\lambda = \pm\left(\frac{d_\alpha^2 - S(\boldsymbol{\theta}_r) + S(\hat{\boldsymbol{\theta}}) + (\boldsymbol{Y}-\boldsymbol{f}(\gamma\boldsymbol{\theta}_r))'\boldsymbol{\omega}^{1/2}\boldsymbol{R}_r\boldsymbol{\omega}^{1/2}(\boldsymbol{Y}-\boldsymbol{f}(\gamma\boldsymbol{\theta}_r))}{\boldsymbol{Q}_r'\boldsymbol{Q}_r}\right)^{1/2}. \tag{A-6}$$

To obtain the solution for the (r+1)th iteration, we write equations A-6 and A-3 in the forms

$$\lambda_{r+1} = \pm\left(\frac{d_\alpha^2 - S(\boldsymbol{\theta}_r) + S(\hat{\boldsymbol{\theta}}) + (\boldsymbol{Y} - \boldsymbol{f}(\gamma\boldsymbol{\theta}_r))' \boldsymbol{\omega}^{1/2} \boldsymbol{R}_r \boldsymbol{\omega}^{1/2} (\boldsymbol{Y} - \boldsymbol{f}(\gamma\boldsymbol{\theta}_r))}{\boldsymbol{Q}_r'\boldsymbol{Q}_r}\right)^{1/2} \qquad \text{(A-7)}$$

and

$$\boldsymbol{\theta}_{r+1} = \boldsymbol{\theta}_r + \lambda_{r+1}(\boldsymbol{Df}_r'\boldsymbol{\omega}\boldsymbol{Df}_r)^{-1}\boldsymbol{Dg}_r' + (\boldsymbol{Df}_r'\boldsymbol{\omega}\boldsymbol{Df}_r)^{-1}\boldsymbol{Df}_r'\boldsymbol{\omega}(\boldsymbol{Y} - \boldsymbol{f}(\gamma\boldsymbol{\theta}_r)). \qquad \text{(A-8)}$$

Prediction Intervals

Extreme values of $g(\gamma\boldsymbol{\theta}) + v$ are derived using the same general method as used for $g(\gamma\boldsymbol{\theta})$. First, we use equations A-1 and A-2 in equation 19 and take derivatives with respect to $\boldsymbol{\theta}$, v, and λ. Then we set the results to zero to obtain

$$\boldsymbol{Df}_r'\boldsymbol{\omega}\boldsymbol{Df}_r(\boldsymbol{\theta} - \boldsymbol{\theta}_r) = \lambda\boldsymbol{Dg}_r' + \boldsymbol{Df}_r'\boldsymbol{\omega}(\boldsymbol{Y} - \boldsymbol{f}(\gamma\boldsymbol{\theta}_r)), \qquad \text{(A-9)}$$

$$\omega_p v = \lambda\,, \qquad \text{(A-10)}$$

$$d_\alpha^2 = S(\boldsymbol{\theta}) - S(\hat{\boldsymbol{\theta}}) + \omega_p v^2. \qquad \text{(A-11)}$$

Second, we use equations A-5 and A-10 in equation A-11 to get

$$d_\alpha^2 = S(\boldsymbol{\theta}_r) - S(\hat{\boldsymbol{\theta}}) + \lambda^2(\boldsymbol{Q}_r'\boldsymbol{Q}_r + \omega_p^{-1}) - (\boldsymbol{Y} - \boldsymbol{f}(\gamma\boldsymbol{\theta}_r))' \boldsymbol{\omega}^{1/2} \boldsymbol{R}_r \boldsymbol{\omega}^{1/2} (\boldsymbol{Y} - \boldsymbol{f}(\gamma\boldsymbol{\theta}_r)),$$

from which

$$\lambda = \pm\left(\frac{d_\alpha^2 - S(\boldsymbol{\theta}_r) + S(\hat{\boldsymbol{\theta}}) + (\boldsymbol{Y} - \boldsymbol{f}(\gamma\boldsymbol{\theta}_r))' \boldsymbol{\omega}^{1/2} \boldsymbol{R}_r \boldsymbol{\omega}^{1/2} (\boldsymbol{Y} - \boldsymbol{f}(\gamma\boldsymbol{\theta}_r))}{\boldsymbol{Q}_r'\boldsymbol{Q}_r + \omega_p^{-1}}\right)^{1/2}. \qquad \text{(A-12)}$$

Iteration equations are obtained directly from equations A-12, A-10, and A-9 and have the form

$$\lambda_{r+1} = \pm\left(\frac{d_\alpha^2 - S(\boldsymbol{\theta}_r) + S(\hat{\boldsymbol{\theta}}) + (\boldsymbol{Y} - \boldsymbol{f}(\gamma\boldsymbol{\theta}_r))' \boldsymbol{\omega}^{1/2} \boldsymbol{R}_r \boldsymbol{\omega}^{1/2} (\boldsymbol{Y} - \boldsymbol{f}(\gamma\boldsymbol{\theta}_r))}{\boldsymbol{Q}_r'\boldsymbol{Q}_r + \omega_p^{-1}}\right)^{1/2}, \qquad \text{(A-13)}$$

$$v_{r+1} = \omega_p^{-1}\lambda_{r+1}\,, \qquad \text{(A-14)}$$

and equation A-8.

APPENDIX B. COMPUTATION OF Q AND R FOR TESTING FOR EQUALITY OF CONSTRAINED AND UNCONSTRAINED RESIDUALS

To show that $\boldsymbol{Q}$ and $\boldsymbol{R}$ must be computed using $\boldsymbol{\theta} \neq \tilde{\boldsymbol{\theta}}$ for the test of equality of constrained and unconstrained weighted residuals, we need to use results from the constrained regression. The constrained regression involves finding the minimum value of $S(\boldsymbol{\theta}), S(\tilde{\boldsymbol{\theta}})$, subject to the constraint $g(\gamma\boldsymbol{\theta}) = g(\gamma\boldsymbol{\theta}_*)$. This is accomplished using the Lagrange function given as equation E-7 in Cooley (2004, p. 145):

$$L(\boldsymbol{\theta}, \lambda) = S(\boldsymbol{\theta}) + 2\lambda\left(g(\gamma\boldsymbol{\theta}_*) - g(\gamma\boldsymbol{\theta})\right). \tag{B-1}$$

The method used is the same one used for equation 8. First, we substitute equations A-1 and A-2, appendix A, into equation B-1, take the derivatives of $L(\boldsymbol{\theta}, \lambda)$ with respect to $\boldsymbol{\theta}$ and λ, and set the results to zero to yield, for iteration r+1

$$\boldsymbol{\theta}_{r+1} - \boldsymbol{\theta}_r = \lambda_{r+1}\left(\boldsymbol{Df}_r'\boldsymbol{\omega}\boldsymbol{Df}_r\right)^{-1}\boldsymbol{D}g_r' + \left(\boldsymbol{Df}_r'\boldsymbol{\omega}\boldsymbol{Df}_r\right)^{-1}\boldsymbol{Df}_r'\boldsymbol{\omega}\left(\boldsymbol{Y} - \boldsymbol{f}(\gamma\boldsymbol{\theta}_r)\right) \tag{B-2}$$

and

$$g(\gamma\boldsymbol{\theta}_*) = g(\gamma\boldsymbol{\theta}_r) + \boldsymbol{D}g_r\left(\boldsymbol{\theta}_{r+1} - \boldsymbol{\theta}_r\right). \tag{B-3}$$

Second, we put equation B-2 into equation B-3 and solve for λ to obtain for iteration r+1

$$\lambda_{r+1} = \frac{g(\gamma\boldsymbol{\theta}_*) - g(\gamma\boldsymbol{\theta}_r) - \boldsymbol{D}g_r\left(\boldsymbol{Df}_r'\boldsymbol{\omega}\boldsymbol{Df}_r\right)^{-1}\boldsymbol{Df}_r'\boldsymbol{\omega}\left(\boldsymbol{Y} - \boldsymbol{f}(\gamma\boldsymbol{\theta}_r)\right)}{\boldsymbol{Q}_r'\boldsymbol{Q}_r}. \tag{B-4}$$

At convergence $\boldsymbol{\theta}_{r+1} \approx \boldsymbol{\theta}_r \approx \tilde{\boldsymbol{\theta}}$ so that equation B-4 can be substituted into equation B-2 to give

$$\begin{aligned}
&\left(\boldsymbol{D}\tilde{\boldsymbol{f}}'\boldsymbol{\omega}\boldsymbol{D}\tilde{\boldsymbol{f}}\right)^{-1}\boldsymbol{D}\tilde{\boldsymbol{f}}'\boldsymbol{\omega}\left(\boldsymbol{Y} - \boldsymbol{f}(\gamma\tilde{\boldsymbol{\theta}})\right) - \frac{\left(\boldsymbol{D}\tilde{\boldsymbol{f}}'\boldsymbol{\omega}\boldsymbol{D}\tilde{\boldsymbol{f}}\right)^{-1}\boldsymbol{D}\tilde{g}'\boldsymbol{D}\tilde{g}\left(\boldsymbol{D}\tilde{\boldsymbol{f}}'\boldsymbol{\omega}\boldsymbol{D}\tilde{\boldsymbol{f}}\right)^{-1}\boldsymbol{D}\tilde{\boldsymbol{f}}'\boldsymbol{\omega}\left(\boldsymbol{Y} - \boldsymbol{f}(\gamma\tilde{\boldsymbol{\theta}})\right)}{\tilde{\boldsymbol{Q}}'\tilde{\boldsymbol{Q}}} \\
&= \left(\boldsymbol{D}\tilde{\boldsymbol{f}}'\boldsymbol{\omega}\boldsymbol{D}\tilde{\boldsymbol{f}}\right)^{-1}\left(\boldsymbol{I} - \frac{\boldsymbol{D}\tilde{g}'\boldsymbol{D}\tilde{g}\left(\boldsymbol{D}\tilde{\boldsymbol{f}}'\boldsymbol{\omega}\boldsymbol{D}\tilde{\boldsymbol{f}}\right)^{-1}}{\tilde{\boldsymbol{Q}}'\tilde{\boldsymbol{Q}}}\right)\boldsymbol{D}\tilde{\boldsymbol{f}}'\boldsymbol{\omega}\left(\boldsymbol{Y} - \boldsymbol{f}(\gamma\tilde{\boldsymbol{\theta}})\right) \\
&= \boldsymbol{0},
\end{aligned} \tag{B-5}$$

where the tildes over variables indicate evaluation using $\tilde{\boldsymbol{\theta}}$. Cooley (2004, equation E-14) showed that equation B-5 can be written in the form

$$\left(\tilde{\boldsymbol{Df}}'\boldsymbol{\omega}\tilde{\boldsymbol{Df}}\right)^{-1}\tilde{\boldsymbol{Df}}'\boldsymbol{\omega}^{1/2}\left(\tilde{\boldsymbol{R}}-\frac{\tilde{\boldsymbol{Q}}\tilde{\boldsymbol{Q}}'}{\tilde{\boldsymbol{Q}}'\tilde{\boldsymbol{Q}}}\right)\boldsymbol{\omega}^{1/2}\left(\boldsymbol{Y}-\boldsymbol{f}\left(\gamma\tilde{\boldsymbol{\theta}}\right)\right)=\boldsymbol{0}. \qquad \text{(B-6)}$$

Premultiplication of equation B-6 by $\boldsymbol{\omega}^{1/2}\tilde{\boldsymbol{Df}}$ and use of the definition and properties of $\tilde{\boldsymbol{R}}$ lead to the result needed to complete the proof:

$$\left(\tilde{\boldsymbol{R}}-\frac{\tilde{\boldsymbol{Q}}\tilde{\boldsymbol{Q}}'}{\tilde{\boldsymbol{Q}}'\tilde{\boldsymbol{Q}}}\right)\boldsymbol{\omega}^{1/2}\left(\boldsymbol{Y}-\boldsymbol{f}\left(\gamma\tilde{\boldsymbol{\theta}}\right)\right)=\boldsymbol{0}. \qquad \text{(B-7)}$$

To derive the equations needed to show that weighted residuals from the constrained regression, defined as $\left(\boldsymbol{I}-\boldsymbol{QQ}'/\boldsymbol{Q}'\boldsymbol{Q}\right)\boldsymbol{\omega}^{1/2}\left(\boldsymbol{Y}-\boldsymbol{f}\left(\gamma\tilde{\boldsymbol{\theta}}\right)\right)$, equal standard weighted residuals $\boldsymbol{\omega}^{1/2}\left(\boldsymbol{Y}-\boldsymbol{f}\left(\gamma\hat{\boldsymbol{\theta}}\right)\right)$ when model intrinsic and model combined intrinsic types of nonlinearity are negligible, we substitute equation 6-17 of Cooley (2004) into the constrained weighted residuals to get

$$\begin{aligned}&\left(\boldsymbol{I}-\frac{\boldsymbol{QQ}'}{\boldsymbol{Q}'\boldsymbol{Q}}\right)\boldsymbol{\omega}^{1/2}\left(\boldsymbol{Y}-\boldsymbol{f}\left(\gamma\tilde{\boldsymbol{\theta}}\right)\right)\\&=\left(\boldsymbol{I}-\boldsymbol{R}\right)\boldsymbol{\omega}^{1/2}\left(\boldsymbol{Y}-\boldsymbol{f}\left(\gamma\boldsymbol{\theta}_*\right)\right)+\left(\boldsymbol{I}-\boldsymbol{R}\right)\boldsymbol{\omega}^{1/2}\left(\boldsymbol{f}\left(\gamma\boldsymbol{\theta}_*\right)-\boldsymbol{f}\left(\gamma\tilde{\boldsymbol{\theta}}\right)\right)+\left(\boldsymbol{R}-\frac{\boldsymbol{QQ}'}{\boldsymbol{Q}'\boldsymbol{Q}}\right)\boldsymbol{\omega}^{1/2}\left(\boldsymbol{Y}-\boldsymbol{f}\left(\gamma\tilde{\boldsymbol{\theta}}\right)\right).\end{aligned} \qquad \text{(B-8)}$$

If model intrinsic nonlinearity is negligible, then from Cooley (2004, equations 6-2 and I-1 - I-5) the first term on the right side of equation B-8 is equal to the weighted residual vector and the second term is negligible. If model combined intrinsic nonlinearity is negligible, then from Cooley (2004, equation I-21) the last term is negligible. However, from equation B-7, if $\tilde{\boldsymbol{R}}$ and $\tilde{\boldsymbol{Q}}$ were used in place of $\boldsymbol{R}$ and $\boldsymbol{Q}$, then this term always would be zero.

APPENDIX C. EXAMPLE SIMULATIONS

The test case presented in this section provides example input and output files for an entire modeling process including parameter estimation using MODFLOW-2000 in the Parameter-Estimation Process (PES) mode, calculation of correction factors using CORFAC-2k, calculation of nonlinearity measures using BEALE2-2k, calculation of quantities needed for residuals and nonlinearity analyses using RESAN2-2k, and calculation of confidence intervals and residuals analysis using MODFLOW-2000 in Uncertainty Process (UNC) mode.

The test example is taken from the synthetic case study of Christensen and Cooley (2003). The dimensions of the two-dimensional flow domain (fig. C1) are 18 by 8, divided into 90 by 40 uniform structural elements. The transmissivity is constant within each structural element. There is a pumping well in the center of the domain where ground water is withdrawn at a rate of 1. Boundary conditions include no flow across the top and bottom boundaries, a constant head of zero along the right boundary, and a constant flux across the left boundary (simulated as recharge with rate equal to 3.1076 over the left-most column of cells). The vector $\boldsymbol{\beta}$ of unknown system characteristics consists of spatially varying log-transmissivity, which is

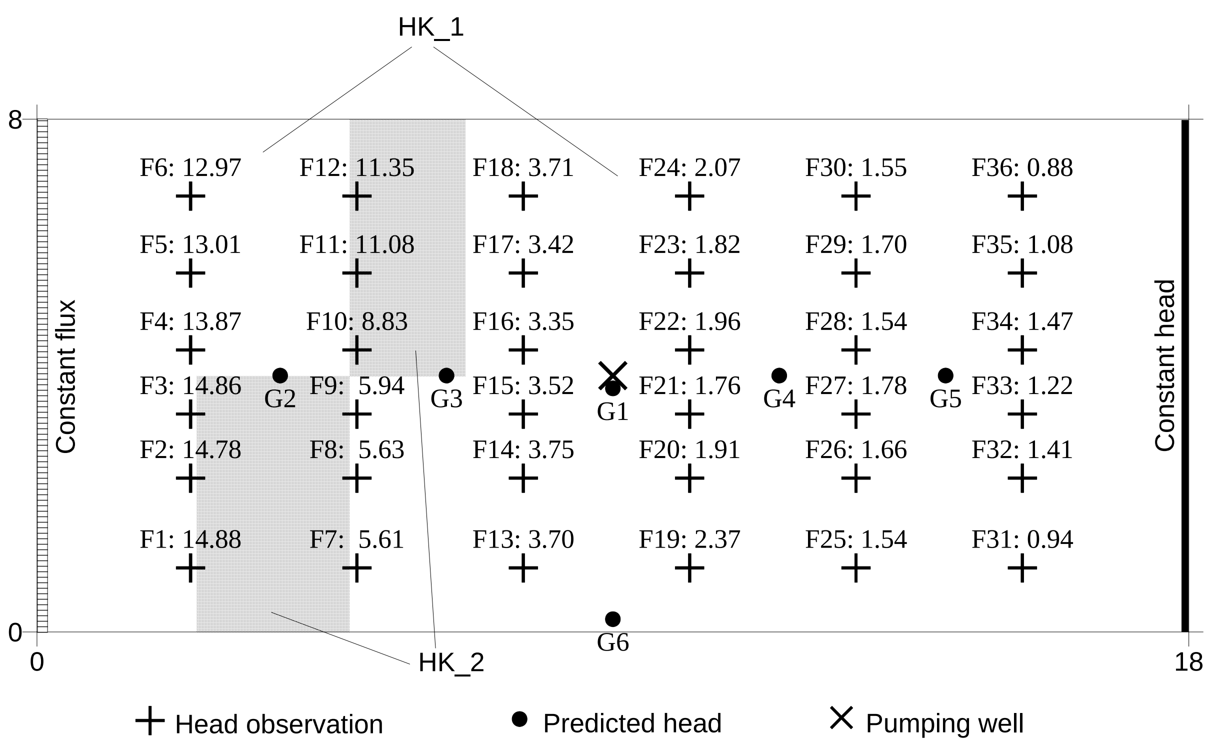

Figure C1. Model domain, boundary conditions, zonation, locations, and values of head observations, and locations of head predictions.

known to be normally distributed with a constant mean of zero and with exponential covariance with a correlation scale of 1.0 and a variance of 4.0.

The observations used for parameter estimation consist of 36 observations of hydraulic head observed at almost uniformly distributed grid points (fig. C1). The observation errors are known to be normally distributed with a variance of 0.01. (In the study of Christensen and Cooley (2003) the variance was 1.0.) The true error second-moment matrix, $\sigma_\varepsilon^2\boldsymbol{\Omega}$, was computed by the same Monte-Carlo method as used by Christensen and Cooley (2003). Weights for the observations are obtained as the inverses of the diagonal elements of $\boldsymbol{\Omega}$.

The numerical model used for parameter estimation and computation of confidence intervals has 91 by 41 elements. The width of the left-most and right-most columns is 0.1, while the remaining column widths are all 0.2. The width of the upper-most and lower-most rows is 0.1, while all other row-widths are 0.2. Based on the available 36 head observations, we divided the transmissivity field of the model into two transmissivity zones (fig. C1), one of presumably higher transmissivity (low hydraulic head gradient), and one of presumably lower transmissivity (high hydraulic head gradient). The model parameters are the log-transmissivities of each of the two zones and are named HK_1 and HK_2, respectively.

Parameter Estimation

The input files for, and the GLOBAL output file from, the parameter estimation are listed in the ‘Parameter Estimation – Input Files’ and the ‘Parameter Estimation – Global Output File’ sections. The diagonal elements of the true error second-moment matrix, $\sigma_\varepsilon^2\boldsymbol{\Omega}$, have values between 2.0 and 7.3. Because σ_ε^2 equals 0.01, the values of the diagonal elements of $\boldsymbol{\Omega}$ vary between 200 and 730. These values are input to MODFLOW-2000 as STATISTIC in item 6 of the head observation input where STAT-FLAG is set equal to 0 (Hill and others, 2000). Thus the weights for the head observations used in the regression are calculated as the inverses of the diagonal elements of $\boldsymbol{\Omega}$.

OUTNAM in the Observation Process input file is specified to be “example.” This defines the names of a number of MODFLOW-2000 output files as explained by Hill and others (2000, p. 27) and in this report.

The initial values of two zonal transmissivity parameters are both set to 1.0, which equals the known expected value of the transmissivity. The estimated parameters HK_1 and HK_2 are both log-transformed zonal transmissivity. HK_1 and HK_2 are estimated by MODFLOW-2000 to be 1.46 and 9.94×10^{-2}, respectively. The high estimate of HK_1 and the low estimate of HK_2 conform with the expectations from the head observations.

The value of the weighted least-squares objective function at the minimum is $S(\hat{\boldsymbol{\theta}}) = 0.014039.$ This value is used later to calculate the critical values needed for the calculation of confidence intervals.

Computation of Correction Factors Using CORFAC-2k

The first step to compute correction factors is to make MODFLOW-2000 create the input file example._cf for CORFAC-2k. This is done by the following.

1. The Uncertainty (UNC) process is activated by adding specification of the UNC input file to the Name File (example.nam).
2. The UNC file (unc.dat) where IACT is set equal to 3 is created. Confidence intervals are specified to be calculated for the two parameters HK_1 and HK_2.
3. The final calibrated parameter values from the example._b file are substituted into the SEN file.
4. Information about the six hydraulic head predictions is added to the HOB file (hob.dat).
5. MODFLOW-2000 is run.

The MODFLOW-2000 input files are listed in the 'Modified Input Files for Generation of CORFAC-2k Input File' section.

The created file, example._cf, is in this case modified by setting ITRN in item 1 equal to 1 and by setting V in item 14 equal to $\boldsymbol{\Omega}$. This modified file is listed in the 'Modified _cf Input File to CORFAC-2k' section. Running CORFAC-2k produces the output file example.#cf, which is listed in the 'Output File from CORFAC-2k' section.

In the output file, example.#cf, the computed correction factor for the confidence region is listed as CR=33.243, whereas the corresponding approximate bound is computed to be CRB=46.859. The approximate bound was calculated using the default effective correlation of 0.8 and not the actual effective correlation C=0.7149 computed by CORFAC-2k. If $\boldsymbol{\Omega}$ had been unknown, CRB would have to be used instead of CR to compute Scheffé type confidence intervals using MODFLOW-2000 with the UNC Process. Using CRB would produce wider Scheffé intervals than using CR.

In example.#cf the correction factors CC computed for the individual confidence intervals for the six head predictions and the two parameters, and the corresponding approximate bounds CCB, have the values given in table C1. Using the CCB would in all these cases produce wider individual confidence intervals than using the CC values.

Table C1. Correction factors, CC, and correction factor bounds, CCB, computed by CORFAC-2k for six head predictions (G1 to G6) and two parameters (HK_1 and HK_2).

	G1	G2	G3	G4	G5	G6	HK_1	HK_2
CC	45.638	15.989	46.966	45.492	45.477	45.875	45.473	10.668
CCB	71.613	25.130	73.142	71.470	71.456	71.842	71.452	37.083

Computation of Nonlinearity Measures Using BEALE2-2k

BEALE2-2k needs four input files, example._b1, example._b2, example._b3, and example._b4, that are generated by MODFLOW-2000 using UNC. The _b1 and _b3 files are generated as follows:

1. In the UNC file (unc.dat) IACT in item 1 is set equal to 1 and CFR and CFI are specified in items 8 and 9, respectively. The values of CFR and CFI equal the CR and CC values found in the example.#cf output file from CORFAC-2k.
2. The final calibrated parameter values from the example._b file are substituted into the SEN input file (sen.dat).
3. MODFLOW-2000 is run.

After the example._b1 and example._b3 files are generated, the example._b2 and example._b4 files are generated by changing the value of IACT to 2 in the UNC file (unc.dat), and then re-running MODFLOW-2000. Finally, BEALE2-2k is executed to produce the output file example.#be. The unc.dat, example._b1, example._b2, example._b3, example._b4, and example.#be files are listed in the 'Input Files Used to Generate BEALE2-2k Input Files', the 'BEALE2-2k Input Files', and the 'BEALE2-2k Output File' sections.

In the example.#be output file the computed measure of total nonlinearity, BNT, is approximately 0.064, and the measure of intrinsic nonlinearity, BNI, is approximately 0.45×10^{-3}. This indicates that the regression model is moderately nonlinear, and the intrinsic nonlinearity is insignificant. The combined intrinsic nonlinearity measures for confidence intervals are listed in table C2. These values indicate that the combined intrinsic nonlinearity is insignificant for the G2 head prediction confidence interval, but moderate for all the other intervals. Because the correction factors computed by CORFAC-2k for the latter seven intervals are only slightly larger than 0.09 (see chapter 2) and are all much less than one, correction factors CC should not be effected much by the omitted intrinsic nonlinearity components, and factors CCB should be conservative.

Table C2. Combined intrinsic nonlinearity measures computed by BEALE2-2k.

	G1	G2	G3	G4	G5	G6	HK_1	HK_2
BMI	0.91136E-01	0.13976E-04	0.80532E-01	0.92049E-01	0.92165E-01	0.89142E-01	0.37137E-01	0.22188E-01
BMF0	0.12232E-01	0.37404E-02	0.99148E-02	0.12468E-01	0.12491E-01	0.11832E-01	0.58584E-12	0.59462E-10
BMG0	0.36826E-01	0.40559E-02	0.34126E-01	0.37003E-01	0.37051E-01	0.36261E-01	0.37137E-01	0.22186E-01
BMIMAX	0.11560	0.80979E-02	0.10036	0.11699	0.11715	0.11280	0.37137E-01	0.22188E-01

Residuals Analysis And Detection of Nonlinearity Using RESAN2-2k

RESAN2-2k needs two input files that for the example are named example._ws and example._rs. The example._ws file was generated during parameter estimation and contains weighted simulated equivalents and residuals (Hill and others, 2000, table 5). The example._rs file is generated in a separate step where the B values for HK_1 and HK_2 are both set to 1.0 in item 3 of the SEN file (sen.dat), and where MAX-ITER is set to 0 in item 1 of the PES file (pes.dat). This means that the example._rs file is generated using values of 1.0 for both parameters but parameter estimation is not carried out (Hill and others, 2000, p. 72, 75, 78, and 79).

Before running RESAN2-2k, the example._rs file is modified by increasing NSETS in item 1 from 4 to 1,000, setting STDV in items 1 to 0.01, setting IERT in item 1 to 1, setting ICOV in item 1 to 1, specifying ET in item 10 to equal the expected values of the true errors, and specifying V in item 11 to equal $\boldsymbol{\Omega}_m$. RESAN2-2k is then run to generate the example.#nr and example._md output files. The input files for, and output files from, RESAN2-2k are listed in the 'RESAN2-2k Input Files' and 'RESAN2-2k Output Files' sections.

The example.#nr output file contains results of the analysis of residusls. The mean weighted residual, EM, is approximately –0.0005, and the slope of the weighted residual plot, SLP, is approximately 0.0036. Because both values are close to zero, they both indicate that model and system types of intrinsic nonlinearity are small. The intrinsic nonlinearity measure, QINT, is approximately 0.0002, which is much smaller than $S(\hat{\boldsymbol{\theta}}) = 0.014039$. This also indicates small model intrinsic nonlinearity. The correlation between weighted residuals and the means of synthetic residuals, CED, is approximately 0.996, and that the probability, PROB, of this or a smaller correlation is 0.988. Figure C2 shows a probability plot of ordered weighted residuals with an approximate 95 percent confidence band. This plot was generated from the results in the example._md file. The weighted residuals fall inside the confidence band. This, together with the high probability of CED, indicates normality of the weighted residuals.

Calculation of Confidence Intervals Using MODFLOW-2000 With the UNC Process

Finally, individual 95 percent confidence intervals are calculated for the six predicted heads, G1 to G6, and for the two model parameters, HK_1 and HK_2. This is accomplished with the following steps:

1. The UNC Process is activated by specifying the UNC file (unc.dat) in the Name File (example.nam). Two DATAGLO data files are specified to be opened in the Name file, one called confint.dat with unit number equal to 61 and the other called weight-res.dat with unit number equal to 62. The summary output of computed confidence limits are to be printed in the former data file, whereas weighted residuals from the constrained regression are to be printed in the latter.

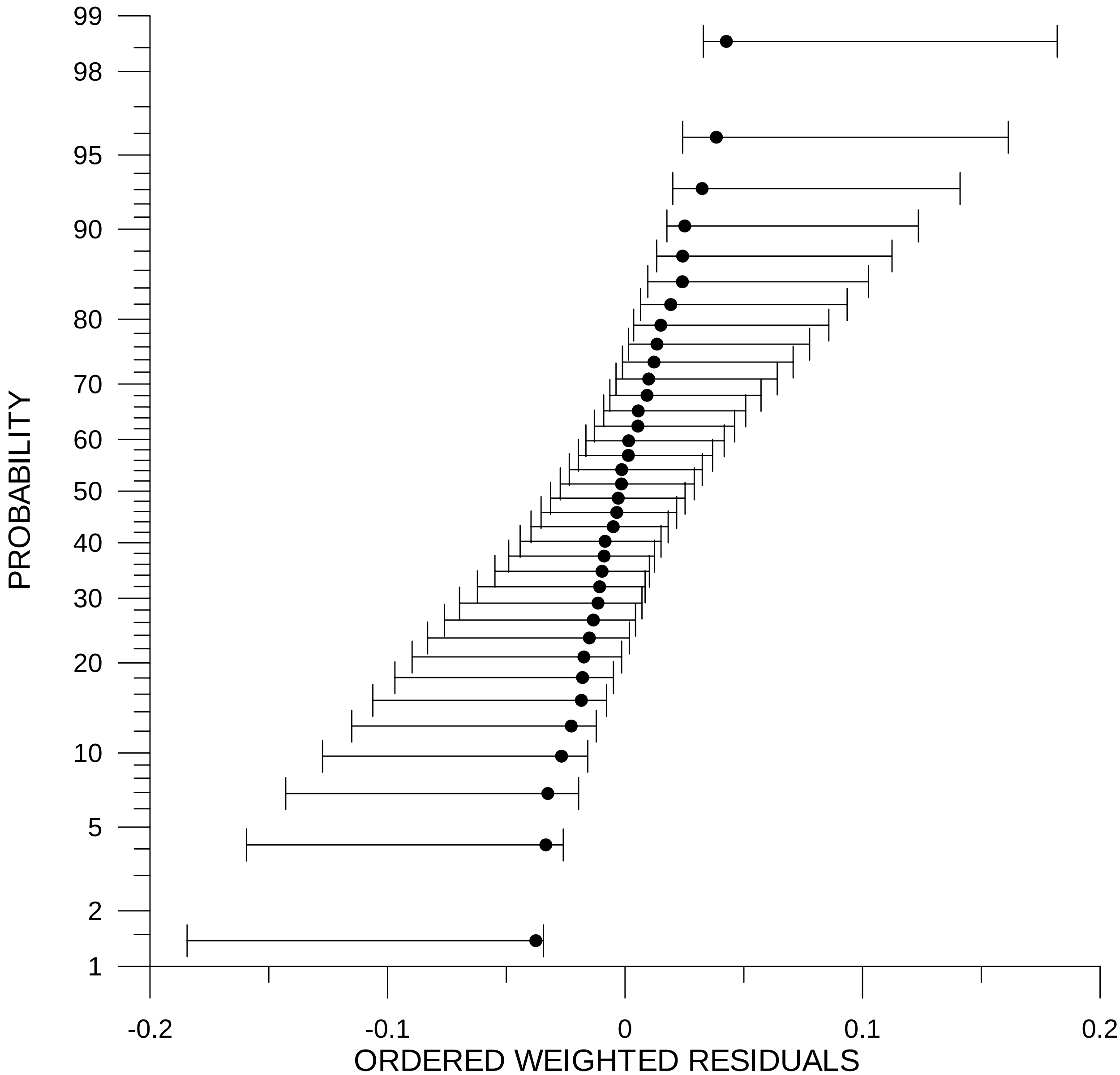

Figure C2. Ordered weighted residuals (dots) plotted with approximate 95 percent confidence band (bars).

2. IACT is set equal to 0, NPI is set equal to 2, IOIN is set equal to 61, IDSQ is set equal to 1, and IWRP is set equal to 62 in item 1 of the UNC file.
3. A critical value is computed from equation 86 for each individual 95 percent confidence interval using the correction factors, CC, in table C1, $t_{2.5}(34) = 2.032,$ and $S(\hat{\theta}) = 0.014039$. The elements of DSQ in item 4 of the UNC file are set equal to the critical values.

4. The two parameters for which confidence intervals are to be computed are specified in item 5 of the UNC file as HK_1 and HK_2, respectively.
5. The initial parameter values in the SEN file (sen.dat) are set equal to the final calibrated values.
6. MODFLOW-2000 is run.

Besides producing the GLOBAL and LIST output files with details concerning the computation of confidence intervals, MODFLOW-2000 in this run also produces the two files mentioned above named confint.dat and weight-res.dat. The input and output files are all listed in the ‘MODFLOW-2000 Input Files For Confidence Interval Calculation’, the ’GLOBAL Output File For Confidence Interval Calculation’, and the ’Summary and Weighted Residuals Output Files’ sections.

The output file named confint.dat contains the following:

```
C.I.  1: FL= 4.1361     ; SSE=0.91894E-01; ITER=4;  PAR:  1.007    0.1538
C.I.  2: FL= 13.439     ; SSE=0.41351E-01; ITER=3;  PAR:  1.519    0.7981E-01
C.I.  3: FL= 6.4088     ; SSE=0.94127E-01; ITER=4;  PAR:  1.003    0.1496
C.I.  4: FL= 3.1090     ; SSE=0.91639E-01; ITER=4;  PAR:  1.008    0.1541
C.I.  5: FL= 1.8458     ; SSE=0.91618E-01; ITER=4;  PAR:  1.007    0.1542
C.I.  6: FL= 4.6167     ; SSE=0.92338E-01; ITER=4;  PAR:  1.006    0.1531
C.I.  7: FL=0.42100     ; SSE=0.91608E-01; ITER=4;  PAR:  2.636    0.6966E-01
C.I.  8: FL=-0.87902    ; SSE=0.32298E-01; ITER=4;  PAR:  1.264    0.1321
C.I. -1: FL= 1.5895     ; SSE=0.91861E-01; ITER=4;  PAR:  2.641    0.6964E-01
C.I. -2: FL= 10.581     ; SSE=0.41295E-01; ITER=4;  PAR:  1.436    0.1282
C.I. -3: FL= 2.5599     ; SSE=0.94083E-01; ITER=4;  PAR:  2.671    0.6945E-01
C.I. -4: FL= 1.1892     ; SSE=0.91594E-01; ITER=4;  PAR:  2.636    0.6967E-01
C.I. -5: FL= 0.70517    ; SSE=0.91630E-01; ITER=4;  PAR:  2.636    0.6967E-01
C.I. -6: FL= 1.7864     ; SSE=0.92292E-01; ITER=4;  PAR:  2.646    0.6961E-01
C.I. -7: FL= 0.32539E-02; SSE=0.91624E-01; ITER=4;  PAR:  1.008    0.1542
C.I. -8: FL= -1.1052    ; SSE=0.32343E-01; ITER=3;  PAR:  1.750    0.7849E-01
```

Each line summarizes the results for one computed confidence limit: C.I. 1 is for the upper limit of the first confidence interval, C.I. 2 is for the upper limit of the second interval, C.I. –1 is for the lower limit of the first interval, and so on. In this case the first six intervals are for head predictions (G1 to G6), whereas the last two intervals are for the parameters (HK_1 and HK_2). The column of numbers preceded by “FL=” is the confidence limit value. The column of numbers preceded by “SSE=” is the value of the objective function at the parameter values corresponding to the confidence limit. The SSE value should be close to the critical value, DSQ, specified for the confidence interval in the UNC file. This is fulfilled for all confidence limits computed in this example. The column of numbers above preceded by “ITER=” is the number of iterations necessary to compute the confidence limit. Finally, the two columns of numbers preceded by "PAR:" are the parameter values corresponding to the computed confidence limit.

The output file named weight-res.dat contains weighted residuals for all computed confidence limits. These weighted residuals are defined as $\left(\boldsymbol{I}-\boldsymbol{Q}\boldsymbol{Q}'/\boldsymbol{Q}'\boldsymbol{Q}\right)\boldsymbol{\omega}^{1/2}\left(\boldsymbol{Y}-\boldsymbol{f}\left(\boldsymbol{\gamma}\tilde{\boldsymbol{\theta}}\right)\right)$ in chapter 2. In figure C3 the weighted residuals at the confidence limits are plotted against the weighted residuals from unconstrained regression (parameter estimation), $\boldsymbol{\omega}^{1/2}\left(\boldsymbol{Y}-\boldsymbol{f}\left(\boldsymbol{\gamma}\hat{\boldsymbol{\theta}}\right)\right)$. In all cases the points fall close to the identity line. This is especially true for the head prediction G2, whereas there is a little more scatter for the other head predictions and for the two parameters. This may indicate small combined intrinsic nonlinearity for the confidence interval of G2, and larger combined intrinsic nonlinearity for the other seven confidence intervals. This conforms with the indications of the combined intrinsic nonlinearity measures computed by BEALE2-2k listed in table C2.

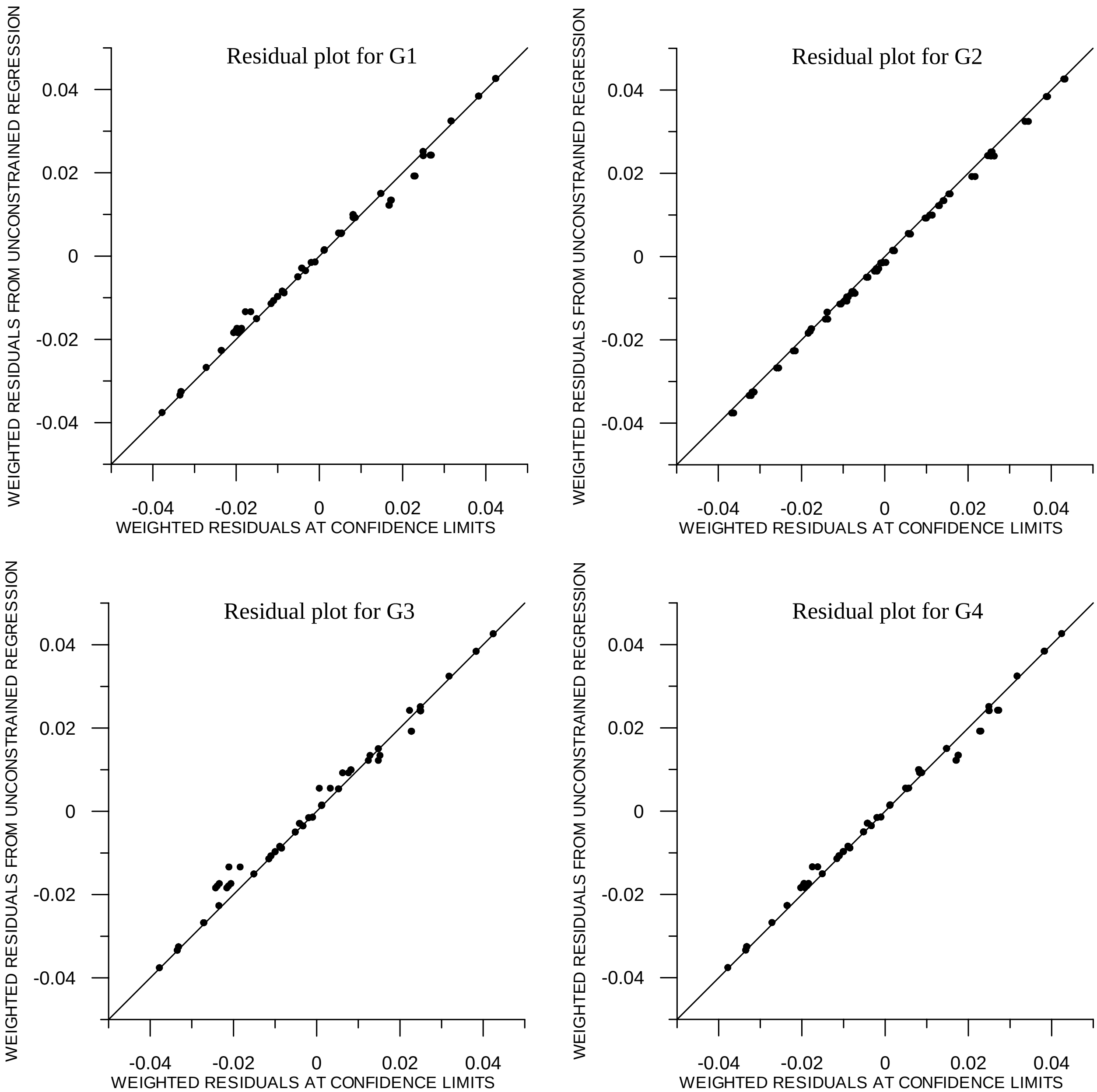

Figure C3. Weighted residuals at confidence limits in relation to weighted residuals from unconstrained regression (parameter estimation). The line is the one-to-one correlation line.

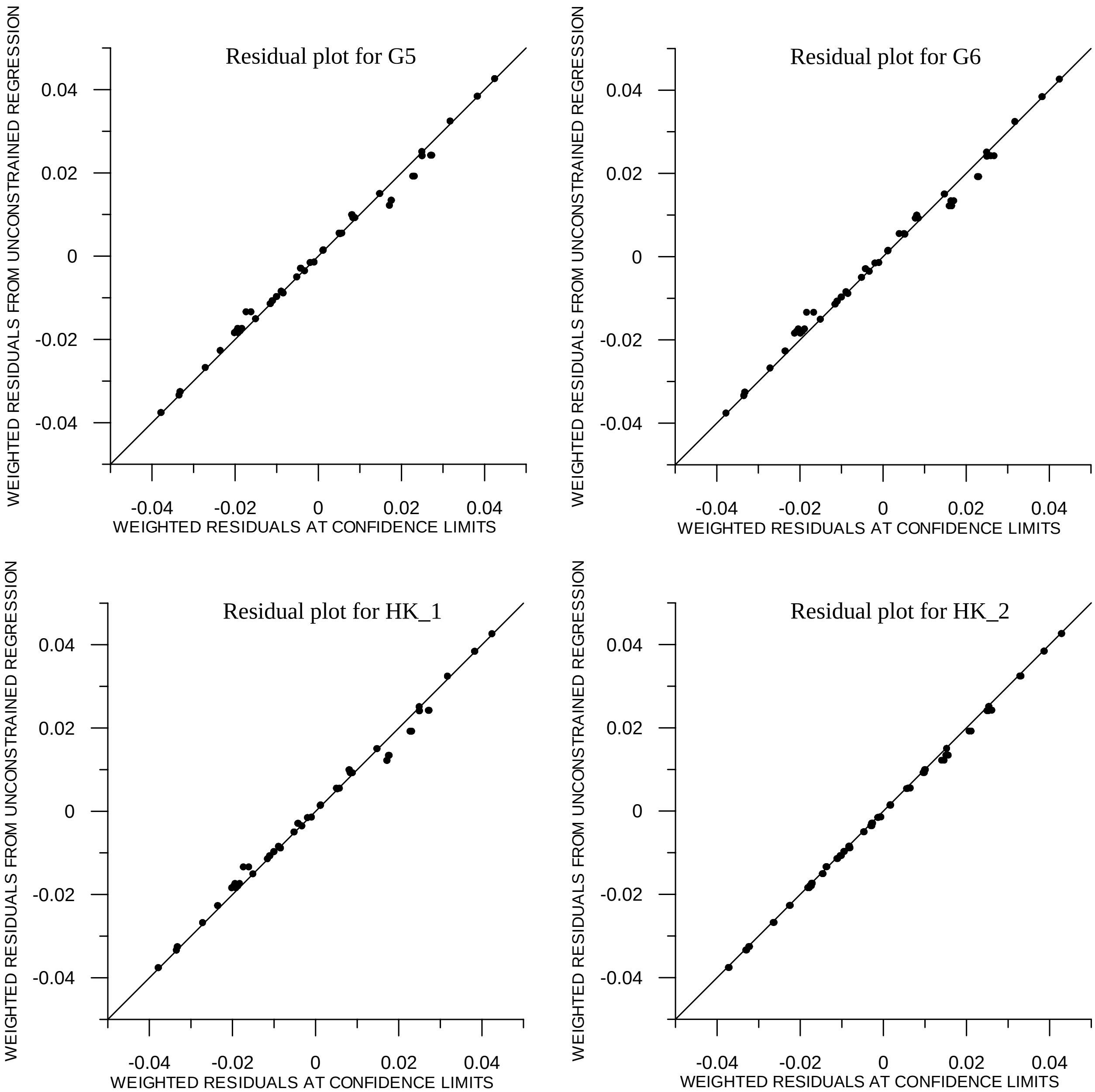

Figure C3 (continued). Weighted residuals at confidence limits in relation to weighted residuals from unconstrained regression (parameter estimation). The line is the one-to-one correlation line.

Parameter Estimation – Input Files

Name file (example.nam):

```
GLOBAL          4 mf2k.global_listing
LIST            3 output.dat
DIS            95 discret.dat
BAS6            1 bas6.dat
ZONE           93 zone.dat
MULT           94 multiple.dat
LPF            31 lpf6.dat
RCH            11 rech6.dat
WEL            12 wel6.dat
PCG            23 pcg2.dat
OC             22 oc.dat
DATA           10 inithead.dat
OBS            40 obs.dat
HOB            41 hob.dat
PES            47 pes.dat
SEN            46 sen.dat
```

DIS file (discret.dat):

```
# Discretization file for MODFLOW-2000, UNC1NLI1 Report Example
        1        41        91         1         1         0
 0
       95         1(16G5.0)                  -1  3. DELR(NCOL)
  0.1  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2
  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2
  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2
  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2
  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2
  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.1
       95         1(16G5.0)                  -1  4. DELC(NROW)
  0.1  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2
  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2
  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.2  0.1
        0         1(20G14.0)                  -1  5. TOP OF SYSTEM
        0         0(20G14.0)                  -1  5. BOTTOM OF OF LAYER 1
            1             1         1 SS
```

BAS6 file (bas6.dat):

```
# Basic package file for MODFLOW-2000, UNC1NLI1 Report Example
FREE
        1         1(40I2)                     -1  2. IBOUND Array for Layer 1
 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
 1 1 1 1 1 1 1 1 1 1-1
 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
```

```
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1-1
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1-1
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
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1 1 1 1 1 1 1 1 1 1-1
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
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1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
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1 1 1 1 1 1 1 1 1 1-1
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1-1
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
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1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1-1
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1-1
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1-1
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1-1
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1-1
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
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1 1 1 1 1 1 1 1 1 1-1
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
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1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
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1 1 1 1 1 1 1 1 1 1-1
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1-1
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
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1 1 1 1 1 1 1 1 1 1-1
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1-1
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
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1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
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 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
 1 1 1 1 1 1 1 1 1 1-1
   -999.99
        10         1(10F8.3)                    -1  4. Starting Heads in Layer 1
```

ZONE file (zone.dat):

```
# Zone file for MODFLOW-2000, UNC1NLI1 Report Example
 2
ZHK1
        93         1(91I1)                      -1  HK zone array for layer 1
1111111111111111111111111222222222111111111111111111111111111111111111111111111111111111111
1111111111111111111111111222222222111111111111111111111111111111111111111111111111111111111
1111111111111111111111111222222222111111111111111111111111111111111111111111111111111111111
1111111111111111111111111222222222111111111111111111111111111111111111111111111111111111111
1111111111111111111111111222222222111111111111111111111111111111111111111111111111111111111
1111111111111111111111111222222222111111111111111111111111111111111111111111111111111111111
1111111111111111111111111222222222111111111111111111111111111111111111111111111111111111111
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1111111111111222222222222111111111111111111111111111111111111111111111111111111111111111111
1111111111111222222222222111111111111111111111111111111111111111111111111111111111111111111
1111111111111222222222222111111111111111111111111111111111111111111111111111111111111111111
```

```
1111111111111222222222222111111111111111111111111111111111111111111111111111111111111111111
1111111111111222222222222111111111111111111111111111111111111111111111111111111111111111111
1111111111111222222222222111111111111111111111111111111111111111111111111111111111111111111
1111111111111222222222222111111111111111111111111111111111111111111111111111111111111111111
1111111111111222222222222111111111111111111111111111111111111111111111111111111111111111111
ZVK1
         0       999(20I4)                     -1  VK zone array for layer 1
```

MULT file (multiple.dat):

```
# Multiplier file for MODFLOW-2000, UNC1NLI1 Report Example
 2
HK1
         0         1(20G14.0)                   -1  4. HK Mult. array
VK1
         0         1(20G14.0)                   -1  4. VK Mult. array
```

LPF file (lpf6.dat):

```
# Layer-Property Flow file for MODFLOW-2000, UNC1NLI1 Report Example
         0      999.         3
 0
 0
 1
 0
 0
HK_1 HK   1  1
 1 HK1 ZHK1 1
HK_2 HK   1  1
 1 HK1 ZHK1 2
VK_0 VK   1  1
 1 VK1 ZVK1 999
        31         1(20G14.0)                   -1  10. HK of layer 1
        31         1(20G14.0)                   -1  11. HANI of layer 1
        31         1(20G14.0)                   -1  12. VK of layer 1
```

RCH file (rech6.dat):

```
# RECH file for MODFLOW-2000, UNC1NLI1 Report Example
1  0  NRCHOP  IRCHCB
1     INRECH
       11    6.2152(91G2.0)                    -1  10. RCH of layer 1
1.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0
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1.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0
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1.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0
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```

WEL file (wel6.dat):

```
# WELL file for MODFLOW-2000, UNC1NLI1 Report Example
#
PARAMETER 1  1
 1  00
WEL_0_1 Q  1 1
         1         21         46           -1
 0  1
WEL_0_1
```

PCG file (pcg2.dat):

```
        50        30          1
      .001      .001          1          1          1          0          1
```

OC file (oc.dat):

```
# Output control file for MODFLOW-2000, UNC1NLI1 Report Example
         0         0         0         0
         1         0         0         0   PERIOD: 1    TIME STEP: 1
         0         0         0         0   LAYER: 1
```

DATA file with initial heads (inithead.dat):

```
  14.549  14.484  14.397  14.309  14.219  14.128  14.036  13.942  13.848  13.753
  13.657  13.561  13.465  13.369  13.274  13.180  13.088  12.996  12.907  12.821
  12.737  12.656  12.579  12.505  12.435  11.913  10.940   9.971   9.005   8.042
   7.082   6.125   5.170   4.216   3.707   3.642   3.577   3.512   3.447   3.381
   3.316   3.250   3.183   3.117   3.051   2.984   2.918   2.851   2.785   2.718
   2.652   2.585   2.519   2.453   2.386   2.320   2.254   2.188   2.122   2.055
   1.989   1.923   1.857   1.790   1.724   1.658   1.591   1.525   1.458   1.391
```

```
  1.325   1.258   1.191   1.124   1.057   0.990   0.923   0.856   0.789   0.722
  0.655   0.588   0.521   0.454   0.387   0.319   0.252   0.185   0.118   0.050
  0.000
 14.549  14.485  14.398  14.309  14.220  14.128  14.036  13.942  13.848  13.753
 13.657  13.561  13.465  13.369  13.274  13.180  13.087  12.996  12.906  12.820
 12.736  12.655  12.577  12.503  12.433  11.912  10.938   9.969   9.002   8.040
  7.081   6.124   5.170   4.217   3.707   3.643   3.578   3.513   3.447   3.382
  3.316   3.250   3.184   3.117   3.051   2.984   2.918   2.851   2.785   2.718
  2.652   2.585   2.519   2.453   2.386   2.320   2.254   2.188   2.122   2.055
  1.989   1.923   1.857   1.790   1.724   1.658   1.591   1.525   1.458   1.391
  1.325   1.258   1.191   1.124   1.057   0.990   0.923   0.856   0.789   0.722
  0.655   0.588   0.521   0.454   0.387   0.319   0.252   0.185   0.118   0.050
  0.000
 14.551  14.487  14.400  14.311  14.222  14.130  14.038  13.944  13.849  13.754
 13.658  13.561  13.465  13.368  13.273  13.178  13.084  12.992  12.903  12.816
 12.731  12.650  12.572  12.498  12.427  11.906  10.932   9.963   8.997   8.035
  7.077   6.122   5.169   4.216   3.708   3.643   3.578   3.513   3.448   3.382
  3.316   3.250   3.184   3.117   3.051   2.984   2.918   2.851   2.785   2.718
  2.652   2.585   2.519   2.453   2.386   2.320   2.254   2.188   2.122   2.055
  1.989   1.923   1.857   1.790   1.724   1.658   1.591   1.525   1.458   1.391
  1.325   1.258   1.191   1.124   1.057   0.990   0.923   0.856   0.789   0.722
  0.655   0.588   0.521   0.454   0.387   0.319   0.252   0.185   0.118   0.050
  0.000
 14.555  14.491  14.404  14.315  14.225  14.133  14.040  13.946  13.851  13.755
 13.658  13.561  13.464  13.367  13.270  13.174  13.080  12.987  12.897  12.808
 12.723  12.641  12.563  12.488  12.418  11.896  10.922   9.953   8.988   8.027
  7.070   6.117   5.166   4.215   3.708   3.644   3.579   3.514   3.448   3.383
  3.317   3.251   3.184   3.118   3.051   2.984   2.918   2.851   2.784   2.718
  2.651   2.585   2.519   2.453   2.386   2.320   2.254   2.188   2.122   2.055
  1.989   1.923   1.857   1.790   1.724   1.658   1.591   1.525   1.458   1.391
  1.325   1.258   1.191   1.124   1.057   0.991   0.924   0.857   0.789   0.722
  0.655   0.588   0.521   0.454   0.387   0.320   0.252   0.185   0.118   0.050
  0.000
 14.560  14.496  14.409  14.320  14.230  14.138  14.044  13.950  13.854  13.757
 13.660  13.562  13.463  13.365  13.267  13.170  13.074  12.980  12.888  12.798
 12.712  12.629  12.550  12.475  12.404  11.881  10.908   9.939   8.975   8.016
  7.061   6.110   5.161   4.214   3.709   3.644   3.580   3.515   3.449   3.384
  3.318   3.251   3.185   3.118   3.051   2.985   2.918   2.851   2.784   2.718
  2.651   2.585   2.519   2.452   2.386   2.320   2.254   2.188   2.122   2.055
  1.989   1.923   1.857   1.791   1.724   1.658   1.591   1.525   1.458   1.392
  1.325   1.258   1.191   1.125   1.058   0.991   0.924   0.857   0.790   0.723
  0.655   0.588   0.521   0.454   0.387   0.319   0.252   0.185   0.118   0.050
  0.000
 14.567  14.503  14.416  14.326  14.236  14.143  14.050  13.954  13.858  13.760
 13.661  13.562  13.462  13.362  13.263  13.164  13.066  12.970  12.877  12.786
 12.698  12.613  12.533  12.457  12.385  11.862  10.888   9.920   8.957   8.000
  7.048   6.100   5.156   4.213   3.710   3.645   3.581   3.516   3.451   3.385
  3.319   3.252   3.185   3.119   3.052   2.985   2.918   2.851   2.784   2.717
  2.651   2.585   2.518   2.452   2.386   2.320   2.254   2.188   2.122   2.056
  1.989   1.923   1.857   1.791   1.724   1.658   1.592   1.525   1.458   1.392
  1.325   1.258   1.192   1.125   1.058   0.991   0.924   0.857   0.790   0.723
  0.655   0.588   0.521   0.454   0.387   0.319   0.252   0.185   0.118   0.050
  0.000
 14.576  14.511  14.424  14.335  14.244  14.151  14.056  13.960  13.863  13.764
 13.664  13.563  13.461  13.360  13.258  13.157  13.057  12.959  12.863  12.769
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12.679  12.593  12.511  12.434  12.362  11.839  10.863   9.895   8.934   7.979
 7.031   6.087   5.148   4.211   3.711   3.647   3.583   3.518   3.452   3.386
 3.320   3.253   3.186   3.119   3.052   2.985   2.917   2.850   2.784   2.717
 2.650   2.584   2.518   2.452   2.386   2.320   2.254   2.188   2.122   2.056
 1.990   1.923   1.857   1.791   1.725   1.658   1.592   1.525   1.459   1.392
 1.325   1.259   1.192   1.125   1.058   0.991   0.924   0.857   0.790   0.723
 0.656   0.588   0.521   0.454   0.387   0.319   0.252   0.185   0.118   0.050
 0.000
14.586  14.522  14.434  14.345  14.253  14.160  14.065  13.968  13.869  13.769
13.667  13.564  13.461  13.357  13.253  13.149  13.046  12.945  12.846  12.750
12.657  12.569  12.485  12.407  12.334  11.809  10.833   9.864   8.904   7.952
 7.008   6.070   5.138   4.208   3.712   3.649   3.585   3.520   3.454   3.388
 3.322   3.254   3.187   3.120   3.052   2.985   2.917   2.850   2.783   2.716
 2.650   2.584   2.517   2.451   2.385   2.320   2.254   2.188   2.122   2.056
 1.990   1.924   1.858   1.791   1.725   1.659   1.592   1.526   1.459   1.392
 1.326   1.259   1.192   1.125   1.058   0.991   0.924   0.857   0.790   0.723
 0.656   0.589   0.521   0.454   0.387   0.320   0.252   0.185   0.118   0.050
 0.000
14.598  14.534  14.446  14.356  14.264  14.171  14.075  13.977  13.877  13.775
13.672  13.567  13.461  13.354  13.247  13.140  13.034  12.929  12.827  12.727
12.631  12.540  12.454  12.373  12.300  11.773  10.794   9.825   8.865   7.917
 6.978   6.048   5.125   4.205   3.715   3.652   3.588   3.523   3.457   3.391
 3.324   3.256   3.188   3.120   3.052   2.984   2.917   2.849   2.782   2.716
 2.649   2.583   2.517   2.451   2.385   2.319   2.254   2.188   2.122   2.056
 1.990   1.924   1.858   1.792   1.725   1.659   1.593   1.526   1.459   1.393
 1.326   1.259   1.192   1.125   1.059   0.992   0.924   0.857   0.790   0.723
 0.656   0.589   0.521   0.454   0.387   0.320   0.252   0.185   0.118   0.050
 0.000
14.613  14.548  14.460  14.370  14.278  14.183  14.087  13.988  13.886  13.783
13.677  13.570  13.461  13.351  13.241  13.130  13.020  12.911  12.804  12.700
12.601  12.505  12.416  12.334  12.258  11.729  10.745   9.774   8.817   7.872
 6.941   6.021   5.109   4.201   3.717   3.655   3.591   3.527   3.461   3.394
 3.326   3.258   3.189   3.121   3.052   2.984   2.916   2.848   2.781   2.714
 2.648   2.582   2.516   2.450   2.385   2.319   2.254   2.188   2.122   2.056
 1.990   1.924   1.858   1.792   1.726   1.660   1.593   1.527   1.460   1.393
 1.326   1.260   1.193   1.126   1.059   0.992   0.925   0.858   0.790   0.723
 0.656   0.589   0.522   0.454   0.387   0.320   0.252   0.185   0.118   0.050
 0.000
14.629  14.565  14.477  14.386  14.293  14.198  14.101  14.001  13.898  13.793
13.685  13.575  13.463  13.350  13.235  13.120  13.005  12.891  12.779  12.670
12.565  12.465  12.372  12.286  12.209  11.674  10.684   9.710   8.753   7.815
 6.893   5.985   5.088   4.196   3.721   3.660   3.596   3.532   3.465   3.398
 3.329   3.260   3.191   3.121   3.052   2.983   2.914   2.847   2.780   2.713
 2.647   2.581   2.515   2.450   2.384   2.319   2.254   2.188   2.122   2.057
 1.991   1.925   1.859   1.793   1.726   1.660   1.594   1.527   1.460   1.394
 1.327   1.260   1.193   1.126   1.059   0.992   0.925   0.858   0.791   0.724
 0.656   0.589   0.522   0.454   0.387   0.320   0.253   0.185   0.118   0.050
 0.000
14.648  14.584  14.495  14.405  14.312  14.216  14.118  14.016  13.912  13.805
13.695  13.582  13.467  13.349  13.229  13.109  12.988  12.868  12.750  12.635
12.524  12.419  12.321  12.231  12.151  11.608  10.608   9.628   8.672   7.740
 6.831   5.939   5.061   4.191   3.726   3.666   3.603   3.538   3.471   3.403
 3.333   3.263   3.192   3.121   3.051   2.981   2.913   2.845   2.778   2.711
 2.645   2.580   2.514   2.449   2.384   2.319   2.254   2.188   2.123   2.057
 1.991   1.926   1.860   1.793   1.727   1.661   1.594   1.528   1.461   1.394
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  1.328   1.261   1.194   1.127   1.060   0.993   0.925   0.858   0.791   0.724
  0.657   0.589   0.522   0.455   0.387   0.320   0.253   0.185   0.118   0.051
  0.000
 14.669  14.605  14.516  14.425  14.332  14.236  14.137  14.035  13.930  13.821
 13.708  13.592  13.473  13.350  13.225  13.098  12.971  12.844  12.719  12.596
 12.478  12.365  12.260  12.165  12.082  11.528  10.510   9.521   8.565   7.643
  6.750   5.880   5.027   4.183   3.733   3.674   3.611   3.546   3.478   3.409
  3.338   3.266   3.194   3.121   3.050   2.979   2.910   2.842   2.775   2.709
  2.643   2.578   2.513   2.449   2.384   2.319   2.254   2.189   2.123   2.058
  1.992   1.926   1.860   1.794   1.728   1.662   1.595   1.528   1.462   1.395
  1.328   1.261   1.194   1.127   1.060   0.993   0.926   0.859   0.791   0.724
  0.657   0.589   0.522   0.455   0.387   0.320   0.253   0.185   0.118   0.051
  0.000
 14.693  14.628  14.540  14.449  14.355  14.259  14.160  14.057  13.951  13.840
 13.725  13.605  13.481  13.353  13.222  13.089  12.954  12.819  12.685  12.553
 12.426  12.304  12.191  12.088  11.999  11.428  10.385   9.382   8.426   7.516
  6.645   5.805   4.985   4.175   3.743   3.685   3.622   3.557   3.488   3.416
  3.343   3.269   3.195   3.121   3.047   2.976   2.906   2.838   2.771   2.706
  2.641   2.576   2.512   2.448   2.384   2.319   2.254   2.189   2.124   2.059
  1.993   1.927   1.861   1.795   1.729   1.662   1.596   1.529   1.462   1.396
  1.329   1.262   1.195   1.128   1.061   0.993   0.926   0.859   0.792   0.724
  0.657   0.590   0.522   0.455   0.388   0.320   0.253   0.185   0.118   0.051
  0.000
 14.719  14.654  14.566  14.475  14.382  14.285  14.186  14.083  13.975  13.863
 13.746  13.623  13.494  13.360  13.222  13.080  12.936  12.792  12.649  12.506
 12.368  12.234  12.110  11.997  11.901  11.302  10.219   9.196   8.241   7.350
  6.510   5.709   4.931   4.165   3.756   3.699   3.637   3.570   3.499   3.426
  3.350   3.273   3.196   3.119   3.043   2.970   2.900   2.832   2.766   2.702
  2.638   2.575   2.511   2.447   2.384   2.319   2.255   2.190   2.125   2.060
  1.994   1.928   1.862   1.796   1.730   1.663   1.597   1.530   1.463   1.396
  1.330   1.263   1.196   1.128   1.061   0.994   0.927   0.859   0.792   0.725
  0.657   0.590   0.523   0.455   0.388   0.320   0.253   0.186   0.118   0.051
  0.000
 14.747  14.682  14.594  14.504  14.410  14.315  14.215  14.113  14.005  13.892
 13.773  13.647  13.513  13.371  13.224  13.073  12.920  12.765  12.610  12.456
 12.304  12.157  12.017  11.889  11.781  11.137   9.992   8.942   7.994   7.132
  6.337   5.588   4.866   4.156   3.775   3.719   3.656   3.587   3.514   3.437
  3.358   3.277   3.196   3.116   3.037   2.962   2.891   2.825   2.760   2.697
  2.635   2.573   2.510   2.447   2.384   2.320   2.256   2.191   2.126   2.061
  1.995   1.929   1.863   1.797   1.731   1.664   1.598   1.531   1.464   1.397
  1.330   1.263   1.196   1.129   1.062   0.995   0.927   0.860   0.793   0.725
  0.658   0.590   0.523   0.455   0.388   0.321   0.253   0.186   0.118   0.051
  0.000
 14.777  14.713  14.625  14.535  14.442  14.347  14.249  14.147  14.040  13.927
 13.807  13.678  13.538  13.388  13.231  13.069  12.905  12.739  12.572  12.404
 12.236  12.071  11.911  11.763  11.636  10.911   9.667   8.588   7.660   6.849
  6.119   5.441   4.790   4.148   3.801   3.746   3.681   3.609   3.532   3.451
  3.368   3.282   3.196   3.110   3.027   2.950   2.879   2.815   2.753   2.692
  2.632   2.571   2.510   2.447   2.384   2.321   2.257   2.192   2.128   2.062
  1.997   1.931   1.865   1.799   1.732   1.666   1.599   1.532   1.465   1.398
  1.331   1.264   1.197   1.130   1.062   0.995   0.928   0.860   0.793   0.726
  0.658   0.591   0.523   0.456   0.388   0.321   0.253   0.186   0.118   0.051
  0.000
 14.809  14.745  14.658  14.568  14.477  14.383  14.286  14.186  14.081  13.970
 13.851  13.720  13.574  13.412  13.241  13.067  12.891  12.713  12.534  12.351
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12.167  11.980  11.794  11.615  11.456  10.571   9.178   8.083   7.210   6.483
 5.848   5.265   4.706   4.146   3.839   3.782   3.713   3.636   3.554   3.468
 3.379   3.288   3.195   3.102   3.012   2.930   2.862   2.801   2.744   2.687
 2.629   2.570   2.510   2.448   2.386   2.323   2.259   2.194   2.129   2.064
 1.999   1.933   1.867   1.800   1.734   1.667   1.600   1.533   1.466   1.399
 1.332   1.265   1.198   1.130   1.063   0.996   0.928   0.861   0.794   0.726
 0.659   0.591   0.523   0.456   0.388   0.321   0.253   0.186   0.118   0.051
 0.000
14.844  14.780  14.693  14.604  14.514  14.422  14.327  14.229  14.128  14.021
13.905  13.777  13.626  13.444  13.256  13.068  12.879  12.690  12.498  12.301
12.098  11.888  11.670  11.446  11.231   9.968   8.391   7.356   6.612   6.026
 5.524   5.066   4.622   4.162   3.893   3.831   3.754   3.669   3.579   3.487
 3.392   3.295   3.194   3.091   2.989   2.896   2.836   2.785   2.735   2.683
 2.628   2.570   2.511   2.450   2.388   2.325   2.261   2.197   2.132   2.066
 2.001   1.935   1.868   1.802   1.735   1.669   1.602   1.535   1.468   1.401
 1.333   1.266   1.199   1.131   1.064   0.996   0.929   0.862   0.794   0.726
 0.659   0.591   0.524   0.456   0.389   0.321   0.254   0.186   0.118   0.051
 0.000
14.879  14.815  14.729  14.641  14.553  14.463  14.371  14.277  14.180  14.080
13.974  13.856  13.711  13.481  13.270  13.068  12.869  12.669  12.466  12.257
12.038  11.805  11.551  11.267  10.951   8.573   7.064   6.335   5.859   5.484
 5.157   4.854   4.553   4.223   3.977   3.895   3.802   3.705   3.608   3.509
 3.408   3.305   3.196   3.080   2.955   2.831   2.800   2.769   2.729   2.681
 2.629   2.572   2.513   2.453   2.391   2.328   2.264   2.199   2.134   2.069
 2.003   1.937   1.870   1.804   1.737   1.670   1.603   1.536   1.469   1.402
 1.334   1.267   1.200   1.132   1.065   0.997   0.930   0.862   0.795   0.727
 0.659   0.592   0.524   0.457   0.389   0.321   0.254   0.186   0.118   0.051
 0.000
14.916  14.852  14.766  14.680  14.593  14.505  14.417  14.327  14.237  14.145
14.053  13.961  13.880  13.631  13.317  13.048  12.791  12.533  12.268  11.986
11.675  11.313  10.847  10.128   8.629   6.255   5.939   5.656   5.402   5.169
 4.950   4.739   4.532   4.325   4.110   3.970   3.852   3.743   3.638   3.533
 3.428   3.319   3.205   3.079   2.921   2.671   2.763   2.762   2.730   2.685
 2.633   2.577   2.518   2.457   2.395   2.331   2.267   2.203   2.137   2.072
 2.005   1.939   1.873   1.806   1.739   1.672   1.605   1.538   1.470   1.403
 1.336   1.268   1.201   1.133   1.065   0.998   0.930   0.863   0.795   0.727
 0.660   0.592   0.524   0.457   0.389   0.321   0.254   0.186   0.118   0.051
 0.000
14.953  14.889  14.805  14.719  14.634  14.549  14.464  14.379  14.294  14.211
14.131  14.058  13.999  13.758  13.362  12.998  12.644  12.286  11.912  11.506
11.046  10.494   9.782   8.774   7.225   5.976   5.763   5.541   5.324   5.115
 4.915   4.720   4.530   4.345   4.169   4.022   3.895   3.778   3.666   3.558
 3.450   3.340   3.227   3.108   2.979   2.852   2.819   2.787   2.745   2.696
 2.642   2.584   2.524   2.463   2.400   2.336   2.271   2.206   2.141   2.075
 2.008   1.942   1.875   1.808   1.741   1.674   1.607   1.539   1.472   1.404
 1.337   1.269   1.202   1.134   1.066   0.999   0.931   0.863   0.796   0.728
 0.660   0.593   0.525   0.457   0.389   0.322   0.254   0.186   0.119   0.051
 0.000
14.990  14.927  14.843  14.759  14.675  14.592  14.510  14.429  14.350  14.274
14.203  14.140  14.089  13.832  13.376  12.936  12.501  12.056  11.589  11.080
10.508   9.836   9.012   7.962   6.613   5.751   5.596   5.420   5.237   5.054
 4.873   4.696   4.524   4.356   4.199   4.056   3.927   3.807   3.692   3.582
 3.473   3.365   3.255   3.145   3.037   2.939   2.874   2.820   2.767   2.712
 2.654   2.594   2.532   2.470   2.406   2.341   2.276   2.211   2.145   2.078
 2.012   1.945   1.878   1.810   1.743   1.676   1.608   1.541   1.473   1.406
```

```
 1.338   1.270   1.203   1.135   1.067   0.999   0.932   0.864   0.796   0.728
 0.661   0.593   0.525   0.457   0.390   0.322   0.254   0.186   0.119   0.051
 0.000
15.028  14.964  14.881  14.798  14.716  14.635  14.556  14.478  14.404  14.333
14.267  14.209  14.161  13.882  13.372  12.870  12.367  11.849  11.305  10.719
10.069   9.330   8.467   7.450   6.265   5.572   5.449   5.306   5.150   4.990
 4.829   4.669   4.511   4.358   4.213   4.076   3.949   3.829   3.715   3.604
 3.496   3.390   3.285   3.181   3.083   2.993   2.919   2.853   2.791   2.730
 2.668   2.605   2.542   2.478   2.413   2.347   2.281   2.215   2.149   2.082
 2.015   1.948   1.880   1.813   1.745   1.678   1.610   1.543   1.475   1.407
 1.339   1.272   1.204   1.136   1.068   1.000   0.932   0.865   0.797   0.729
 0.661   0.593   0.526   0.458   0.390   0.322   0.254   0.186   0.119   0.051
 0.000
15.064  15.001  14.918  14.836  14.755  14.676  14.599  14.525  14.453  14.386
14.323  14.268  14.220  13.918  13.361  12.806  12.245  11.669  11.065  10.421
 9.721   8.945   8.078   7.105   6.033   5.427   5.324   5.203   5.069   4.928
 4.783   4.638   4.494   4.353   4.217   4.088   3.964   3.847   3.734   3.624
 3.518   3.414   3.312   3.213   3.119   3.032   2.954   2.882   2.814   2.748
 2.683   2.618   2.552   2.486   2.420   2.354   2.287   2.220   2.153   2.086
 2.018   1.951   1.883   1.816   1.748   1.680   1.612   1.544   1.476   1.408
 1.341   1.273   1.205   1.137   1.069   1.001   0.933   0.865   0.797   0.730
 0.662   0.594   0.526   0.458   0.390   0.322   0.254   0.187   0.119   0.051
 0.000
15.099  15.036  14.954  14.872  14.793  14.716  14.640  14.568  14.499  14.433
14.373  14.318  14.270  13.948  13.348  12.748  12.140  11.516  10.866  10.180
 9.447   8.654   7.792   6.858   5.862   5.309   5.218   5.112   4.994   4.868
 4.738   4.606   4.474   4.343   4.216   4.093   3.974   3.859   3.749   3.641
 3.537   3.435   3.336   3.240   3.149   3.063   2.983   2.907   2.836   2.766
 2.698   2.630   2.563   2.495   2.428   2.360   2.293   2.225   2.158   2.090
 2.022   1.954   1.886   1.818   1.750   1.682   1.614   1.546   1.478   1.410
 1.342   1.274   1.206   1.138   1.070   1.002   0.934   0.866   0.798   0.730
 0.662   0.594   0.526   0.458   0.390   0.323   0.255   0.187   0.119   0.051
 0.000
15.133  15.070  14.988  14.907  14.829  14.753  14.679  14.608  14.540  14.476
14.417  14.362  14.313  13.972  13.336  12.697  12.051  11.389  10.704   9.988
 9.233   8.431   7.578   6.675   5.729   5.210   5.128   5.033   4.927   4.813
 4.695   4.574   4.452   4.330   4.210   4.093   3.979   3.868   3.760   3.655
 3.553   3.454   3.357   3.263   3.174   3.088   3.007   2.929   2.855   2.783
 2.712   2.642   2.573   2.504   2.436   2.367   2.299   2.231   2.162   2.094
 2.026   1.957   1.889   1.821   1.753   1.684   1.616   1.548   1.480   1.411
 1.343   1.275   1.207   1.139   1.071   1.003   0.935   0.867   0.799   0.731
 0.663   0.595   0.527   0.459   0.391   0.323   0.255   0.187   0.119   0.051
 0.000
15.165  15.102  15.020  14.940  14.863  14.787  14.715  14.645  14.578  14.515
14.456  14.401  14.351  13.993  13.325  12.655  11.976  11.284  10.572   9.834
 9.065   8.259   7.415   6.535   5.624   5.127   5.051   4.964   4.867   4.764
 4.655   4.543   4.429   4.316   4.202   4.091   3.981   3.874   3.769   3.667
 3.567   3.469   3.375   3.283   3.194   3.109   3.027   2.948   2.872   2.798
 2.725   2.654   2.583   2.513   2.443   2.374   2.305   2.236   2.167   2.098
 2.029   1.961   1.892   1.823   1.755   1.686   1.618   1.550   1.481   1.413
 1.344   1.276   1.208   1.140   1.072   1.003   0.935   0.867   0.799   0.731
 0.663   0.595   0.527   0.459   0.391   0.323   0.255   0.187   0.119   0.051
 0.000
15.195  15.132  15.051  14.971  14.894  14.819  14.747  14.678  14.612  14.549
14.490  14.435  14.384  14.012  13.317  12.620  11.916  11.200  10.467   9.712
```

```
  8.933   8.125   7.288   6.425   5.539   5.058   4.986   4.904   4.815   4.719
  4.618   4.514   4.407   4.300   4.193   4.086   3.981   3.877   3.775   3.675
  3.578   3.482   3.389   3.299   3.211   3.126   3.044   2.964   2.887   2.811
  2.737   2.664   2.593   2.521   2.451   2.381   2.311   2.241   2.171   2.102
  2.033   1.964   1.895   1.826   1.757   1.688   1.620   1.551   1.483   1.414
  1.346   1.277   1.209   1.141   1.072   1.004   0.936   0.868   0.800   0.732
  0.663   0.595   0.527   0.459   0.391   0.323   0.255   0.187   0.119   0.051
  0.000
 15.223  15.160  15.079  15.000  14.923  14.849  14.777  14.708  14.643  14.580
 14.521  14.465  14.413  14.029  13.312  12.593  11.867  11.132  10.382   9.615
  8.828   8.020   7.189   6.337   5.469   4.999   4.930   4.853   4.769   4.679
  4.585   4.487   4.386   4.284   4.182   4.080   3.979   3.878   3.780   3.682
  3.587   3.493   3.401   3.312   3.225   3.140   3.058   2.978   2.900   2.823
  2.748   2.674   2.601   2.529   2.458   2.387   2.316   2.246   2.176   2.106
  2.036   1.967   1.898   1.829   1.759   1.691   1.622   1.553   1.484   1.416
  1.347   1.278   1.210   1.142   1.073   1.005   0.937   0.868   0.800   0.732
  0.664   0.596   0.528   0.459   0.391   0.323   0.255   0.187   0.119   0.051
  0.000
 15.249  15.186  15.105  15.026  14.949  14.876  14.804  14.736  14.670  14.608
 14.548  14.492  14.439  14.045  13.309  12.572  11.829  11.078  10.315   9.539
  8.746   7.936   7.110   6.267   5.411   4.949   4.882   4.809   4.729   4.644
  4.554   4.462   4.366   4.269   4.172   4.073   3.976   3.878   3.782   3.687
  3.594   3.502   3.411   3.323   3.237   3.152   3.070   2.990   2.911   2.834
  2.758   2.683   2.609   2.537   2.464   2.393   2.321   2.251   2.180   2.110
  2.040   1.970   1.900   1.831   1.762   1.692   1.623   1.554   1.486   1.417
  1.348   1.280   1.211   1.142   1.074   1.006   0.937   0.869   0.801   0.732
  0.664   0.596   0.528   0.460   0.392   0.323   0.255   0.187   0.119   0.051
  0.000
 15.272  15.210  15.128  15.050  14.973  14.900  14.829  14.760  14.695  14.632
 14.572  14.516  14.462  14.060  13.308  12.556  11.799  11.035  10.262   9.478
  8.681   7.871   7.047   6.210   5.363   4.906   4.842   4.771   4.694   4.613
  4.528   4.439   4.348   4.255   4.161   4.067   3.972   3.877   3.784   3.691
  3.599   3.509   3.420   3.332   3.247   3.163   3.080   3.000   2.921   2.843
  2.766   2.691   2.617   2.543   2.470   2.398   2.326   2.255   2.184   2.113
  2.043   1.973   1.903   1.833   1.764   1.694   1.625   1.556   1.487   1.418
  1.349   1.281   1.212   1.143   1.075   1.006   0.938   0.869   0.801   0.733
  0.665   0.596   0.528   0.460   0.392   0.324   0.255   0.187   0.119   0.051
  0.000
 15.293  15.231  15.150  15.071  14.995  14.921  14.850  14.782  14.716  14.653
 14.593  14.536  14.482  14.073  13.309  12.544  11.775  11.002  10.221   9.430
  8.630   7.818   6.996   6.164   5.323   4.870   4.807   4.738   4.665   4.586
  4.504   4.419   4.332   4.242   4.151   4.060   3.968   3.876   3.784   3.693
  3.603   3.514   3.426   3.340   3.255   3.171   3.089   3.008   2.929   2.851
  2.774   2.698   2.623   2.549   2.476   2.403   2.331   2.259   2.188   2.117
  2.046   1.975   1.905   1.835   1.766   1.696   1.627   1.557   1.488   1.419
  1.350   1.281   1.213   1.144   1.075   1.007   0.938   0.870   0.802   0.733
  0.665   0.597   0.528   0.460   0.392   0.324   0.256   0.187   0.119   0.051
  0.000
 15.312  15.249  15.168  15.090  15.014  14.940  14.869  14.801  14.735  14.672
 14.612  14.554  14.499  14.085  13.310  12.535  11.757  10.976  10.188   9.393
  8.589   7.777   6.956   6.127   5.290   4.840   4.778   4.711   4.639   4.563
  4.484   4.402   4.317   4.230   4.142   4.053   3.964   3.874   3.784   3.695
  3.606   3.518   3.431   3.346   3.261   3.178   3.096   3.015   2.936   2.858
  2.780   2.704   2.629   2.554   2.480   2.407   2.335   2.262   2.191   2.119
  2.048   1.978   1.907   1.837   1.767   1.698   1.628   1.559   1.489   1.420
```

```
  1.351   1.282   1.213   1.145   1.076   1.007   0.939   0.870   0.802   0.734
  0.665   0.597   0.529   0.460   0.392   0.324   0.256   0.188   0.119   0.051
  0.000
 15.328  15.265  15.184  15.106  15.030  14.956  14.885  14.817  14.751  14.688
 14.627  14.569  14.514  14.095  13.312  12.529  11.744  10.955  10.162   9.363
  8.557   7.744   6.924   6.097   5.263   4.815   4.754   4.688   4.618   4.544
  4.467   4.387   4.305   4.220   4.134   4.047   3.960   3.872   3.784   3.696
  3.608   3.522   3.436   3.351   3.267   3.184   3.102   3.021   2.942   2.863
  2.786   2.709   2.634   2.559   2.484   2.411   2.338   2.266   2.194   2.122
  2.051   1.980   1.909   1.839   1.769   1.699   1.629   1.560   1.490   1.421
  1.352   1.283   1.214   1.145   1.077   1.008   0.939   0.871   0.802   0.734
  0.666   0.597   0.529   0.461   0.392   0.324   0.256   0.188   0.119   0.051
  0.000
 15.342  15.279  15.198  15.120  15.044  14.970  14.899  14.831  14.765  14.701
 14.641  14.582  14.526  14.104  13.314  12.525  11.734  10.940  10.143   9.341
  8.533   7.719   6.899   6.073   5.242   4.795   4.734   4.669   4.600   4.528
  4.453   4.374   4.294   4.211   4.127   4.042   3.956   3.870   3.783   3.696
  3.610   3.524   3.439   3.354   3.271   3.188   3.107   3.026   2.946   2.868
  2.790   2.713   2.638   2.562   2.488   2.414   2.341   2.268   2.196   2.124
  2.053   1.982   1.911   1.840   1.770   1.700   1.630   1.561   1.491   1.422
  1.353   1.284   1.215   1.146   1.077   1.008   0.940   0.871   0.803   0.734
  0.666   0.597   0.529   0.461   0.392   0.324   0.256   0.188   0.119   0.051
  0.000
 15.353  15.290  15.209  15.131  15.055  14.981  14.910  14.842  14.776  14.712
 14.651  14.593  14.536  14.111  13.317  12.522  11.727  10.929  10.128   9.323
  8.514   7.699   6.879   6.054   5.224   4.779   4.718   4.654   4.586   4.515
  4.441   4.364   4.285   4.204   4.122   4.038   3.953   3.868   3.782   3.696
  3.611   3.526   3.441   3.357   3.274   3.192   3.110   3.030   2.950   2.872
  2.794   2.717   2.641   2.565   2.491   2.417   2.343   2.270   2.198   2.126
  2.054   1.983   1.912   1.842   1.771   1.701   1.631   1.561   1.492   1.423
  1.353   1.284   1.215   1.146   1.077   1.009   0.940   0.871   0.803   0.734
  0.666   0.598   0.529   0.461   0.393   0.324   0.256   0.188   0.119   0.051
  0.000
 15.362  15.299  15.218  15.139  15.063  14.990  14.919  14.850  14.784  14.721
 14.660  14.601  14.544  14.117  13.319  12.520  11.722  10.921  10.118   9.311
  8.500   7.685   6.864   6.040   5.211   4.767   4.706   4.643   4.576   4.505
  4.432   4.356   4.278   4.199   4.117   4.034   3.950   3.866   3.781   3.696
  3.612   3.527   3.443   3.359   3.277   3.194   3.113   3.033   2.953   2.874
  2.797   2.720   2.643   2.568   2.493   2.419   2.345   2.272   2.200   2.127
  2.056   1.984   1.913   1.843   1.772   1.702   1.632   1.562   1.493   1.423
  1.354   1.285   1.216   1.147   1.078   1.009   0.940   0.872   0.803   0.735
  0.666   0.598   0.529   0.461   0.393   0.324   0.256   0.188   0.119   0.051
  0.000
 15.368  15.305  15.224  15.146  15.070  14.996  14.925  14.857  14.790  14.727
 14.665  14.607  14.550  14.121  13.320  12.520  11.719  10.916  10.111   9.302
  8.490   7.674   6.854   6.030   5.202   4.758   4.698   4.635   4.568   4.498
  4.426   4.351   4.274   4.195   4.114   4.032   3.949   3.865   3.781   3.696
  3.612   3.528   3.444   3.361   3.278   3.196   3.115   3.035   2.955   2.876
  2.799   2.721   2.645   2.570   2.495   2.420   2.347   2.273   2.201   2.128
  2.057   1.985   1.914   1.843   1.773   1.702   1.632   1.563   1.493   1.423
  1.354   1.285   1.216   1.147   1.078   1.009   0.941   0.872   0.803   0.735
  0.666   0.598   0.529   0.461   0.393   0.324   0.256   0.188   0.120   0.051
  0.000
 15.372  15.309  15.228  15.149  15.073  15.000  14.929  14.860  14.794  14.730
 14.669  14.610  14.553  14.124  13.322  12.519  11.717  10.913  10.107   9.297
```

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   8.484   7.668   6.848   6.024   5.196   4.753   4.693   4.630   4.563   4.494
   4.422   4.347   4.271   4.192   4.112   4.030   3.948   3.864   3.780   3.696
   3.612   3.528   3.445   3.362   3.279   3.197   3.116   3.036   2.956   2.878
   2.800   2.723   2.646   2.571   2.496   2.421   2.347   2.274   2.201   2.129
   2.057   1.986   1.915   1.844   1.773   1.703   1.633   1.563   1.493   1.424
   1.354   1.285   1.216   1.147   1.078   1.009   0.941   0.872   0.803   0.735
   0.666   0.598   0.530   0.461   0.393   0.324   0.256   0.188   0.120   0.051
   0.000
  15.373  15.310  15.229  15.150  15.074  15.001  14.930  14.861  14.795  14.731
  14.670  14.611  14.554  14.125  13.322  12.519  11.716  10.911  10.105   9.295
   8.482   7.666   6.846   6.022   5.195   4.751   4.692   4.629   4.562   4.493
   4.421   4.347   4.270   4.191   4.111   4.030   3.947   3.864   3.780   3.696
   3.612   3.529   3.445   3.362   3.279   3.198   3.116   3.036   2.957   2.878
   2.800   2.723   2.646   2.571   2.496   2.421   2.348   2.274   2.201   2.129
   2.057   1.986   1.915   1.844   1.773   1.703   1.633   1.563   1.493   1.424
   1.354   1.285   1.216   1.147   1.078   1.009   0.941   0.872   0.803   0.735
   0.666   0.598   0.530   0.461   0.393   0.324   0.256   0.188   0.120   0.051
   0.000
```

OBS file (obs.dat):

```
# OBS file for MODFLOW-2000, UNC1NLI1 Report Example
Example         1
```

HOB file (hob.dat):

```
# HOBS file for MODFLOW-2000, UNC1NLI1 Report Example
 36  0  0
 1  1
F1   1  37  13  1  0  0  0  14.88  7.2928  0  1    1
F2   1  30  13  1  0  0  0  14.78  6.9068  0  1    1
F3   1  25  13  1  0  0  0  14.86  6.6802  0  1    1
F4   1  20  13  1  0  0  0  13.87  6.9935  0  1    1
F5   1  14  13  1  0  0  0  13.01  7.2859  0  1    1
F6   1   8  13  1  0  0  0  12.97  7.4680  0  1    1
F7   1  37  26  1  0  0  0   5.61  6.4327  0  1    1
F8   1  30  26  1  0  0  0   5.63  6.6651  0  1    1
F9   1  25  26  1  0  0  0   5.94  6.8781  0  1    1
F10  1  20  26  1  0  0  0   8.83  7.2128  0  1    1
F11  1  14  26  1  0  0  0  11.08  7.1766  0  1    1
F12  1   8  26  1  0  0  0  11.35  7.3150  0  1    1
F13  1  37  39  1  0  0  0    3.7  6.4067  0  1    1
F14  1  30  39  1  0  0  0   3.75  6.4828  0  1    1
F15  1  25  39  1  0  0  0   3.52  6.1912  0  1    1
F16  1  20  39  1  0  0  0   3.35  6.0780  0  1    1
F17  1  14  39  1  0  0  0   3.42  6.3866  0  1    1
F18  1   8  39  1  0  0  0   3.71  6.2947  0  1    1
F19  1  37  52  1  0  0  0   2.37  5.4804  0  1    1
F20  1  30  52  1  0  0  0   1.91  5.3105  0  1    1
F21  1  25  52  1  0  0  0   1.76  5.2649  0  1    1
F22  1  20  52  1  0  0  0   1.96  5.3133  0  1    1
F23  1  14  52  1  0  0  0   1.82  5.4639  0  1    1
F24  1   8  52  1  0  0  0   2.06  5.4263  0  1    1
```

```
F25  1  37  65  1  0  0  0   1.54  4.2383  0  1    1
F26  1  30  65  1  0  0  0   1.66  4.2794  0  1    1
F27  1  25  65  1  0  0  0   1.78  4.2922  0  1    1
F28  1  20  65  1  0  0  0   1.54  4.2612  0  1    1
F29  1  14  65  1  0  0  0    1.7  4.3214  0  1    1
F30  1   8  65  1  0  0  0   1.55  4.4493  0  1    1
F31  1  37  78  1  0  0  0    .94  1.5312  0  1    1
F32  1  30  78  1  0  0  0   1.41  1.9728  0  1    1
F33  1  25  78  1  0  0  0   1.22  1.9722  0  1    1
F34  1  20  78  1  0  0  0   1.47  2.0206  0  1    1
F35  1  14  78  1  0  0  0   1.08  2.1253  0  1    1
F36  1   8  78  1  0  0  0    .88  2.0226  0  1    1
```

PES file (pes.dat):

```
# PES file for MODFLOW-2000, UNC1NLI1 Report Example
#
 50  2  .01  0                 Item 1
 0  0  0  0  0  0  .001  1.5  0  Item 2
 1  0  0                       Item 3
  .08  0  1                    Item 4
 0  0  0                       Item 5
```

SEN file (sen.dat):

```
# SEN file for MODFLOW-2000, UNC1NLI1 Report Example
#
 2  0  0  2                           Item 1
 1  0   0  0                          Item 2
HK_1 1  1   1.00000  .01  100  1E-10  Item 3
HK_2 1  1   1.00000  .01  100  1E-10  Item 3
```

Parameter Estimation – GLOBAL Output File

GLOBAL Output File (mf2k.global_listing):

```
      U.S. GEOLOGICAL SURVEY MODULAR FINITE-DIFFERENCE GROUND-WATER FLOW MODEL
                           VERSION 1.6SC1 ¨25/02/2003


 This model run produced both GLOBAL and LIST files.  This is the GLOBAL file.

 GLOBAL LISTING FILE: mf2k.global_listing
                         UNIT   4

 OPENING output.dat
 FILE TYPE:LIST   UNIT   3   STATUS:REPLACE
 FORMAT:FORMATTED              ACCESS:SEQUENTIAL

 OPENING discret.dat
 FILE TYPE:DIS   UNIT  95   STATUS:OLD
 FORMAT:FORMATTED              ACCESS:SEQUENTIAL

 OPENING bas6.dat
 FILE TYPE:BAS6   UNIT   1   STATUS:OLD
 FORMAT:FORMATTED              ACCESS:SEQUENTIAL

 OPENING zone.dat
 FILE TYPE:ZONE   UNIT  93   STATUS:OLD
 FORMAT:FORMATTED              ACCESS:SEQUENTIAL

 OPENING multiple.dat
 FILE TYPE:MULT   UNIT  94   STATUS:OLD
 FORMAT:FORMATTED              ACCESS:SEQUENTIAL

 OPENING lpf6.dat
 FILE TYPE:LPF   UNIT  31   STATUS:OLD
 FORMAT:FORMATTED              ACCESS:SEQUENTIAL

 OPENING rech6.dat
 FILE TYPE:RCH   UNIT  11   STATUS:OLD
 FORMAT:FORMATTED              ACCESS:SEQUENTIAL

 OPENING wel6.dat
 FILE TYPE:WEL   UNIT  12   STATUS:OLD
 FORMAT:FORMATTED              ACCESS:SEQUENTIAL

 OPENING pcg2.dat
 FILE TYPE:PCG   UNIT  23   STATUS:OLD
 FORMAT:FORMATTED              ACCESS:SEQUENTIAL

 OPENING oc.dat
 FILE TYPE:OC   UNIT  22   STATUS:OLD
 FORMAT:FORMATTED              ACCESS:SEQUENTIAL
```

```
 OPENING inithead.dat
 FILE TYPE:DATA   UNIT  10   STATUS:UNKNOWN
 FORMAT:FORMATTED              ACCESS:SEQUENTIAL

 OPENING obs.dat
 FILE TYPE:OBS   UNIT  40   STATUS:OLD
 FORMAT:FORMATTED              ACCESS:SEQUENTIAL

 OPENING hob.dat
 FILE TYPE:HOB   UNIT  41   STATUS:OLD
 FORMAT:FORMATTED              ACCESS:SEQUENTIAL

 OPENING pes.dat
 FILE TYPE:PES   UNIT  47   STATUS:OLD
 FORMAT:FORMATTED              ACCESS:SEQUENTIAL

 OPENING sen.dat
 FILE TYPE:SEN   UNIT  46   STATUS:OLD
 FORMAT:FORMATTED              ACCESS:SEQUENTIAL
#UNC           60 unc.dat
#DATA            61 ci-res.dat
 THE FREE FORMAT OPTION HAS BEEN SELECTED

 DISCRETIZATION INPUT DATA READ FROM UNIT 95
 # Discretization file for MODFLOW-2000, UNC1NLI1 Report Example
    1 LAYERS        41 ROWS        91 COLUMNS
   1 STRESS PERIOD(S) IN SIMULATION
 MODEL TIME UNIT IS SECONDS
 MODEL LENGTH UNIT IS UNDEFINED
 THE GROUND-WATER TRANSPORT PROCESS IS INACTIVE

 THE OBSERVATION PROCESS IS ACTIVE
 THE SENSITIVITY PROCESS IS ACTIVE
 THE PARAMETER-ESTIMATION PROCESS IS ACTIVE

 MODE: PARAMETER ESTIMATION


 ZONE OPTION, INPUT READ FROM UNIT 93
 # Zone file for MODFLOW-2000, UNC1NLI1 Report Example
     2 ZONE ARRAYS

 MULTIPLIER OPTION, INPUT READ FROM UNIT 94
 # Multiplier file for MODFLOW-2000, UNC1NLI1 Report Example
   2 MULTIPLIER ARRAYS
  Confining bed flag for each layer:
   0

      41173  ELEMENTS OF GX ARRAY USED OUT OF      41173
       3731  ELEMENTS OF GZ ARRAY USED OUT OF       3731
      11193  ELEMENTS OF IG ARRAY USED OUT OF      11193


                              DELR
```

```
READING ON UNIT  95 WITH FORMAT: (16G5.0)



                              DELC
READING ON UNIT  95 WITH FORMAT: (16G5.0)

TOP ELEVATION OF LAYER 1 =   1.00000

  MODEL LAYER BOTTOM EL. =   0.00000     FOR LAYER   1

STRESS PERIOD     LENGTH       TIME STEPS     MULTIPLIER FOR DELT    SS FLAG
----------------------------------------------------------------------------
       1         1.000000          1                    1.000         SS

STEADY-STATE SIMULATION




 MULT. ARRAY: HK1        =   1.00000

 MULT. ARRAY: VK1        =   1.00000



            ZONE ARRAY: ZHK1
READING ON UNIT  93 WITH FORMAT: (91I1)

  ZONE ARRAY: ZVK1       =            999

LPF1 -- LAYER PROPERTY FLOW PACKAGE, VERSION 1, 1/11/2000
        INPUT READ FROM UNIT 31
# Layer-Property Flow file for MODFLOW-2000, UNC1NLI1 Report Example
HEAD AT CELLS THAT CONVERT TO DRY=   999.00
    3 Named Parameters

  LAYER FLAGS:
LAYER       LAYTYP        LAYAVG         CHANI        LAYVKA        LAYWET
---------------------------------------------------------------------------
   1             0             0     1.000E+00             0             0

  INTERPRETATION OF LAYER FLAGS:
                       INTERBLOCK     HORIZONTAL    DATA IN
        LAYER TYPE   TRANSMISSIVITY   ANISOTROPY   ARRAY VKA   WETTABILITY
LAYER      (LAYTYP)      (LAYAVG)       (CHANI)      (LAYVKA)      (LAYWET)
---------------------------------------------------------------------------
   1      CONFINED      HARMONIC     1.000E+00    VERTICAL K  NON-WETTABLE

      7462 ELEMENTS IN X ARRAY ARE USED BY LPF
         6 ELEMENTS IN IX ARRAY ARE USED BY LPF

PCG2 -- CONJUGATE GRADIENT SOLUTION PACKAGE, VERSION 2.4, 12/29/98
MAXIMUM OF     50 CALLS OF SOLUTION ROUTINE
```

```
MAXIMUM OF     30 INTERNAL ITERATIONS PER CALL TO SOLUTION ROUTINE
MATRIX PRECONDITIONING TYPE :    1
     14193 ELEMENTS IN X ARRAY ARE USED BY PCG
     10500 ELEMENTS IN IX ARRAY ARE USED BY PCG
      7462 ELEMENTS IN Z ARRAY ARE USED BY PCG

SEN1BAS6 -- SENSITIVITY PROCESS, VERSION 1.0, 10/15/98
INPUT READ FROM UNIT  46
# SEN file for MODFLOW-2000, UNC1NLI1 Report Example
#

NUMBER OF PARAMETER VALUES TO BE READ FROM SEN FILE:    2
ISENALL...........................................:    0
SENSITIVITIES WILL BE STORED IN MEMORY
FOR UP TO   2 PARAMETERS

      3745 ELEMENTS IN X ARRAY ARE USED FOR SENSITIVITIES
      3731 ELEMENTS IN Z ARRAY ARE USED FOR SENSITIVITIES
         4 ELEMENTS IN IX ARRAY ARE USED FOR SENSITIVITIES

PES1BAS6 -- PARAMETER-ESTIMATION PROCESS, VERSION 1.0, 07/22/99
INPUT READ FROM UNIT  47
# PES file for MODFLOW-2000, UNC1NLI1 Report Example
#

MAXIMUM NUMBER OF PARAMETER-ESTIMATION ITERATIONS (MAX-ITER)  =    50
MAXIMUM PARAMETER CORRECTION (MAX-CHANGE) ------------------- =  2.0000
CLOSURE CRITERION (TOL) ------------------------------------- = 0.10000E-01
SUM OF SQUARES CLOSURE CRITERION (SOSC) --------------------- =  0.0000

FLAG TO GENERATE INPUT NEEDED BY BEALE-2000 (IBEFLG) -------- =     0
FLAG TO GENERATE INPUT NEEDED BY YCINT-2000 (IYCFLG) -------- =     0
OMIT PRINTING TO SCREEN (IF = 1) (IOSTAR) ------------------- =     0
ADJUST GAUSS-NEWTON MATRIX WITH NEWTON UPDATES (IF = 1)(NOPT) =     0
NUMBER OF FLETCHER-REEVES ITERATIONS (NFIT) ----------------- =     0
CRITERION FOR ADDING MATRIX R (SOSR) ------------------------ =  0.0000
VALUE USED TO INCREMENT MARQUARDT PARAMETER (RMAR) ---------- = 0.10000E-02
MARQUARDT PARAMETER MULTIPLIER (RMARM) ---------------------- =  1.5000
APPLY MAX-CHANGE IN REGRESSION SPACE (IF = 1) (IAP) --------- =     0

FORMAT CODE FOR COVARIANCE AND CORRELATION MATRICES (IPRCOV)  =     1
PRINT PARAMETER-ESTIMATION STATISTICS
    EACH ITERATION (IF > 0)  (IPRINT) ----------------------- =     0
PRINT EIGENVALUES AND EIGENVECTORS OF
    COVARIANCE MATRIX (IF > 0)  (LPRINT) -------------------- =     0

SEARCH DIRECTION ADJUSTMENT PARAMETER (CSA) ----------------- = 0.80000E-01
MODIFY CONVERGENCE CRITERIA (IF > 0) (FCONV) ---------------- =  0.0000
CALCULATE SENSITIVITIES USING FINAL
    PARAMETER ESTIMATES (IF > 0) (LASTX) -------------------- =     1

NUMBER OF USUALLY POS. PARAMETERS THAT MAY BE NEGATIVE (NPNG) =     0
NUMBER OF PARAMETERS WITH CORRELATED PRIOR INFORMATION (IPR)  =     0
NUMBER OF PRIOR-INFORMATION EQUATIONS (MPR) ----------------- =     0
```

```
   479 ELEMENTS IN X ARRAY ARE USED FOR PARAMETER ESTIMATION
    81 ELEMENTS IN Z ARRAY ARE USED FOR PARAMETER ESTIMATION
    52 ELEMENTS IN IX ARRAY ARE USED FOR PARAMETER ESTIMATION

OBS1BAS6 -- OBSERVATION PROCESS, VERSION 1.0, 4/27/99
INPUT READ FROM UNIT  40
# OBS file for MODFLOW-2000, UNC1NLI1 Report Example
OBSERVATION GRAPH-DATA OUTPUT FILES
WILL BE PRINTED AND NAMED USING THE BASE: Example
DIMENSIONLESS SCALED OBSERVATION SENSITIVITIES WILL BE PRINTED

HEAD OBSERVATIONS -- INPUT READ FROM UNIT  41
# HOBS file for MODFLOW-2000, UNC1NLI1 Report Example

NUMBER OF HEADS....................................:   36
  NUMBER OF MULTILAYER HEADS.......................:    0
  MAXIMUM NUMBER OF LAYERS FOR MULTILAYER HEADS....:    0

    718 ELEMENTS IN X ARRAY ARE USED FOR OBSERVATIONS
      2 ELEMENTS IN Z ARRAY ARE USED FOR OBSERVATIONS
    363 ELEMENTS IN IX ARRAY ARE USED FOR OBSERVATIONS

COMMON ERROR VARIANCE FOR ALL OBSERVATIONS SET TO:       1.000

     26597  ELEMENTS OF X ARRAY USED OUT OF      26597
     11276  ELEMENTS OF Z ARRAY USED OUT OF      11276
     10925  ELEMENTS OF IX ARRAY USED OUT OF      10925
      7462  ELEMENTS OF XHS ARRAY USED OUT OF       7462

INFORMATION ON PARAMETERS LISTED IN SEN FILE
                                             LOWER         UPPER       ALTERNATE
                         VALUE IN SEN     REASONABLE    REASONABLE     SCALING
   NAME     ISENS  LN    INPUT FILE         LIMIT         LIMIT         FACTOR
----------  -----  --  ------------  ------------  ------------  ------------
HK_1          1     1    1.0000       0.10000E-01    100.00       0.10000E-09
HK_2          1     1    1.0000       0.10000E-01    100.00       0.10000E-09
----------------------------------------------------------------------------
FOR THE PARAMETERS LISTED IN THE TABLE ABOVE, PARAMETER VALUES IN INDIVIDUAL
PACKAGE INPUT FILES ARE REPLACED BY THE VALUES FROM THE SEN INPUT FILE.  THE
ALTERNATE SCALING FACTOR IS USED TO SCALE SENSITIVITIES IF IT IS LARGER THAN
THE PARAMETER VALUE IN ABSOLUTE VALUE AND THE PARAMETER IS NOT LOG-TRANSFORMED.

ISENS IS GREATER THAN ZERO FOR    2 PARAMETERS

HEAD OBSERVATION VARIANCES ARE MULTIPLIED BY:       1.000

OBSERVED HEAD DATA -- TIME OFFSETS ARE MULTIPLIED BY:   1.0000

                   REFER.
      OBSERVATION  STRESS    TIME                                 STATISTIC   PLOT
 OBS#     NAME     PERIOD   OFFSET    OBSERVATION  STATISTIC        TYPE      SYM.
    1 F1               1    0.000       14.88       729.3       VARIANCE       1
    2 F2               1    0.000       14.78       690.7       VARIANCE       1
    3 F3               1    0.000       14.86       668.0       VARIANCE       1
    4 F4               1    0.000       13.87       699.3       VARIANCE       1
```

5	F5	1	0.000	13.01	728.6	VARIANCE	1
6	F6	1	0.000	12.97	746.8	VARIANCE	1
7	F7	1	0.000	5.610	643.3	VARIANCE	1
8	F8	1	0.000	5.630	666.5	VARIANCE	1
9	F9	1	0.000	5.940	687.8	VARIANCE	1
10	F10	1	0.000	8.830	721.3	VARIANCE	1
11	F11	1	0.000	11.08	717.7	VARIANCE	1
12	F12	1	0.000	11.35	731.5	VARIANCE	1
13	F13	1	0.000	3.700	640.7	VARIANCE	1
14	F14	1	0.000	3.750	648.3	VARIANCE	1
15	F15	1	0.000	3.520	619.1	VARIANCE	1
16	F16	1	0.000	3.350	607.8	VARIANCE	1
17	F17	1	0.000	3.420	638.7	VARIANCE	1
18	F18	1	0.000	3.710	629.5	VARIANCE	1
19	F19	1	0.000	2.370	548.0	VARIANCE	1
20	F20	1	0.000	1.910	531.0	VARIANCE	1
21	F21	1	0.000	1.760	526.5	VARIANCE	1
22	F22	1	0.000	1.960	531.3	VARIANCE	1
23	F23	1	0.000	1.820	546.4	VARIANCE	1
24	F24	1	0.000	2.060	542.6	VARIANCE	1
25	F25	1	0.000	1.540	423.8	VARIANCE	1
26	F26	1	0.000	1.660	427.9	VARIANCE	1
27	F27	1	0.000	1.780	429.2	VARIANCE	1
28	F28	1	0.000	1.540	426.1	VARIANCE	1
29	F29	1	0.000	1.700	432.1	VARIANCE	1
30	F30	1	0.000	1.550	444.9	VARIANCE	1
31	F31	1	0.000	0.9400	153.1	VARIANCE	1
32	F32	1	0.000	1.410	197.3	VARIANCE	1
33	F33	1	0.000	1.220	197.2	VARIANCE	1
34	F34	1	0.000	1.470	202.1	VARIANCE	1
35	F35	1	0.000	1.080	212.5	VARIANCE	1
36	F36	1	0.000	0.8800	202.3	VARIANCE	1

OBS#	OBSERVATION NAME	LAY	ROW	COL	ROW OFFSET	COL OFFSET	HEAD CHANGE REFERENCE OBSERVATION (IF > 0)
1	F1	1	37	13	0.000	0.000	0
2	F2	1	30	13	0.000	0.000	0
3	F3	1	25	13	0.000	0.000	0
4	F4	1	20	13	0.000	0.000	0
5	F5	1	14	13	0.000	0.000	0
6	F6	1	8	13	0.000	0.000	0
7	F7	1	37	26	0.000	0.000	0
8	F8	1	30	26	0.000	0.000	0
9	F9	1	25	26	0.000	0.000	0
10	F10	1	20	26	0.000	0.000	0
11	F11	1	14	26	0.000	0.000	0
12	F12	1	8	26	0.000	0.000	0
13	F13	1	37	39	0.000	0.000	0
14	F14	1	30	39	0.000	0.000	0
15	F15	1	25	39	0.000	0.000	0
16	F16	1	20	39	0.000	0.000	0
17	F17	1	14	39	0.000	0.000	0
18	F18	1	8	39	0.000	0.000	0

```
   19  F19             1   37   52   0.000   0.000        0
   20  F20             1   30   52   0.000   0.000        0
   21  F21             1   25   52   0.000   0.000        0
   22  F22             1   20   52   0.000   0.000        0
   23  F23             1   14   52   0.000   0.000        0
   24  F24             1    8   52   0.000   0.000        0
   25  F25             1   37   65   0.000   0.000        0
   26  F26             1   30   65   0.000   0.000        0
   27  F27             1   25   65   0.000   0.000        0
   28  F28             1   20   65   0.000   0.000        0
   29  F29             1   14   65   0.000   0.000        0
   30  F30             1    8   65   0.000   0.000        0
   31  F31             1   37   78   0.000   0.000        0
   32  F32             1   30   78   0.000   0.000        0
   33  F33             1   25   78   0.000   0.000        0
   34  F34             1   20   78   0.000   0.000        0
   35  F35             1   14   78   0.000   0.000        0
   36  F36             1    8   78   0.000   0.000        0


                                        SOLUTION BY THE CONJUGATE-GRADIENT METHOD
                                       ------------------------------------------
                    MAXIMUM NUMBER OF CALLS TO PCG ROUTINE =       50
                        MAXIMUM ITERATIONS PER CALL TO PCG =       30
                               MATRIX PRECONDITIONING TYPE =        1
       RELAXATION FACTOR (ONLY USED WITH PRECOND. TYPE 1) =    0.10000E+01
PARAMETER OF POLYNOMIAL PRECOND. = 2 (2) OR IS CALCULATED :        1
                         HEAD CHANGE CRITERION FOR CLOSURE =    0.10000E-02
                     RESIDUAL CHANGE CRITERION FOR CLOSURE =    0.10000E-02
            PCG HEAD AND RESIDUAL CHANGE PRINTOUT INTERVAL =        1
    PRINTING FROM SOLVER IS LIMITED(1) OR SUPPRESSED (>1) =        0
                                         DAMPING PARAMETER =    0.10000E+01

CONVERGENCE CRITERIA FOR SENSITIVITIES
PARAMETER      HCLOSE        RCLOSE
----------  ------------  ------------
HK_1         0.10000E-04   0.10000E-04
HK_2         0.10000E-04   0.10000E-04
--------------------------------------

WETTING CAPABILITY IS NOT ACTIVE IN ANY LAYER

PARAMETERS DEFINED IN THE LPF PACKAGE

PARAMETER NAME:HK_1         TYPE:HK     CLUSTERS:   1
Parameter value from package file is:    1.0000
               LAYER:  1    MULTIPLIER ARRAY: HK1    ZONE ARRAY: ZHK1
               ZONE VALUES:    1

PARAMETER NAME:HK_2         TYPE:HK     CLUSTERS:   1
Parameter value from package file is:    1.0000
               LAYER:  1    MULTIPLIER ARRAY: HK1    ZONE ARRAY: ZHK1
               ZONE VALUES:    2
```

```
PARAMETER NAME:VK_0         TYPE:VK     CLUSTERS:   1
Parameter value from package file is:    1.0000
               LAYER:  1    MULTIPLIER ARRAY: VK1    ZONE ARRAY: ZVK1
               ZONE VALUES:  999

   HYD. COND. ALONG ROWS FOR LAYER   1 WILL BE DEFINED BY PARAMETERS
(PRINT FLAG=  31)

     VERTICAL HYD. COND. FOR LAYER   1 WILL BE DEFINED BY PARAMETERS
(PRINT FLAG=  31)


    1 Well parameters

PARAMETER NAME:WEL_0_1      TYPE:Q
Parameter value from package file is:    1.0000
  NUMBER OF ENTRIES:      1

WELL NO.  LAYER   ROW   COL   STRESS FACTOR
----------------------------------------------
     1      1     21     46      -1.000


    0 Recharge parameters

  4 PARAMETERS HAVE BEEN DEFINED IN ALL PACKAGES.
(SPACE IS ALLOCATED FOR  500 PARAMETERS.)

OBSERVATION SENSITIVITY TABLE(S) FOR PARAMETER-ESTIMATION ITERATION     1

DIMENSIONLESS SCALED SENSITIVITIES (SCALED BY B*(WT**.5))

        PARAMETER:   HK_1        HK_2
OBS #  OBSERVATION
    1  F1            -0.261      -0.556E-01
    2  F2            -0.269      -0.564E-01
    3  F3            -0.275      -0.557E-01
    4  F4            -0.275      -0.482E-01
    5  F5            -0.274      -0.425E-01
    6  F6            -0.272      -0.408E-01
    7  F7            -0.270      -0.346E-02
    8  F8            -0.263      -0.518E-02
    9  F9            -0.255      -0.899E-02
   10  F10           -0.236      -0.218E-01
   11  F11           -0.226      -0.324E-01
   12  F12           -0.221      -0.350E-01
   13  F13           -0.209      -0.244E-02
   14  F14           -0.206      -0.228E-02
   15  F15           -0.210      -0.158E-02
   16  F16           -0.213       0.431E-03
   17  F17           -0.212       0.221E-02
   18  F18           -0.215       0.245E-02
   19  F19           -0.165      -0.106E-02
   20  F20           -0.166      -0.771E-03
   21  F21           -0.165      -0.381E-03
```

```
  22  F22           -0.164       0.100E-03
  23  F23           -0.164       0.625E-03
  24  F24           -0.168       0.968E-03
  25  F25           -0.124      -0.433E-03
  26  F26           -0.123      -0.296E-03
  27  F27           -0.123      -0.141E-03
  28  F28           -0.124       0.364E-04
  29  F29           -0.123       0.238E-03
  30  F30           -0.122       0.379E-03
  31  F31           -0.102      -0.229E-03
  32  F32           -0.900E-01  -0.138E-03
  33  F33           -0.900E-01  -0.656E-04
  34  F34           -0.890E-01   0.165E-04
  35  F35           -0.869E-01   0.107E-03
  36  F36           -0.892E-01   0.178E-03

      COMPOSITE SCALED SENSITIVITIES ((SUM OF THE SQUARED VALUES)/ND)**.5
                     0.196       0.224E-01

 PARAMETER    COMPOSITE SCALED SENSITIVITY
 ----------   ----------------------------
 HK_1           1.95517E-01
 HK_2           2.24057E-02

STARTING VALUES OF REGRESSION PARAMETERS :

  HK_1         HK_2

   1.000        1.000

SUMS OF SQUARED, WEIGHTED RESIDUALS:
  ALL DEPENDENT VARIABLES:  0.40901
  DEP. VARIABLES PLUS PARAMETERS:  0.40901

-----------------------------------------------------------------------
PARAMETER VALUES AND STATISTICS FOR ALL PARAMETER-ESTIMATION ITERATIONS
-----------------------------------------------------------------------

    MODIFIED GAUSS-NEWTON CONVERGES IF THE ABSOLUTE VALUE OF THE MAXIMUM
FRACTIONAL PARAMETER CHANGE (MAX CALC. CHANGE) IS LESS THAN TOL OR IF THE
SUM OF SQUARED, WEIGHTED RESIDUALS CHANGES LESS THAN SOSC OVER TWO
PARAMETER-ESTIMATION ITERATIONS.

MODIFIED GAUSS-NEWTON PROCEDURE FOR PARAMETER-ESTIMATION ITERATION NO. =     1

VALUES FROM SOLVING THE NORMAL EQUATION :
  MARQUARDT PARAMETER ------------------- =  0.0000
  MAX. FRAC. PAR. CHANGE (TOL= 0.100E-01) = -.99783
       OCCURRED FOR PARAMETER  "HK_2      " TYPE N

CALCULATION OF DAMPING PARAMETER
  MAX-CHANGE SPECIFIED:   2.0       USED:   2.0
  OSCILL. CONTROL FACTOR (1, NO EFFECT)-- =  1.0000
  DAMPING PARAMETER (RANGE 0 TO 1) ------ =  1.0000
       CONTROLLED BY PARAMETER "HK_2      " TYPE N
```

```
UPDATED ESTIMATES OF REGRESSION PARAMETERS :

  HK_1         HK_2

   1.404       2.1694E-03

SUMS OF SQUARED, WEIGHTED RESIDUALS:
  ALL DEPENDENT VARIABLES:   1022.7
  DEP. VARIABLES PLUS PARAMETERS:   1022.7

MODIFIED GAUSS-NEWTON PROCEDURE FOR PARAMETER-ESTIMATION ITERATION NO. =     2

VALUES FROM SOLVING THE NORMAL EQUATION :
  MARQUARDT PARAMETER ------------------- =  0.0000
  MAX. FRAC. PAR. CHANGE (TOL= 0.100E-01) =  1.6663
       OCCURRED FOR PARAMETER  "HK_2      " TYPE P

CALCULATION OF DAMPING PARAMETER
  MAX-CHANGE SPECIFIED:   2.0       USED:   2.0
  OSCILL. CONTROL FACTOR (1, NO EFFECT)-- = 0.98277
  DAMPING PARAMETER (RANGE 0 TO 1) ------ = 0.98277
       CONTROLLED BY PARAMETER "HK_2      " TYPE P

UPDATED ESTIMATES OF REGRESSION PARAMETERS :

  HK_1         HK_2

   1.476       5.6874E-03

SUMS OF SQUARED, WEIGHTED RESIDUALS:
  ALL DEPENDENT VARIABLES:   139.07
  DEP. VARIABLES PLUS PARAMETERS:   139.07

MODIFIED GAUSS-NEWTON PROCEDURE FOR PARAMETER-ESTIMATION ITERATION NO. =     3

VALUES FROM SOLVING THE NORMAL EQUATION :
  MARQUARDT PARAMETER ------------------- =  0.0000
  MAX. FRAC. PAR. CHANGE (TOL= 0.100E-01) =  1.5827
       OCCURRED FOR PARAMETER  "HK_2      " TYPE P

CALCULATION OF DAMPING PARAMETER
  MAX-CHANGE SPECIFIED:   2.0       USED:   2.0
  OSCILL. CONTROL FACTOR (1, NO EFFECT)-- =  1.0000
  DAMPING PARAMETER (RANGE 0 TO 1) ------ =  1.0000
       CONTROLLED BY PARAMETER "HK_2      " TYPE P

UPDATED ESTIMATES OF REGRESSION PARAMETERS :

  HK_1         HK_2

   1.477       1.4689E-02

SUMS OF SQUARED, WEIGHTED RESIDUALS:
  ALL DEPENDENT VARIABLES:   17.395
```

```
  DEP. VARIABLES PLUS PARAMETERS:   17.395

MODIFIED GAUSS-NEWTON PROCEDURE FOR PARAMETER-ESTIMATION ITERATION NO. =     4

VALUES FROM SOLVING THE NORMAL EQUATION :
  MARQUARDT PARAMETER ------------------- =  0.0000
  MAX. FRAC. PAR. CHANGE (TOL= 0.100E-01) =  1.3735
       OCCURRED FOR PARAMETER  "HK_2      " TYPE P

CALCULATION OF DAMPING PARAMETER
  MAX-CHANGE SPECIFIED:   2.0       USED:   2.0
  OSCILL. CONTROL FACTOR (1, NO EFFECT)-- =  1.0000
  DAMPING PARAMETER (RANGE 0 TO 1) ------ =  1.0000
       CONTROLLED BY PARAMETER "HK_2      " TYPE P

UPDATED ESTIMATES OF REGRESSION PARAMETERS :

  HK_1         HK_2

   1.472       3.4864E-02

SUMS OF SQUARED, WEIGHTED RESIDUALS:
  ALL DEPENDENT VARIABLES:   1.8804
  DEP. VARIABLES PLUS PARAMETERS:   1.8804

MODIFIED GAUSS-NEWTON PROCEDURE FOR PARAMETER-ESTIMATION ITERATION NO. =     5

VALUES FROM SOLVING THE NORMAL EQUATION :
  MARQUARDT PARAMETER ------------------- =  0.0000
  MAX. FRAC. PAR. CHANGE (TOL= 0.100E-01) = 0.94318
       OCCURRED FOR PARAMETER  "HK_2      " TYPE P

CALCULATION OF DAMPING PARAMETER
  MAX-CHANGE SPECIFIED:   2.0       USED:   2.0
  OSCILL. CONTROL FACTOR (1, NO EFFECT)-- =  1.0000
  DAMPING PARAMETER (RANGE 0 TO 1) ------ =  1.0000
       CONTROLLED BY PARAMETER "HK_2      " TYPE P

UPDATED ESTIMATES OF REGRESSION PARAMETERS :

  HK_1         HK_2

   1.465       6.7748E-02

SUMS OF SQUARED, WEIGHTED RESIDUALS:
  ALL DEPENDENT VARIABLES:  0.14038
  DEP. VARIABLES PLUS PARAMETERS:  0.14038

MODIFIED GAUSS-NEWTON PROCEDURE FOR PARAMETER-ESTIMATION ITERATION NO. =     6

VALUES FROM SOLVING THE NORMAL EQUATION :
  MARQUARDT PARAMETER ------------------- =  0.0000
  MAX. FRAC. PAR. CHANGE (TOL= 0.100E-01) = 0.38419
       OCCURRED FOR PARAMETER  "HK_2      " TYPE P
```

```
CALCULATION OF DAMPING PARAMETER
  MAX-CHANGE SPECIFIED:   2.0       USED:   2.0
  OSCILL. CONTROL FACTOR (1, NO EFFECT)-- =  1.0000
  DAMPING PARAMETER (RANGE 0 TO 1) ------ =  1.0000
       CONTROLLED BY PARAMETER "HK_2      " TYPE P

UPDATED ESTIMATES OF REGRESSION PARAMETERS :

  HK_1         HK_2

   1.462       9.3776E-02

SUMS OF SQUARED, WEIGHTED RESIDUALS:
  ALL DEPENDENT VARIABLES:  0.16299E-01
  DEP. VARIABLES PLUS PARAMETERS:  0.16299E-01

MODIFIED GAUSS-NEWTON PROCEDURE FOR PARAMETER-ESTIMATION ITERATION NO. =     7

VALUES FROM SOLVING THE NORMAL EQUATION :
  MARQUARDT PARAMETER ------------------- =  0.0000
  MAX. FRAC. PAR. CHANGE (TOL= 0.100E-01) = 0.59154E-01
       OCCURRED FOR PARAMETER  "HK_2      " TYPE P

CALCULATION OF DAMPING PARAMETER
  MAX-CHANGE SPECIFIED:   2.0       USED:   2.0
  OSCILL. CONTROL FACTOR (1, NO EFFECT)-- =  1.0000
  DAMPING PARAMETER (RANGE 0 TO 1) ------ =  1.0000
       CONTROLLED BY PARAMETER "HK_2      " TYPE P

UPDATED ESTIMATES OF REGRESSION PARAMETERS :

  HK_1         HK_2

   1.463       9.9323E-02

SUMS OF SQUARED, WEIGHTED RESIDUALS:
  ALL DEPENDENT VARIABLES:  0.14039E-01
  DEP. VARIABLES PLUS PARAMETERS:  0.14039E-01

MODIFIED GAUSS-NEWTON PROCEDURE FOR PARAMETER-ESTIMATION ITERATION NO. =     8

VALUES FROM SOLVING THE NORMAL EQUATION :
  MARQUARDT PARAMETER ------------------- =  0.0000
  MAX. FRAC. PAR. CHANGE (TOL= 0.100E-01) = 0.11102E-02
       OCCURRED FOR PARAMETER  "HK_2      " TYPE P

CALCULATION OF DAMPING PARAMETER
  MAX-CHANGE SPECIFIED:   2.0       USED:   2.0
  OSCILL. CONTROL FACTOR (1, NO EFFECT)-- =  1.0000
  DAMPING PARAMETER (RANGE 0 TO 1) ------ =  1.0000
       CONTROLLED BY PARAMETER "HK_2      " TYPE P

UPDATED ESTIMATES OF REGRESSION PARAMETERS :

  HK_1         HK_2
```

```
   1.464       9.9433E-02

 *** PARAMETER ESTIMATION CONVERGED BY SATISFYING THE TOL CRITERION ***


OBSERVATION SENSITIVITY TABLE(S) FOR PARAMETER-ESTIMATION ITERATION     8

 DIMENSIONLESS SCALED SENSITIVITIES (SCALED BY B*(WT**.5))

        PARAMETER:   HK_1        HK_2
 OBS #  OBSERVATION
     1  F1           -0.258      -0.281
     2  F2           -0.262      -0.287
     3  F3           -0.262      -0.289
     4  F4           -0.243      -0.276
     5  F5           -0.232      -0.268
     6  F6           -0.229      -0.264
     7  F7           -0.189      -0.950E-04
     8  F8           -0.190      -0.366E-02
     9  F9           -0.197      -0.101E-01
    10  F10          -0.185      -0.135
    11  F11          -0.181      -0.246
    12  F12          -0.186      -0.251
    13  F13          -0.148      -0.182E-02
    14  F14          -0.146      -0.228E-02
    15  F15          -0.148      -0.225E-02
    16  F16          -0.146      -0.706E-03
    17  F17          -0.140       0.169E-02
    18  F18          -0.141       0.299E-02
    19  F19          -0.115      -0.974E-03
    20  F20          -0.115      -0.800E-03
    21  F21          -0.114      -0.496E-03
    22  F22          -0.112      -0.399E-04
    23  F23          -0.111       0.567E-03
    24  F24          -0.112       0.105E-02
    25  F25          -0.858E-01  -0.425E-03
    26  F26          -0.849E-01  -0.305E-03
    27  F27          -0.843E-01  -0.160E-03
    28  F28          -0.843E-01   0.170E-04
    29  F29          -0.835E-01   0.233E-03
    30  F30          -0.823E-01   0.396E-03
    31  F31          -0.703E-01  -0.230E-03
    32  F32          -0.618E-01  -0.141E-03
    33  F33          -0.617E-01  -0.700E-04
    34  F34          -0.608E-01   0.131E-04
    35  F35          -0.591E-01   0.107E-03
    36  F36          -0.605E-01   0.184E-03

        COMPOSITE SCALED SENSITIVITIES ((SUM OF THE SQUARED VALUES)/ND)**.5
                      0.154       0.130

  PARAMETER    COMPOSITE SCALED SENSITIVITY
  ----------   ----------------------------
  HK_1           1.53635E-01
```

```
 HK_2           1.29572E-01

FINAL PARAMETER VALUES AND STATISTICS:

PARAMETER NAME(S) AND VALUE(S):

  HK_1         HK_2

   1.464       9.9433E-02

SUMS OF SQUARED WEIGHTED RESIDUALS:
  OBSERVATIONS   PRIOR INFO.    TOTAL
   0.140E-01      0.00         0.140E-01

----------------------------------------------------------------------

SELECTED STATISTICS FROM MODIFIED GAUSS-NEWTON ITERATIONS

       MAX. PARAMETER CALC. CHANGE   MAX. CHANGE     DAMPING
ITER.     PARNAM     MAX. CHANGE       ALLOWED      PARAMETER
-----   ----------  -------------   -------------  ------------
   1    HK_2        -0.997831         2.00000        1.0000
   2    HK_2          1.66634         2.00000       0.98277
   3    HK_2          1.58271         2.00000        1.0000
   4    HK_2          1.37349         2.00000        1.0000
   5    HK_2         0.943184         2.00000        1.0000
   6    HK_2         0.384188         2.00000        1.0000
   7    HK_2         0.591537E-01     2.00000        1.0000
   8    HK_2         0.111021E-02     2.00000        1.0000

SUMS OF SQUARED WEIGHTED RESIDUALS FOR EACH ITERATION

        SUMS OF SQUARED WEIGHTED RESIDUALS
ITER.  OBSERVATIONS  PRIOR INFO.      TOTAL
    1   0.40901        0.0000       0.40901
    2    1022.7        0.0000        1022.7
    3    139.07        0.0000        139.07
    4    17.395        0.0000        17.395
    5    1.8804        0.0000        1.8804
    6   0.14038        0.0000       0.14038
    7   0.16299E-01    0.0000       0.16299E-01
    8   0.14039E-01    0.0000       0.14039E-01
FINAL   0.14039E-01    0.0000       0.14039E-01

*** PARAMETER ESTIMATION CONVERGED BY SATISFYING THE TOL CRITERION ***

----------------------------------------------------------------------

         VARIANCE-COVARIANCE MATRIX FOR THE PARAMETERS
         ---------------------------------------------

           HK_1       HK_2
................................
HK_1        1.083E-03 -9.540E-04
HK_2       -9.540E-04  1.523E-03
```

```
_________________

PARAMETER SUMMARY
_________________

________________________________________________________________________

PARAMETER VALUES IN "REGRESSION" SPACE --- LOG TRANSFORMED AS APPLICABLE
________________________________________________________________________

PARAMETER:         HK_1       HK_2
* = LOG TRNS:         *          *


UPPER 95% C.I.     1.95E-01  -9.68E-01
FINAL VALUES       1.65E-01  -1.00E+00
LOWER 95% C.I.     1.36E-01  -1.04E+00

STD. DEV.          1.43E-02   1.69E-02

COEF. OF VAR. (STD. DEV. / FINAL VALUE); "--" IF FINAL VALUE = 0.0
                   8.64E-02   1.69E-02

------------------------------------------------------------------------
------------------------------------------------------------------------

________________________________________________________________________

PHYSICAL PARAMETER VALUES --- EXP10 OF LOG TRANSFORMED PARAMETERS
________________________________________________________________________

PARAMETER:         HK_1       HK_2
* = LOG TRNS:         *          *

UPPER 95% C.I.     1.57E+00   1.08E-01
FINAL VALUES       1.46E+00   9.94E-02
LOWER 95% C.I.     1.37E+00   9.18E-02

    REASONABLE
   UPPER LIMIT     1.00E+02   1.00E+02
    REASONABLE
   LOWER LIMIT     1.00E-02   1.00E-02

ESTIMATE ABOVE (1)
BELOW(-1)LIMITS        0          0
ENTIRE CONF. INT.
ABOVE(1)BELOW(-1)      0          0


         -------------------------------------
         CORRELATION MATRIX FOR THE PARAMETERS
         -------------------------------------
```

```
           HK_1       HK_2
................................
HK_1         1.00     -0.743
HK_2       -0.743       1.00

THE CORRELATION OF THE FOLLOWING PARAMETER PAIRS >= .95
    PARAMETER   PARAMETER   CORRELATION

THE CORRELATION OF THE FOLLOWING PARAMETER PAIRS IS BETWEEN .90 AND .95
    PARAMETER   PARAMETER   CORRELATION

THE CORRELATION OF THE FOLLOWING PARAMETER PAIRS IS BETWEEN .85 AND .90
    PARAMETER   PARAMETER   CORRELATION


 LEAST-SQUARES OBJ FUNC (DEP.VAR. ONLY)- = 0.14039E-01
 LEAST-SQUARES OBJ FUNC (W/PARAMETERS)-- = 0.14039E-01
 CALCULATED ERROR VARIANCE-------------- = 0.41292E-03
 STANDARD ERROR OF THE REGRESSION------- = 0.20320E-01
 CORRELATION COEFFICIENT---------------- = 0.99322
      W/PARAMETERS---------------------- = 0.99322
 ITERATIONS----------------------------- =       8

 MAX LIKE OBJ FUNC =  289.19
 AIC STATISTIC---- =  293.19
 BIC STATISTIC---- =  296.36

SMALLEST AND LARGEST WEIGHTED RESIDUALS

     SMALLEST WEIGHTED RESIDUALS      |       LARGEST WEIGHTED RESIDUALS
               WEIGHTED   PERCENT OF  |                 WEIGHTED   PERCENT OF
NAME           RESIDUAL    OBJ FUNC   |  NAME           RESIDUAL    OBJ FUNC
F21           -0.376E-01    10.05     |  F34            0.427E-01    12.96
F20           -0.334E-01     7.93     |  F32            0.384E-01    10.52
F23           -0.325E-01     7.54     |  F7             0.325E-01     7.51
F22           -0.267E-01     5.09     |  F33            0.251E-01     4.50
F24           -0.226E-01     3.65     |  F3             0.242E-01     4.19

STATISTICS FOR ALL RESIDUALS :
AVERAGE WEIGHTED RESIDUAL  :-0.500E-03
# RESIDUALS >= 0. :     16
# RESIDUALS < 0.  :     20
NUMBER OF RUNS  :    9  IN   36 OBSERVATIONS

INTERPRETING THE CALCULATED RUNS STATISTIC VALUE OF     -3.18
NOTE: THE FOLLOWING APPLIES ONLY IF
       # RESIDUALS >= 0 . IS GREATER THAN 10 AND
       # RESIDUALS < 0.   IS GREATER THAN 10
THE NEGATIVE VALUE MAY INDICATE TOO FEW RUNS:
   IF THE VALUE IS LESS THAN -1.28, THERE IS LESS THAN A 10 PERCENT
      CHANCE THE VALUES ARE RANDOM,
   IF THE VALUE IS LESS THAN -1.645, THERE IS LESS THAN A 5 PERCENT
      CHANCE THE VALUES ARE RANDOM,
   IF THE VALUE IS LESS THAN -1.96, THERE IS LESS THAN A 2.5 PERCENT
      CHANCE THE VALUES ARE RANDOM.
```

```
CORRELATION BETWEEN ORDERED WEIGHTED RESIDUALS AND NORMAL ORDER STATISTICS
FOR OBSERVATIONS =    0.988

-------------------------------------------------------------------------
COMMENTS ON THE INTERPRETATION OF THE CORRELATION BETWEEN
WEIGHTED RESIDUALS AND NORMAL ORDER STATISTICS:

The critical value for correlation at the 5% significance level is 0.944

IF the reported CORRELATION is GREATER than the 5% critical value, ACCEPT
the hypothesis that the weighted residuals are INDEPENDENT AND NORMALLY
DISTRIBUTED at the 5% significance level.  The probability that this
conclusion is wrong is less than 5%.

IF the reported correlation IS LESS THAN the 5% critical value REJECT the,
hypothesis that the weighted residuals are INDEPENDENT AND NORMALLY
DISTRIBUTED at the 5% significance level.

The analysis can also be done using the 10% significance level.
The associated critical value is 0.953
-------------------------------------------------------------------------


*** PARAMETER ESTIMATION CONVERGED BY SATISFYING THE TOL CRITERION ***
```

Modified Input Files For Generation of CORFAC-2k Input File

Name file (example.nam):

```
GLOBAL          4 mf2k.global_listing
LIST            3 output.dat
DIS            95 discret.dat
BAS6            1 bas6.dat
ZONE           93 zone.dat
MULT           94 multiple.dat
LPF            31 lpf6.dat
RCH            11 rech6.dat
WEL            12 wel6.dat
PCG            23 pcg2.dat
OC             22 oc.dat
DATA           10 inithead.dat
OBS            40 obs.dat
HOB            41 hob.dat
PES            47 pes.dat
SEN            46 sen.dat
UNC            60 unc.dat
```

UNC file (example.unc):

```
    3    2    0    0    1    0   61  0    1    0    4    0
.01 .1 .1
  0.0
HK_1 .0
HK_2 .0
```

SEN file (sen.dat):

```
# SEN file for MODFLOW-2000, UNC1NLI1 Report Example
#
 2  0  0  2                           Item 1
 1  0   0  0                          Item 2
HK_1 1  1   1.46378  .01  100  1E-10  Item 3
HK_2 1  1  .0994330  .01  100  1E-10  Item 3
```

HOB file (hob.dat):

```
# HOBS file for MODFLOW-2000, UNC1NLI1 Report Example
 42  0  0  6
 1  1
F1   1  37  13  1  0  0  0  14.88  729.28  0  1
F2   1  30  13  1  0  0  0  14.78  690.68  0  1
F3   1  25  13  1  0  0  0  14.86  668.02  0  1
F4   1  20  13  1  0  0  0  13.87  699.35  0  1
F5   1  14  13  1  0  0  0  13.01  728.59  0  1
```

```
F6   1   8  13  1  0  0  0  12.97  746.80  0  1
F7   1  37  26  1  0  0  0   5.61  643.27  0  1
F8   1  30  26  1  0  0  0   5.63  666.51  0  1
F9   1  25  26  1  0  0  0   5.94  687.81  0  1
F10  1  20  26  1  0  0  0   8.83  721.28  0  1
F11  1  14  26  1  0  0  0  11.08  717.66  0  1
F12  1   8  26  1  0  0  0  11.35  731.50  0  1
F13  1  37  39  1  0  0  0    3.7  640.67  0  1
F14  1  30  39  1  0  0  0   3.75  648.28  0  1
F15  1  25  39  1  0  0  0   3.52  619.12  0  1
F16  1  20  39  1  0  0  0   3.35  607.80  0  1
F17  1  14  39  1  0  0  0   3.42  638.66  0  1
F18  1   8  39  1  0  0  0   3.71  629.47  0  1
F19  1  37  52  1  0  0  0   2.37  548.04  0  1
F20  1  30  52  1  0  0  0   1.91  531.05  0  1
F21  1  25  52  1  0  0  0   1.76  526.49  0  1
F22  1  20  52  1  0  0  0   1.96  531.33  0  1
F23  1  14  52  1  0  0  0   1.82  546.39  0  1
F24  1   8  52  1  0  0  0   2.06  542.63  0  1
F25  1  37  65  1  0  0  0   1.54  423.83  0  1
F26  1  30  65  1  0  0  0   1.66  427.94  0  1
F27  1  25  65  1  0  0  0   1.78  429.22  0  1
F28  1  20  65  1  0  0  0   1.54  426.12  0  1
F29  1  14  65  1  0  0  0    1.7  432.14  0  1
F30  1   8  65  1  0  0  0   1.55  444.93  0  1
F31  1  37  78  1  0  0  0    .94  153.12  0  1
F32  1  30  78  1  0  0  0   1.41  197.28  0  1
F33  1  25  78  1  0  0  0   1.22  197.22  0  1
F34  1  20  78  1  0  0  0   1.47  202.06  0  1
F35  1  14  78  1  0  0  0   1.08  212.53  0  1
F36  1   8  78  1  0  0  0    .88  202.26  0  1
G1   1  22  46  1  0  0  0      0  1037.4  0  1
G2   1  21  20  1  0  0  0      0  723.55  0  1
G3   1  21  33  1  0  0  0      0  620.74  0  1
G4   1  21  59  1  0  0  0      0  488.07  0  1
G5   1  21  72  1  0  0  0      0  329.80  0  1
G6   1  40  46  1  0  0  0      0  597.63  0  1
```

Modified _cf Input File to CORFAC-2k

Modified _cf Input File to CORFAC-2k (example._cf):

```
         2        36           0          0          0  0.412962E-03  -1.00000
1
HK_1       HK_2
F1            F2            F3            F4            F5            F6
F7            F8            F9            F10           F11           F12
F13           F14           F15           F16           F17           F18
F19           F20           F21           F22           F23           F24
F25           F26           F27           F28           F29           F30
F31           F32           F33           F34           F35           F36
 0.37029926E-01 0.38050603E-01 0.38690582E-01 0.37814010E-01 0.37047457E-01
0.36592986E-01 0.39427873E-01 0.38734384E-01
 0.38129907E-01 0.37234716E-01 0.37328508E-01 0.36973692E-01 0.39507795E-01
0.39275225E-01 0.40189497E-01 0.40562026E-01
 0.39569918E-01 0.39857723E-01 0.42716324E-01 0.43394260E-01 0.43581776E-01
0.43382823E-01 0.42780772E-01 0.42928737E-01
 0.48574030E-01 0.48340213E-01 0.48268080E-01 0.48443336E-01 0.48104730E-01
0.47408275E-01 0.80813520E-01 0.71196474E-01
 0.71207300E-01 0.70349306E-01 0.68594590E-01 0.70314519E-01
 -6.95528     -7.59430
 -6.88616     -7.54031
 -6.76804     -7.46494
 -6.43567     -7.28740
 -6.26939     -7.22403
 -6.24739     -7.22516
 -4.78414    -0.240649E-02
 -4.91206    -0.944998E-01
 -5.17005    -0.265524
 -4.96155     -3.61991
 -4.84161     -6.59591
 -5.02165     -6.79714
 -3.74236    -0.460639E-01
 -3.72761    -0.580034E-01
 -3.68348    -0.559502E-01
 -3.59604    -0.174140E-01
 -3.53574     0.426478E-01
 -3.53499     0.750806E-01
 -2.69891    -0.227933E-01
 -2.66038    -0.184378E-01
 -2.61047    -0.113816E-01
 -2.57549    -0.919775E-03
 -2.59367     0.132558E-01
 -2.61204     0.244984E-01
 -1.76582    -0.875923E-02
 -1.75638    -0.630512E-02
 -1.74753    -0.331463E-02
 -1.74041     0.349868E-03
 -1.73644     0.484277E-02
 -1.73592     0.835407E-02
-0.870245    -0.284664E-02
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-0.868096    -0.198254E-02
-0.865989    -0.983839E-03
-0.863890     0.186636E-03
-0.862079     0.156564E-02
-0.861022     0.261434E-02
         8         6         0         2         1         0
G1           G2           G3           G4           G5           G6
  HK_1         HK_2
 0.31047517E-01 0.37176263E-01 0.40137023E-01 0.45264628E-01 0.55064879E-01
0.40905699E-01  0.0000000      0.0000000
 -2.84418    -0.123538E-01
 -5.29811     -6.69752
 -4.37059    -0.168617
 -2.13973    -0.106125E-02
 -1.27031    -0.137881E-03
 -3.16943    -0.333658E-01
  1.00000      0.00000
  0.00000      1.00000
729.28    667.57    615.68    586.33    557.59    534.25    584.85    598.77
591.88    569.46    549.34    541.11    477.64    485.80    477.81    474.03
490.18    486.31    326.73    325.31    323.54    332.79    344.61    339.91
208.67    221.75    226.29    225.34    240.21    245.61    68.870    101.52
103.49    110.91    118.31    98.075
667.57    690.68    654.63    620.72    586.71    561.51    589.59    601.63
595.99    577.41    559.76    549.42    478.84    483.95    474.92    467.99
483.29    478.43    321.55    318.49    315.94    322.14    333.98    331.21
214.14    224.01    227.44    222.64    233.67    236.83    72.997    106.27
108.19    114.37    119.57    96.373
615.68    654.63    668.02    651.43    618.29    587.79    577.61    590.09
588.78    576.27    558.71    553.40    467.96    471.16    460.22    452.06
465.32    460.42    308.79    303.50    300.50    304.75    314.61    312.42
202.47    210.94    215.14    210.02    220.51    221.90    72.489    104.27
105.26    110.19    114.24    92.439
586.33    620.72    651.43    699.35    686.13    649.67    562.03    574.93
574.79    566.42    550.59    553.37    452.96    452.53    440.17    430.63
441.05    439.34    293.55    290.00    287.19    289.52    297.87    293.66
193.48    201.20    204.83    198.65    206.20    206.93    69.506    99.734
99.477    103.72    107.11    87.286
557.59    586.71    618.29    686.13    728.59    707.08    543.25    559.94
561.06    555.06    538.05    538.75    443.24    442.05    428.49    417.27
424.38    421.98    288.46    285.79    281.38    283.14    288.82    282.64
192.57    200.60    204.67    197.13    203.52    203.09    69.115    99.001
98.459    104.13    107.79    87.132
534.25    561.51    587.79    649.67    707.08    746.80    525.38    543.55
547.06    545.23    529.14    527.88    437.16    436.68    423.31    411.63
418.82    415.31    289.42    286.38    280.51    281.62    286.86    279.57
191.49    200.05    202.37    193.86    198.61    197.71    65.800    95.801
95.834    100.16    103.22    82.084
584.85    589.59    577.61    562.03    543.25    525.38    643.27    632.46
614.20    600.57    577.59    562.10    507.35    507.86    491.01    477.72
483.99    476.30    331.83    326.31    325.01    329.89    338.91    334.53
216.78    225.84    232.23    227.82    238.01    242.82    71.272    107.29
108.79    114.71    123.51    104.54
598.77    601.63    590.09    574.93    559.94    543.55    632.46    666.51
657.18    644.11    618.41    599.20    524.83    525.59    509.64    499.58
510.39    501.63    346.45    338.31    333.05    337.30    349.23    345.68
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221.67    230.89    237.21    232.60    242.72    247.01    73.206    109.94
110.31    115.26    124.50    105.37
591.88    595.99    588.78    574.79    561.06    547.06    614.20    657.18
687.81    686.21    659.29    637.88    537.68    541.81    526.18    517.05
531.07    522.43    362.45    354.14    347.07    349.82    361.59    358.58
232.67    240.53    246.07    242.48    250.68    254.24    78.717    114.03
114.30    119.04    127.26    106.76
569.46    577.41    576.27    566.42    555.06    545.23    600.57    644.11
686.21    721.28    701.42    676.61    554.47    562.74    551.08    543.76
558.91    552.38    379.87    372.12    363.43    363.69    375.96    372.75
242.19    249.08    254.99    254.22    261.06    263.36    84.298    120.19
120.19    124.31    131.48    110.02
549.34    559.76    558.71    550.59    538.05    529.14    577.59    618.41
659.29    701.42    717.66    702.17    553.51    566.83    558.53    551.51
566.99    560.49    382.08    375.64    366.97    367.21    378.36    374.44
245.30    252.08    257.29    255.75    261.15    262.41    88.611    121.30
120.89    124.28    131.52    112.32
541.11    549.42    553.40    553.37    538.75    527.88    562.10    599.20
637.88    676.61    702.17    731.50    549.20    564.90    560.42    557.96
574.98    566.97    382.48    378.58    371.67    371.59    381.56    374.77
248.91    256.43    261.51    258.12    261.74    261.68    91.934    123.40
123.28    127.11    134.16    113.32
477.64    478.84    467.96    452.96    443.24    437.16    507.35    524.83
537.68    554.47    553.51    549.20    640.67    626.22    591.51    563.61
555.08    535.82    453.45    447.14    440.73    438.31    441.10    423.05
295.30    305.66    312.49    311.97    316.94    320.88    105.64    144.94
148.93    153.49    165.66    142.97
485.80    483.95    471.16    452.53    442.05    436.68    507.86    525.59
541.81    562.74    566.83    564.90    626.22    648.28    618.24    588.02
580.79    558.88    460.96    454.52    448.96    446.67    449.88    432.98
303.50    313.53    320.28    319.66    325.02    328.34    111.31    149.19
151.82    155.30    165.42    142.83
477.81    474.92    460.22    440.17    428.49    423.31    491.01    509.64
526.18    551.08    558.53    560.42    591.51    618.24    619.12    597.36
588.69    566.62    452.11    449.96    444.33    443.98    453.68    439.92
300.25    308.91    315.03    313.82    319.76    324.34    108.06    145.56
148.64    152.55    161.93    139.60
474.03    467.99    452.06    430.63    417.27    411.63    477.72    499.58
517.05    543.76    551.51    557.96    563.61    588.02    597.36    607.80
599.81    577.83    445.39    443.84    438.99    440.63    456.72    446.56
296.70    305.68    312.57    310.46    316.16    321.64    106.61    144.37
146.88    150.81    159.16    137.11
490.18    483.29    465.32    441.05    424.38    418.82    483.99    510.39
531.07    558.91    566.99    574.98    555.08    580.79    588.69    599.81
638.66    617.67    438.33    438.82    437.99    440.62    458.55    449.80
292.93    303.57    309.94    308.99    313.48    315.66    105.79    143.49
145.72    148.31    155.68    131.83
486.31    478.43    460.42    439.34    421.98    415.31    476.30    501.63
522.43    552.38    560.49    566.97    535.82    558.88    566.62    577.83
617.67    629.47    428.62    428.57    430.59    437.01    456.18    447.76
288.83    299.85    307.41    307.76    311.41    313.08    105.58    143.63
146.56    150.52    156.68    132.63
326.73    321.55    308.79    293.55    288.46    289.42    331.83    346.45
362.45    379.87    382.08    382.48    453.45    460.96    452.11    445.39
438.33    428.62    548.04    522.35    500.04    484.78    471.74    454.53
379.15    390.62    392.18    383.88    378.94    379.17    137.98    179.29
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184.21    190.21    201.84    174.92
325.31    318.49    303.50    290.00    285.79    286.38    326.31    338.31
354.14    372.12    375.64    378.58    447.14    454.52    449.96    443.84
438.82    428.57    522.35    531.05    515.27    499.46    486.02    465.12
377.99    389.36    391.95    384.08    380.66    379.82    139.14    177.36
182.01    187.59    198.06    171.04
323.54    315.94    300.50    287.19    281.38    280.51    325.01    333.05
347.07    363.43    366.97    371.67    440.73    448.96    444.33    438.99
437.99    430.59    500.04    515.27    526.49    517.52    502.76    477.30
381.07    395.46    399.39    394.44    392.14    390.23    145.44    183.03
188.11    193.42    204.07    177.28
332.79    322.14    304.75    289.52    283.14    281.62    329.89    337.30
349.82    363.69    367.21    371.59    438.31    446.67    443.98    440.63
440.62    437.01    484.78    499.46    517.52    531.33    522.51    497.03
371.13    389.59    396.26    394.86    398.34    402.69    143.86    182.63
188.43    193.53    205.17    179.10
344.61    333.98    314.61    297.87    288.82    286.86    338.91    349.23
361.59    375.96    378.36    381.56    441.10    449.88    453.68    456.72
458.55    456.18    471.74    486.02    502.76    522.51    546.39    526.83
360.58    381.27    390.93    393.82    401.50    409.36    141.58    181.57
187.82    192.83    203.97    177.63
339.91    331.21    312.42    293.66    282.64    279.57    334.53    345.68
358.58    372.75    374.44    374.77    423.05    432.98    439.92    446.56
449.80    447.76    454.53    465.12    477.30    497.03    526.83    542.63
346.27    367.35    378.05    383.54    394.49    404.22    134.42    174.09
180.86    186.84    198.00    171.15
208.67    214.14    202.47    193.48    192.57    191.49    216.78    221.67
232.67    242.19    245.30    248.91    295.30    303.50    300.25    296.70
292.93    288.83    379.15    377.99    381.07    371.13    360.58    346.27
423.83    409.60    393.71    366.08    338.05    324.23    170.89    210.96
207.57    202.51    198.52    162.88
221.75    224.01    210.94    201.20    200.60    200.05    225.84    230.89
240.53    249.08    252.08    256.43    305.66    313.53    308.91    305.68
303.57    299.85    390.62    389.36    395.46    389.59    381.27    367.35
409.60    427.94    417.14    392.68    365.92    350.74    173.99    216.39
216.19    214.18    214.04    179.48
226.29    227.44    215.14    204.83    204.67    202.37    232.23    237.21
246.07    254.99    257.29    261.51    312.49    320.28    315.03    312.57
309.94    307.41    392.18    391.95    399.39    396.26    390.93    378.05
393.71    417.14    429.22    411.90    388.36    372.38    172.20    216.59
217.49    217.96    221.48    188.33
225.34    222.64    210.02    198.65    197.13    193.86    227.82    232.60
242.48    254.22    255.75    258.12    311.97    319.66    313.82    310.46
308.99    307.76    383.88    384.08    394.44    394.86    393.82    383.54
366.08    392.68    411.90    426.12    411.10    395.28    165.65    211.41
215.82    218.80    226.66    197.82
240.21    233.67    220.51    206.20    203.52    198.61    238.01    242.72
250.68    261.06    261.15    261.74    316.94    325.02    319.76    316.16
313.48    311.41    378.94    380.66    392.14    398.34    401.50    394.49
338.05    365.92    388.36    411.10    432.14    425.39    160.29    207.36
214.39    219.04    231.88    204.96
245.61    236.83    221.90    206.93    203.09    197.71    242.82    247.01
254.24    263.36    262.41    261.68    320.88    328.34    324.34    321.64
315.66    313.08    379.17    379.82    390.23    402.69    409.36    404.22
324.23    350.74    372.38    395.28    425.39    444.93    153.77    201.63
210.36    217.26    232.57    206.41
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68.870    72.997    72.489    69.506    69.115    65.800    71.272    73.206
78.717    84.298    88.611    91.934    105.64    111.31    108.06    106.61
105.79    105.58    137.98    139.14    145.44    143.86    141.58    134.42
170.89    173.99    172.20    165.65    160.29    153.77    153.12    155.86
140.83    128.13    111.47    93.066
101.52    106.27    104.27    99.734    99.001    95.801    107.29    109.94
114.03    120.19    121.30    123.40    144.94    149.19    145.56    144.37
143.49    143.63    179.29    177.36    183.03    182.63    181.57    174.09
210.96    216.39    216.59    211.41    207.36    201.63    155.86    197.28
185.59    173.70    156.95    128.51
103.49    108.19    105.26    99.477    98.459    95.834    108.79    110.31
114.30    120.19    120.89    123.28    148.93    151.82    148.64    146.88
145.72    146.56    184.21    182.01    188.11    188.43    187.82    180.86
207.57    216.19    217.49    215.82    214.39    210.36    140.83    185.59
197.22    190.73    175.32    147.00
110.91    114.37    110.19    103.72    104.13    100.16    114.71    115.26
119.04    124.31    124.28    127.11    153.49    155.30    152.55    150.81
148.31    150.52    190.21    187.59    193.42    193.53    192.83    186.84
202.51    214.18    217.96    218.80    219.04    217.26    128.13    173.70
190.73    202.06    192.15    162.93
118.31    119.57    114.24    107.11    107.79    103.22    123.51    124.50
127.26    131.48    131.52    134.16    165.66    165.42    161.93    159.16
155.68    156.68    201.84    198.06    204.07    205.17    203.97    198.00
198.52    214.04    221.48    226.66    231.88    232.57    111.47    156.95
175.32    192.15    212.53    188.12
98.075    96.373    92.439    87.286    87.132    82.084    104.54    105.37
106.76    110.02    112.32    113.32    142.97    142.83    139.60    137.11
131.83    132.63    174.92    171.04    177.28    179.10    177.63    171.15
162.88    179.48    188.33    197.82    204.96    206.41    93.066    128.51
147.00    162.93    188.12    202.26
```

Output File from CORFAC-2k

Output File from CORFAC-2k (example.#cf):

```
                                    CORFAC

                 MODFLOW-2000 POST-PROCESSING PROGRAM TO CALCULATE
 CORRECTION FACTORS FOR CONFIDENCE REGION AND CONFIDENCE AND PREDICTION
INTERVALS
                              Version 1.0.0 31/10/2003

 NUMBER OF ESTIMATED PARAMETERS..................:    2
 NUMBER OF HEAD OBSERVATIONS.....................:   36
 NUMBER OF ALL OTHER OBSERVATIONS................:    0
 TOTAL NUMBER OF OBSERVATIONS....................:   36

 NUMBER OF PRIOR-INFORMATION EQUATIONS...........:    0
 NUMBER OF PRIOR INFORMATION W/ FULL WEIGHT MATRIX:    0
 CALCULATED ERROR VARIANCE.......................: 0.41296E-03

 EFFECTIVE CORRELATION (EC)......................: 0.80000    (WAS RESET
BECAUSE IN INPUT FILE EC<0.0)

 TRANSFORM WITH OBS. COV. MATRIX? (YES,NO)=(1,0)..:    1


          SQUARE-ROOT OF WEIGHTS FOR SAMPLE INFORMATION
   NO. OBSERVATION      W          NO. OBSERVATION      W
  HEADS:
     1  F1           0.37030E-01    19  F19          0.42716E-01
     2  F2           0.38051E-01    20  F20          0.43394E-01
     3  F3           0.38691E-01    21  F21          0.43582E-01
     4  F4           0.37814E-01    22  F22          0.43383E-01
     5  F5           0.37047E-01    23  F23          0.42781E-01
     6  F6           0.36593E-01    24  F24          0.42929E-01
     7  F7           0.39428E-01    25  F25          0.48574E-01
     8  F8           0.38734E-01    26  F26          0.48340E-01
     9  F9           0.38130E-01    27  F27          0.48268E-01
    10  F10          0.37235E-01    28  F28          0.48443E-01
    11  F11          0.37329E-01    29  F29          0.48105E-01
    12  F12          0.36974E-01    30  F30          0.47408E-01
    13  F13          0.39508E-01    31  F31          0.80814E-01
    14  F14          0.39275E-01    32  F32          0.71196E-01
    15  F15          0.40189E-01    33  F33          0.71207E-01
    16  F16          0.40562E-01    34  F34          0.70349E-01
    17  F17          0.39570E-01    35  F35          0.68595E-01
    18  F18          0.39858E-01    36  F36          0.70315E-01

 SENSITIVITIES FOR OPTIMUM PARAMETERS

 PARAMETER   F1           F2           F3           F4           F5
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 HK_1         -6.9553      -6.8862      -6.7680      -6.4357      -6.2694
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HK_2	-7.5943	-7.5403	-7.4649	-7.2874	-7.2240

PARAMETER	F6	F7	F8	F9	F10
HK_1	-6.2474	-4.7841	-4.9121	-5.1701	-4.9616
HK_2	-7.2252	-0.24065E-02	-0.94500E-01	-0.26552	-3.6199

PARAMETER	F11	F12	F13	F14	F15
HK_1	-4.8416	-5.0216	-3.7424	-3.7276	-3.6835
HK_2	-6.5959	-6.7971	-0.46064E-01	-0.58003E-01	-0.55950E-01

PARAMETER	F16	F17	F18	F19	F20
HK_1	-3.5960	-3.5357	-3.5350	-2.6989	-2.6604
HK_2	-0.17414E-01	0.42648E-01	0.75081E-01	-0.22793E-01	-0.18438E-01

PARAMETER	F21	F22	F23	F24	F25
HK_1	-2.6105	-2.5755	-2.5937	-2.6120	-1.7658
HK_2	-0.11382E-01	-0.91977E-03	0.13256E-01	0.24498E-01	-0.87592E-02

PARAMETER	F26	F27	F28	F29	F30
HK_1	-1.7564	-1.7475	-1.7404	-1.7364	-1.7359
HK_2	-0.63051E-02	-0.33146E-02	0.34987E-03	0.48428E-02	0.83541E-02

PARAMETER	F31	F32	F33	F34	F35
HK_1	-0.87024	-0.86810	-0.86599	-0.86389	-0.86208
HK_2	-0.28466E-02	-0.19825E-02	-0.98384E-03	0.18664E-03	0.15656E-02

PARAMETER	F36
HK_1	-0.86102
HK_2	0.26143E-02

SQUARE-ROOT OF WEIGHTS FOR INTERVALS

NO.	INTERVAL	W	NO.	INTERVAL	W
1	G1	0.0000	5	G5	0.0000
2	G2	0.0000	6	G6	0.0000
3	G3	0.0000	7	HK_1	0.0000
4	G4	0.0000	8	HK_2	0.0000

SENSITIVITIES FOR OPTIMUM PARAMETERS

PARAMETER	G1	G2	G3	G4	G5
HK_1	-2.8442	-5.2981	-4.3706	-2.1397	-1.2703
HK_2	-0.12354E-01	-6.6975	-0.16862	-0.10612E-02	-0.13788E-03

PARAMETER	G6	HK_1	HK_2
HK_1	-3.1694	1.0000	0.0000
HK_2	-0.33366E-01	0.0000	1.0000

```
****** CORRECTION FACTOR COMPUTED FOR CONFIDENCE REGION


CORRECTION FACTOR FOR N-P (A) ---- =  11.910
SCALING FACTOR (B) --------------- =  1.0000
EFFECTIVE CORRELATION (C) -------- = 0.71490
(N-P)/(N-A*P) VALUE (FAC) -------- =  2.7913
CORRECTION FACTOR (CR) ----------- =  33.243


APPROXIMATE N-A*P VALUE (DFB) ---- =  9.5836
APPROX. (N-P)/(N-A*P) VALUE (FACB) =  3.5477
APPROXIMATE BOUND FOR CR (CRB) --- =  46.859



****** CORRECTION FACTORS COMPUTED FOR CONFIDENCE INTERVALS


TOTAL NUMBER OF INTERVALS (NOINT)......................:    8
NUMBER OF INTERVALS FOR HEAD (NHI).....................:    6
NUMBER OF INTERVALS FOR HEAD DEPENDENT FLOWS (NQI).....:    0
NUMBER OF INTERVALS FOR PARAMETERS (NPI)...............:    2
INTERVAL TYPE (1=CONFIDENCE,2=PREDICTION)..............:    1
HEAD AND FLOW INTERVALS ON DIFFERENCES (0,1)=(NO,YES)..:    0

          SQUARE-ROOT OF WEIGHTS FOR INTERVALS
   NO.   INTERVAL       W          NO.   INTERVAL       W
    1  G1            0.0000         5  G5            0.0000
    2  G2            0.0000         6  G6            0.0000
    3  G3            0.0000         7    HK_1        0.0000
    4  G4            0.0000         8    HK_2        0.0000

SENSITIVITIES FOR OPTIMUM PARAMETERS

PARAMETER   G1           G2           G3           G4           G5
----------  ------------ ------------ ------------ ------------ ------------
HK_1         -2.8442      -5.2981      -4.3706      -2.1397      -1.2703
HK_2        -0.12354E-01  -6.6975     -0.16862     -0.10612E-02 -0.13788E-03

PARAMETER   G6             HK_1         HK_2
----------  ------------ ------------ ------------
HK_1         -3.1694       1.0000       0.0000
HK_2        -0.33366E-01   0.0000       1.0000


** CONFIDENCE INTERVAL NO.   1, FOR G1

 CORRECTION FACTOR XI FOR C. I. ------ =  16.350
 CORRECTION FACTOR (CC) -------------- =  45.638

 ESTIMATED VARIANCE OF PREDICTION (VE) = 0.86984E-02
 BOUND FOR XI USING POS. VALUES (XIPB) =  24.982
 BOUND FOR XI USING NEG. VALUES (XINB) = 0.15332E-01
```

```
 APPROXIMATE BOUND FOR CC (CCB) ------ =  71.613


** CONFIDENCE INTERVAL NO.   2, FOR G2

 CORRECTION FACTOR XI FOR C. I. ------ =  5.7280
 CORRECTION FACTOR (CC) -------------- =  15.989

 ESTIMATED VARIANCE OF PREDICTION (VE) = 0.31039E-01
 BOUND FOR XI USING POS. VALUES (XIPB) =  8.6042
 BOUND FOR XI USING NEG. VALUES (XINB) = 0.27022
 APPROXIMATE BOUND FOR CC (CCB) ------ =  25.130


** CONFIDENCE INTERVAL NO.   3, FOR G3

 CORRECTION FACTOR XI FOR C. I. ------ =  16.826
 CORRECTION FACTOR (CC) -------------- =  46.966

 ESTIMATED VARIANCE OF PREDICTION (VE) = 0.19335E-01
 BOUND FOR XI USING POS. VALUES (XIPB) =  25.521
 BOUND FOR XI USING NEG. VALUES (XINB) = 0.91738E-02
 APPROXIMATE BOUND FOR CC (CCB) ------ =  73.142


** CONFIDENCE INTERVAL NO.   4, FOR G4

 CORRECTION FACTOR XI FOR C. I. ------ =  16.298
 CORRECTION FACTOR (CC) -------------- =  45.492

 ESTIMATED VARIANCE OF PREDICTION (VE) = 0.49567E-02
 BOUND FOR XI USING POS. VALUES (XIPB) =  24.932
 BOUND FOR XI USING NEG. VALUES (XINB) = 0.16355E-01
 APPROXIMATE BOUND FOR CC (CCB) ------ =  71.470


** CONFIDENCE INTERVAL NO.   5, FOR G5

 CORRECTION FACTOR XI FOR C. I. ------ =  16.292
 CORRECTION FACTOR (CC) -------------- =  45.477

 ESTIMATED VARIANCE OF PREDICTION (VE) = 0.17482E-02
 BOUND FOR XI USING POS. VALUES (XIPB) =  24.927
 BOUND FOR XI USING NEG. VALUES (XINB) = 0.16459E-01
 APPROXIMATE BOUND FOR CC (CCB) ------ =  71.456


** CONFIDENCE INTERVAL NO.   6, FOR G6

 CORRECTION FACTOR XI FOR C. I. ------ =  16.435
 CORRECTION FACTOR (CC) -------------- =  45.875

 ESTIMATED VARIANCE OF PREDICTION (VE) = 0.10685E-01
 BOUND FOR XI USING POS. VALUES (XIPB) =  25.063
 BOUND FOR XI USING NEG. VALUES (XINB) = 0.13742E-01
 APPROXIMATE BOUND FOR CC (CCB) ------ =  71.842
```

```
** CONFIDENCE INTERVAL NO.   7, FOR   HK_1

 CORRECTION FACTOR XI FOR C. I. ------ =  16.291
 CORRECTION FACTOR (CC) -------------- =  45.473

 ESTIMATED VARIANCE OF PREDICTION (VE) = 0.10836E-02
 BOUND FOR XI USING POS. VALUES (XIPB) = 0.16488E-01
 BOUND FOR XI USING NEG. VALUES (XINB) =  24.925
 APPROXIMATE BOUND FOR CC (CCB) ------ =  71.452


** CONFIDENCE INTERVAL NO.   8, FOR   HK_2

 CORRECTION FACTOR XI FOR C. I. ------ =  3.8218
 CORRECTION FACTOR (CC) -------------- =  10.668

 ESTIMATED VARIANCE OF PREDICTION (VE) = 0.15234E-02
 BOUND FOR XI USING POS. VALUES (XIPB) =  12.816
 BOUND FOR XI USING NEG. VALUES (XINB) =  3.8470
 APPROXIMATE BOUND FOR CC (CCB) ------ =  37.083
```

Input Files Used to Generate BEALE2-2k Input Files

Name file (example.nam):

```
GLOBAL          4 mf2k.global_listing
LIST            3 output.dat
DIS            95 discret.dat
BAS6            1 bas6.dat
ZONE           93 zone.dat
MULT           94 multiple.dat
LPF            31 lpf6.dat
RCH            11 rech6.dat
WEL            12 wel6.dat
PCG            23 pcg2.dat
OC             22 oc.dat
DATA           10 inithead.dat
OBS            40 obs.dat
HOB            41 hob.dat
PES            47 pes.dat
SEN            46 sen.dat
UNC            60 unc.dat
```

UNC file (unc.dat):

```
    1    2    0   00    1    0   61  0    1    0    4    0
.01 .1 .1
  0.0
HK_1 .0
HK_2 .0
33.243
45.638  15.989  46.966  45.492  45.477  45.875  45.473  10.668
```

SEN file (sen.dat):

```
# SEN file for MODFLOW-2000, UNC1NLI1 Report Example
#
 2  0  0  2                           Item 1
 1  0   0  0                          Item 2
HK_1 1  1   1.46378  .01  100  1E-10  Item 3
HK_2 1  1  .0994330  .01  100  1E-10  Item 3
```

BEALE2-2k Input Files

_b1 file (example._b1):

```
         2        36         0         0         0  0.412962E-03   33.2430
HK_1       HK_2
  1.46378     0.994330E-01
F1           F2           F3           F4           F5           F6
F7           F8           F9           F10          F11          F12
F13          F14          F15          F16          F17          F18
F19          F20          F21          F22          F23          F24
F25          F26          F27          F28          F29          F30
F31          F32          F33          F34          F35          F36
  14.5496      14.4265      14.2330      13.7231      13.4935      13.4726
  4.78655      5.00656      5.43558      8.58150      11.4376      11.8188
  3.78842      3.78562      3.73943      3.61346      3.49310      3.45992
  2.72171      2.67882      2.62185      2.57641      2.58042      2.58755
  1.77458      1.76269      1.75084      1.74006      1.73160      1.72757
 0.873092     0.870080     0.866973     0.863704     0.860516     0.858411
  14.8800      14.7800      14.8600      13.8700      13.0100      12.9700
  5.61000      5.63000      5.94000      8.83000      11.0800      11.3500
  3.70000      3.75000      3.52000      3.35000      3.42000      3.71000
  2.37000      1.91000      1.76000      1.96000      1.82000      2.06000
  1.54000      1.66000      1.78000      1.54000      1.70000      1.55000
 0.940000      1.41000      1.22000      1.47000      1.08000     0.880000
 0.13712154E-02 0.14478485E-02 0.14969611E-02 0.14298992E-02 0.13725139E-02
0.13390466E-02 0.15545571E-02 0.15003525E-02
 0.14538899E-02 0.13864241E-02 0.13934176E-02 0.13670539E-02 0.15608660E-02
0.15425433E-02 0.16151958E-02 0.16452781E-02
 0.15657784E-02 0.15886382E-02 0.18246844E-02 0.18830620E-02 0.18993714E-02
0.18820695E-02 0.18301945E-02 0.18428763E-02
 0.23594366E-02 0.23367761E-02 0.23298075E-02 0.23467569E-02 0.23140649E-02
0.22475447E-02 0.65308255E-02 0.50689378E-02
 0.50704796E-02 0.49490249E-02 0.47052181E-02 0.49441312E-02
 -6.95528     -7.59430
 -6.88616     -7.54031
 -6.76804     -7.46494
 -6.43567     -7.28740
 -6.26939     -7.22403
 -6.24739     -7.22516
 -4.78414    -0.240649E-02
 -4.91206    -0.944998E-01
 -5.17005    -0.265524
 -4.96155     -3.61991
 -4.84161     -6.59591
 -5.02165     -6.79714
 -3.74236    -0.460639E-01
 -3.72761    -0.580034E-01
 -3.68348    -0.559502E-01
 -3.59604    -0.174140E-01
 -3.53574     0.426478E-01
 -3.53499     0.750806E-01
 -2.69891    -0.227933E-01
```

```
 -2.66038    -0.184378E-01
 -2.61047    -0.113816E-01
 -2.57549    -0.919775E-03
 -2.59367     0.132558E-01
 -2.61204     0.244984E-01
 -1.76582    -0.875923E-02
 -1.75638    -0.630512E-02
 -1.74753    -0.331463E-02
 -1.74041     0.349868E-03
 -1.73644     0.484277E-02
 -1.73592     0.835407E-02
-0.870245    -0.284664E-02
-0.868096    -0.198254E-02
-0.865989    -0.983839E-03
-0.863890     0.186636E-03
-0.862079     0.156564E-02
-0.861022     0.261434E-02
         1          1
 THE PARAMETER SETS FOLLOW
  1.11920     0.125942
  1.91444     0.785038E-01
  1.78665     0.723296E-01
  1.19926     0.136693
```

_b2 file (example._b2):

```
  1.11920     0.125942
  14.9125      14.7902      14.5913      14.0530      13.7994      13.7717
  6.25830      6.48017      6.91921      9.29229      11.4711      11.8419
  4.92199      4.90968      4.85074      4.71361      4.59867      4.57772
  3.54356      3.49045      3.42087      3.36873      3.38397      3.40104
  2.31476      2.30107      2.28757      2.27605      2.26799      2.26511
  1.13968      1.13657      1.13324      1.12992      1.12660      1.12444
  1.91444     0.785038E-01
  14.7982      14.6854      14.5117      14.0612      13.8643      13.8490
  3.66131      3.86141      4.24862      8.33661      12.0036      12.3774
  2.91287      2.91490      2.87901      2.76949      2.65662      2.61988
  2.08898      2.05466      2.00876      1.97049      1.96871      1.97038
  1.35974      1.34991      1.33980      1.33040      1.32244      1.31831
 0.668514     0.665898     0.663172     0.660340     0.657408     0.655526
  1.78665     0.723296E-01
  15.9823      15.8606      15.6737      15.1897      14.9787      14.9621
  3.92336      4.13889      4.55545      8.99430      12.9751      13.3778
  3.12183      3.12423      3.08576      2.96817      2.84692      2.80706
  2.23880      2.20211      2.15289      2.11173      2.10983      2.11143
  1.45719      1.44666      1.43587      1.42568      1.41723      1.41261
 0.716377     0.713626     0.710627     0.707445     0.704398     0.702631
  1.19926     0.136693
  13.8379      13.7248      13.5404      13.0412      12.8058      12.7800
  5.84041      6.04568      6.45219      8.63549      10.6408      10.9837
  4.59238      4.58067      4.52578      4.39841      4.29207      4.27328
  3.30650      3.25695      3.19203      3.14359      3.15788      3.17407
  2.15999      2.14697      2.13451      2.12386      2.11640      2.11393
  1.06347      1.06053      1.05755      1.05446      1.05147      1.04941
```

_b3 file (example._b3):

```
         8         6         0         2         1         0
G1            G2            G3            G4            G5            G6
  HK_1          HK_2
  2.85654      11.9957      4.53921      2.14079      1.27045      3.20279
 0.381022     -2.30827
 0.96394832E-03 0.13820746E-02 0.16109805E-02 0.20488864E-02 0.30321409E-02
0.16732761E-02  0.0000000      0.0000000
 -2.84418    -0.123538E-01
 -5.29811     -6.69752
 -4.37059    -0.168617
 -2.13973    -0.106125E-02
 -1.27031    -0.137881E-03
 -3.16943    -0.333658E-01
  1.00000      0.00000
  0.00000      1.00000
   45.6380       15.9890       46.9660       45.4920       45.4770
45.8750
   45.4730       10.6680
 THE PARAMETER SETS FOLLOW
  1.82832     0.818010E-01
  1.17192     0.120866
  1.44237     0.111757
  1.48551     0.884681E-01
  1.83400     0.819924E-01
  1.16830     0.120583
  1.82767     0.817822E-01
  1.17234     0.120893
  1.82760     0.817804E-01
  1.17238     0.120896
  1.82936     0.818321E-01
  1.17126     0.120820
  1.17239     0.120897
  1.82759     0.817798E-01
  1.58544     0.875319E-01
  1.35145     0.112952
```

_b4 file (example._b4):

```
  1.82832     0.818010E-01
  14.7031      14.5883      14.4106      13.9490      13.7463      13.7301
  3.83359      4.03804      4.43404      8.34384      11.8579      12.2337
  3.04753      3.04903      3.01155      2.89900      2.78433      2.74775
  2.18610      2.15054      2.10289      2.06339      2.06235      2.06468
  1.42344      1.41320      1.40288      1.39314      1.38505      1.38092
 0.699981     0.697227     0.694390     0.691413     0.688442     0.686534
  2.29123
  1.17192     0.120866
  14.8142      14.6905      14.4912      13.9546      13.7038      13.6772
  5.97744      6.20061      6.64103      9.13822      11.4268      11.8017
  4.70650      4.69607      4.63942      4.50362      4.38650      4.36281
  3.38693      3.33566      3.26840      3.21743      3.23023      3.24517
  2.21175      2.19841      2.18516      2.17367      2.16539      2.16223
```

```
  1.08887      1.08568      1.08239      1.07904      1.07577      1.07355
  3.56090
  1.44237     0.111757
  13.8048      13.6878      13.5018      13.0087      12.7843      12.7628
  4.85767      5.06823      5.48016      8.25290      10.7782      11.1389
  3.83863      3.83402      3.78730      3.66483      3.55091      3.52183
  2.75907      2.71604      2.65919      2.61444      2.62048      2.62922
  1.79967      1.78799      1.77638      1.76594      1.75790      1.75430
 0.885609     0.882716     0.879694     0.876626     0.873547     0.871495
  11.3327
  1.48551     0.884681E-01
  15.3788      15.2506      15.0503      14.5253      14.2911      14.2707
  4.71698      4.94540      5.38994      8.95448      12.1801      12.5825
  3.73883      3.73768      3.69200      3.56306      3.43687      3.39986
  2.68481      2.64204      2.58503      2.53892      2.54111      2.54671
  1.74967      1.73767      1.72564      1.71458      1.70570      1.70139
 0.860568     0.857560     0.854368     0.851076     0.847743     0.845575
  12.7448
  1.83400     0.819924E-01
  14.6641      14.5494      14.3722      13.9116      13.7094      13.6933
  3.82153      4.02530      4.42007      8.32080      11.8267      12.2014
  3.03798      3.03949      3.00215      2.88999      2.77559      2.73910
  2.17938      2.14389      2.09638      2.05699      2.05588      2.05819
  1.41909      1.40891      1.39851      1.38883      1.38071      1.37654
 0.697785     0.695042     0.692217     0.689299     0.686325     0.684411
  3.67501
  1.16830     0.120583
  14.8549      14.7309      14.5310      13.9929      13.7415      13.7148
  5.99579      6.21957      6.66124      9.16414      11.4580      11.8340
  4.72094      4.71058      4.65378      4.51760      4.40014      4.37634
  3.39745      3.34600      3.27849      3.22733      3.24017      3.25521
  2.21855      2.20513      2.19184      2.18036      2.17210      2.16895
  1.09215      1.08902      1.08574      1.08239      1.07911      1.07688
  5.59279
  1.82767     0.817822E-01
  14.7071      14.5921      14.4143      13.9522      13.7493      13.7331
  3.83480      4.03922      4.43524      8.34582      11.8606      12.2365
  3.04848      3.04998      3.01250      2.89997      2.78520      2.74860
  2.18690      2.15128      2.10361      2.06408      2.06299      2.06532
  1.42397      1.41377      1.40334      1.39364      1.38550      1.38132
 0.700185     0.697445     0.694615     0.691690     0.688705     0.686784
  1.71507
  1.17234     0.120893
  14.8097      14.6861      14.4868      13.9503      13.6996      13.6731
  5.97510      6.19822      6.63859      9.13533      11.4235      11.7984
  4.70472      4.69442      4.63782      4.50206      4.38493      4.36117
  3.38579      3.33450      3.26720      3.21620      3.22897      3.24395
  2.21092      2.19753      2.18428      2.17283      2.16460      2.16146
  1.08839      1.08527      1.08200      1.07866      1.07538      1.07316
  2.67229
  1.82760     0.817804E-01
  14.7076      14.5926      14.4148      13.9527      13.7498      13.7336
  3.83486      4.03932      4.43540      8.34612      11.8609      12.2369
  3.04855      3.05003      3.01255      2.89998      2.78521      2.74862
  2.18688      2.15123      2.10356      2.06405      2.06301      2.06537
  1.42387      1.41370      1.40331      1.39364      1.38554      1.38138
```

```
0.700138     0.697450     0.694631     0.691702     0.688741     0.686813
 1.01752
 1.17238     0.120896
 14.8094      14.6857      14.4864      13.9499      13.6993      13.6727
 5.97499      6.19809      6.63841      9.13506      11.4232      11.7980
 4.70460      4.69424      4.63764      4.50189      4.38479      4.36106
 3.38564      3.33438      3.26712      3.21614      3.22892      3.24387
 2.21088      2.19752      2.18426      2.17279      2.16453      2.16138
 1.08840      1.08524      1.08196      1.07862      1.07534      1.07313
 1.58623
 1.82936     0.818321E-01
 14.6962      14.5812      14.4036      13.9419      13.7392      13.7231
 3.83115      4.03541      4.43112      8.33939      11.8521      12.2277
 3.04560      3.04711      3.00969      2.89727      2.78262      2.74605
 2.18484      2.14928      2.10167      2.06218      2.06110      2.06341
 1.42266      1.41247      1.40205      1.39235      1.38422      1.38004
0.699548     0.696803     0.693973     0.691048     0.688069     0.686150
 2.57305
 1.17126     0.120820
 14.8212      14.6975      14.4980      13.9611      13.7102      13.6837
 5.98058      6.20385      6.64455      9.14273      11.4323      11.8074
 4.70899      4.69870      4.64208      4.50623      4.38903      4.36527
 3.38891      3.33760      3.27026      3.21921      3.23200      3.24697
 2.21301      2.19960      2.18633      2.17485      2.16660      2.16346
 1.08942      1.08627      1.08300      1.07965      1.07638      1.07415
 3.98442
 1.17239     0.120897
 14.8092      14.6856      14.4863      13.9498      13.6992      13.6726
 5.97494      6.19805      6.63837      9.13499      11.4231      11.7979
 4.70457      4.69421      4.63759      4.50184      4.38474      4.36101
 3.38560      3.33434      3.26708      3.21610      3.22889      3.24384
 2.21085      2.19750      2.18424      2.17277      2.16452      2.16136
 1.08839      1.08523      1.08195      1.07861      1.07534      1.07312
0.159044
 1.82759     0.817798E-01
 14.7081      14.5931      14.4153      13.9533      13.7504      13.7341
 3.83506      4.03960      4.43576      8.34654      11.8614      12.2374
 3.04889      3.05034      3.01284      2.90027      2.78548      2.74884
 2.18712      2.15151      2.10380      2.06422      2.06315      2.06546
 1.42406      1.41382      1.40341      1.39367      1.38556      1.38139
0.700221     0.697469     0.694638     0.691677     0.688748     0.686813
0.602998
 1.58544     0.875319E-01
 15.0249      14.9012      14.7088      14.2056      13.9821      13.9632
 4.42082      4.64083      5.06867      8.68673      11.9547      12.3465
 3.50652      3.50644      3.46367      3.34027      3.21826      3.18160
 2.51721      2.47698      2.42324      2.37953      2.38072      2.38536
 1.64010      1.62869      1.61732      1.60674      1.59826      1.59412
0.806684     0.803738     0.800670     0.797407     0.794164     0.792197
-2.43575
 1.35145     0.112952
 14.1905      14.0700      13.8780      13.3672      13.1334      13.1104
 5.18382      5.40041      5.82518      8.55177      11.0393      11.4081
 4.09258      4.08664      4.03706      3.90959      3.79305      3.76468
 2.94271      2.89710      2.83698      2.79010      2.79766      2.80790
 1.92002      1.90771      1.89553      1.88469      1.87651      1.87290
```

```
0.944902      0.941932      0.938851      0.935610      0.932412      0.930263
-2.18079
```

BEALE2-2k Output File

#be Output File (example.#be):

```
                              NLBEALE

            MODFLOW-2000 POST-PROCESSING PROGRAM TO CALCULATE
        MEASURES OF TOTAL, INTRINSIC, AND COMBINED INTRINSIC NONLINEARITY
                       Version 1.0.0 31/10/2003

NUMBER OF ESTIMATED PARAMETERS..................:    2
NUMBER OF HEAD OBSERVATIONS.....................:   36
NUMBER OF ALL OTHER OBSERVATIONS................:    0
TOTAL NUMBER OF OBSERVATIONS....................:   36

NUMBER OF PRIOR-INFORMATION EQUATIONS...........:    0
NUMBER OF PRIOR INFORMATION W/ FULL WEIGHT MATRIX:    0
NUMBER OF DATA SETS USED FOR BEALES MEASURE......:    4

CALCULATED ERROR VARIANCE.......................: 0.41296E-03

CORRECTION FACTOR FOR CONFIDENCE REGION..........:  33.243

                      OPTIMUM PARAMETERS
   NO. NAME           BOPT        NO. NAME           BOPT
    1  HK_1        1.4638          2  HK_2       0.99433E-01

     DEPENDENT VARIABLES COMPUTED WITH OPTIMUM PARAMETERS
   NO. OBSERVATION     FOPT         NO. OBSERVATION     FOPT
    1  F1             14.550        19  F19            2.7217
    2  F2             14.427        20  F20            2.6788
    3  F3             14.233        21  F21            2.6219
    4  F4             13.723        22  F22            2.5764
    5  F5             13.493        23  F23            2.5804
    6  F6             13.473        24  F24            2.5875
    7  F7             4.7866        25  F25            1.7746
    8  F8             5.0066        26  F26            1.7627
    9  F9             5.4356        27  F27            1.7508
   10  F10            8.5815        28  F28            1.7401
   11  F11            11.438        29  F29            1.7316
   12  F12            11.819        30  F30            1.7276
   13  F13            3.7884        31  F31           0.87309
   14  F14            3.7856        32  F32           0.87008
   15  F15            3.7394        33  F33           0.86697
   16  F16            3.6135        34  F34           0.86370
   17  F17            3.4931        35  F35           0.86052
   18  F18            3.4599        36  F36           0.85841

          OBSERVED VALUES OF THE DEPENDENT VARIABLES
   NO. OBSERVATION     FOBS         NO. OBSERVATION     FOBS
    1  F1             14.880        19  F19            2.3700
    2  F2             14.780        20  F20            1.9100
    3  F3             14.860        21  F21            1.7600
```

4	F4	13.870	22	F22	1.9600
5	F5	13.010	23	F23	1.8200
6	F6	12.970	24	F24	2.0600
7	F7	5.6100	25	F25	1.5400
8	F8	5.6300	26	F26	1.6600
9	F9	5.9400	27	F27	1.7800
10	F10	8.8300	28	F28	1.5400
11	F11	11.080	29	F29	1.7000
12	F12	11.350	30	F30	1.5500
13	F13	3.7000	31	F31	0.94000
14	F14	3.7500	32	F32	1.4100
15	F15	3.5200	33	F33	1.2200
16	F16	3.3500	34	F34	1.4700
17	F17	3.4200	35	F35	1.0800
18	F18	3.7100	36	F36	0.88000

RELIABILITY WEIGHTS FOR SAMPLE INFORMATION

NO.	OBSERVATION	W	NO.	OBSERVATION	W
HEADS:					
1	F1	0.13712E-02	19	F19	0.18247E-02
2	F2	0.14478E-02	20	F20	0.18831E-02
3	F3	0.14970E-02	21	F21	0.18994E-02
4	F4	0.14299E-02	22	F22	0.18821E-02
5	F5	0.13725E-02	23	F23	0.18302E-02
6	F6	0.13390E-02	24	F24	0.18429E-02
7	F7	0.15546E-02	25	F25	0.23594E-02
8	F8	0.15004E-02	26	F26	0.23368E-02
9	F9	0.14539E-02	27	F27	0.23298E-02
10	F10	0.13864E-02	28	F28	0.23468E-02
11	F11	0.13934E-02	29	F29	0.23141E-02
12	F12	0.13671E-02	30	F30	0.22475E-02
13	F13	0.15609E-02	31	F31	0.65308E-02
14	F14	0.15425E-02	32	F32	0.50689E-02
15	F15	0.16152E-02	33	F33	0.50705E-02
16	F16	0.16453E-02	34	F34	0.49490E-02
17	F17	0.15658E-02	35	F35	0.47052E-02
18	F18	0.15886E-02	36	F36	0.49441E-02

SENSITIVITIES FOR OPTIMUM PARAMETERS

PARAMETER	F1	F2	F3	F4	F5
HK_1	-6.9553	-6.8862	-6.7680	-6.4357	-6.2694
HK_2	-7.5943	-7.5403	-7.4649	-7.2874	-7.2240

PARAMETER	F6	F7	F8	F9	F10
HK_1	-6.2474	-4.7841	-4.9121	-5.1701	-4.9616
HK_2	-7.2252	-0.24065E-02	-0.94500E-01	-0.26552	-3.6199

PARAMETER	F11	F12	F13	F14	F15
HK_1	-4.8416	-5.0216	-3.7424	-3.7276	-3.6835
HK_2	-6.5959	-6.7971	-0.46064E-01	-0.58003E-01	-0.55950E-01

PARAMETER F16 F17 F18 F19 F20

```
----------  ------------ ------------ ------------ ------------ ------------
HK_1          -3.5960      -3.5357      -3.5350      -2.6989      -2.6604
HK_2        -0.17414E-01  0.42648E-01  0.75081E-01 -0.22793E-01 -0.18438E-01

PARAMETER   F21          F22          F23          F24          F25
----------  ------------ ------------ ------------ ------------ ------------
HK_1          -2.6105      -2.5755      -2.5937      -2.6120      -1.7658
HK_2        -0.11382E-01 -0.91977E-03  0.13256E-01  0.24498E-01 -0.87592E-02

PARAMETER   F26          F27          F28          F29          F30
----------  ------------ ------------ ------------ ------------ ------------
HK_1          -1.7564      -1.7475      -1.7404      -1.7364      -1.7359
HK_2        -0.63051E-02 -0.33146E-02  0.34987E-03  0.48428E-02  0.83541E-02

PARAMETER   F31          F32          F33          F34          F35
----------  ------------ ------------ ------------ ------------ ------------
HK_1        -0.87024     -0.86810     -0.86599     -0.86389     -0.86208
HK_2        -0.28466E-02 -0.19825E-02 -0.98384E-03  0.18664E-03  0.15656E-02

PARAMETER   F36
----------  ------------
HK_1        -0.86102
HK_2         0.26143E-02

        PARAMETER
  NO.     NAME        LN
    1   HK_1           1
    2   HK_2           1

                    PARAMETERS FOR SAMPLE NO.   1
   NO. NAME             B         NO. NAME             B
    1  HK_1        1.1192          2  HK_2       0.12594

        DEPENDENT VARIABLES COMPUTED FOR SAMPLE NO.   1
   NO. OBSERVATION       FC          NO. OBSERVATION       FC
    1  F1              14.913        19  F19             3.5436
    2  F2              14.790        20  F20             3.4904
    3  F3              14.591        21  F21             3.4209
    4  F4              14.053        22  F22             3.3687
    5  F5              13.799        23  F23             3.3840
    6  F6              13.772        24  F24             3.4010
    7  F7              6.2583        25  F25             2.3148
    8  F8              6.4802        26  F26             2.3011
    9  F9              6.9192        27  F27             2.2876
   10  F10             9.2923        28  F28             2.2761
   11  F11             11.471        29  F29             2.2680
   12  F12             11.842        30  F30             2.2651
   13  F13             4.9220        31  F31             1.1397
   14  F14             4.9097        32  F32             1.1366
   15  F15             4.8507        33  F33             1.1332
   16  F16             4.7136        34  F34             1.1299
   17  F17             4.5987        35  F35             1.1266
   18  F18             4.5777        36  F36             1.1244

                    PARAMETERS FOR SAMPLE NO.   2
   NO. NAME             B         NO. NAME             B
```

```
 1  HK_1        1.9144         2  HK_2       0.78504E-01

     DEPENDENT VARIABLES COMPUTED FOR SAMPLE NO.   2
NO. OBSERVATION       FC          NO. OBSERVATION      FC
 1  F1             14.798         19  F19            2.0890
 2  F2             14.685         20  F20            2.0547
 3  F3             14.512         21  F21            2.0088
 4  F4             14.061         22  F22            1.9705
 5  F5             13.864         23  F23            1.9687
 6  F6             13.849         24  F24            1.9704
 7  F7             3.6613         25  F25            1.3597
 8  F8             3.8614         26  F26            1.3499
 9  F9             4.2486         27  F27            1.3398
10  F10            8.3366         28  F28            1.3304
11  F11            12.004         29  F29            1.3224
12  F12            12.377         30  F30            1.3183
13  F13            2.9129         31  F31           0.66851
14  F14            2.9149         32  F32           0.66590
15  F15            2.8790         33  F33           0.66317
16  F16            2.7695         34  F34           0.66034
17  F17            2.6566         35  F35           0.65741
18  F18            2.6199         36  F36           0.65553

                 PARAMETERS FOR SAMPLE NO.   3
NO. NAME             B          NO. NAME            B
 1  HK_1        1.7866         2  HK_2       0.72330E-01

     DEPENDENT VARIABLES COMPUTED FOR SAMPLE NO.   3
NO. OBSERVATION       FC          NO. OBSERVATION      FC
 1  F1             15.982         19  F19            2.2388
 2  F2             15.861         20  F20            2.2021
 3  F3             15.674         21  F21            2.1529
 4  F4             15.190         22  F22            2.1117
 5  F5             14.979         23  F23            2.1098
 6  F6             14.962         24  F24            2.1114
 7  F7             3.9234         25  F25            1.4572
 8  F8             4.1389         26  F26            1.4467
 9  F9             4.5554         27  F27            1.4359
10  F10            8.9943         28  F28            1.4257
11  F11            12.975         29  F29            1.4172
12  F12            13.378         30  F30            1.4126
13  F13            3.1218         31  F31           0.71638
14  F14            3.1242         32  F32           0.71363
15  F15            3.0858         33  F33           0.71063
16  F16            2.9682         34  F34           0.70745
17  F17            2.8469         35  F35           0.70440
18  F18            2.8071         36  F36           0.70263

                 PARAMETERS FOR SAMPLE NO.   4
NO. NAME             B          NO. NAME            B
 1  HK_1        1.1993         2  HK_2       0.13669

     DEPENDENT VARIABLES COMPUTED FOR SAMPLE NO.   4
NO. OBSERVATION       FC          NO. OBSERVATION      FC
 1  F1             13.838         19  F19            3.3065
 2  F2             13.725         20  F20            3.2569
```

```
    3  F3             13.540        21  F21            3.1920
    4  F4             13.041        22  F22            3.1436
    5  F5             12.806        23  F23            3.1579
    6  F6             12.780        24  F24            3.1741
    7  F7             5.8404        25  F25            2.1600
    8  F8             6.0457        26  F26            2.1470
    9  F9             6.4522        27  F27            2.1345
   10  F10            8.6355        28  F28            2.1239
   11  F11            10.641        29  F29            2.1164
   12  F12            10.984        30  F30            2.1139
   13  F13            4.5924        31  F31            1.0635
   14  F14            4.5807        32  F32            1.0605
   15  F15            4.5258        33  F33            1.0575
   16  F16            4.3984        34  F34            1.0545
   17  F17            4.2921        35  F35            1.0515
   18  F18            4.2733        36  F36            1.0494


TOTAL NONLINEARITY (BNT).......... = 0.63930E-01
INTRINSIC NONLINEARITY (BNI)...... = 0.45443E-03




****** NONLINEARITY MEASURES FOR CONFIDENCE INTERVALS


TOTAL NUMBER OF INTERVALS (NOINT)......................:    8
NUMBER OF INTERVALS FOR HEAD (NHI).....................:    6
NUMBER OF INTERVALS FOR HEAD DEPENDENT FLOWS (NQI).....:    0
NUMBER OF INTERVALS FOR PARAMETERS (NPI)...............:    2
INTERVAL TYPE (1=CONFIDENCE,2=PREDICTION)..............:    1
HEAD AND FLOW INTERVALS ON DIFFERENCES (0,1)=(NO,YES)..:    0

     INTERVAL VARIABLES COMPUTED WITH OPTIMUM PARAMETERS
   NO.  INTERVAL       GOPT        NO.  INTERVAL       GOPT
    1  G1             2.8565         5  G5             1.2704
    2  G2             11.996         6  G6             3.2028
    3  G3             4.5392         7    HK_1       0.38102
    4  G4             2.1408         8    HK_2       -2.3083

          RELIABILITY WEIGHTS FOR INTERVAL SAMPLE
   NO.   INTERVAL       W          NO.   INTERVAL       W
    1  G1             0.0000         5  G5             0.0000
    2  G2             0.0000         6  G6             0.0000
    3  G3             0.0000         7    HK_1         0.0000
    4  G4             0.0000         8    HK_2         0.0000

SENSITIVITIES FOR OPTIMUM PARAMETERS

PARAMETER   G1           G2           G3           G4           G5
----------  ------------ ------------ ------------ ------------ ------------
HK_1          -2.8442      -5.2981      -4.3706      -2.1397      -1.2703
HK_2        -0.12354E-01  -6.6975     -0.16862     -0.10612E-02 -0.13788E-03
```

```
PARAMETER   G6             HK_1         HK_2
----------  ------------ ------------ ------------
HK_1         -3.1694       1.0000       0.0000
HK_2        -0.33366E-01   0.0000       1.0000

CORRECTION FACTORS
    1  G1             45.638         5  G5             45.477
    2  G2             15.989         6  G6             45.875
    3  G3             46.966         7    HK_1         45.473
    4  G4             45.492         8    HK_2         10.668


*** INTERVAL NO.   1

                    PARAMETERS FOR SAMPLE NO.   1
   NO. NAME            B          NO. NAME            B
    1  HK_1        1.8283          2  HK_2       0.81801E-01

        DEPENDENT VARIABLES COMPUTED FOR SAMPLE NO.   1
   NO. OBSERVATION      FC          NO. OBSERVATION      FC
    1  F1             14.703        19  F19            2.1861
    2  F2             14.588        20  F20            2.1505
    3  F3             14.411        21  F21            2.1029
    4  F4             13.949        22  F22            2.0634
    5  F5             13.746        23  F23            2.0624
    6  F6             13.730        24  F24            2.0647
    7  F7             3.8336        25  F25            1.4234
    8  F8             4.0380        26  F26            1.4132
    9  F9             4.4340        27  F27            1.4029
   10  F10            8.3438        28  F28            1.3931
   11  F11            11.858        29  F29            1.3851
   12  F12            12.234        30  F30            1.3809
   13  F13            3.0475        31  F31           0.69998
   14  F14            3.0490        32  F32           0.69723
   15  F15            3.0115        33  F33           0.69439
   16  F16            2.8990        34  F34           0.69141
   17  F17            2.7843        35  F35           0.68844
   18  F18            2.7478        36  F36           0.68653


PREDICTED VALUE, GP=  2.2912

                    PARAMETERS FOR SAMPLE NO.   2
   NO. NAME            B          NO. NAME            B
    1  HK_1        1.1719          2  HK_2       0.12087

        DEPENDENT VARIABLES COMPUTED FOR SAMPLE NO.   2
   NO. OBSERVATION      FC          NO. OBSERVATION      FC
    1  F1             14.814        19  F19            3.3869
    2  F2             14.691        20  F20            3.3357
    3  F3             14.491        21  F21            3.2684
    4  F4             13.955        22  F22            3.2174
    5  F5             13.704        23  F23            3.2302
    6  F6             13.677        24  F24            3.2452
    7  F7             5.9774        25  F25            2.2118
    8  F8             6.2006        26  F26            2.1984
```

9	F9	6.6410	27	F27	2.1852
10	F10	9.1382	28	F28	2.1737
11	F11	11.427	29	F29	2.1654
12	F12	11.802	30	F30	2.1622
13	F13	4.7065	31	F31	1.0889
14	F14	4.6961	32	F32	1.0857
15	F15	4.6394	33	F33	1.0824
16	F16	4.5036	34	F34	1.0790
17	F17	4.3865	35	F35	1.0758
18	F18	4.3628	36	F36	1.0735

PREDICTED VALUE, GP= 3.5609

*** INTERVAL NO.   2

PARAMETERS FOR SAMPLE NO.   1

NO.	NAME	B	NO.	NAME	B
1	HK_1	1.4424	2	HK_2	0.11176

DEPENDENT VARIABLES COMPUTED FOR SAMPLE NO.   1

NO.	OBSERVATION	FC	NO.	OBSERVATION	FC
1	F1	13.805	19	F19	2.7591
2	F2	13.688	20	F20	2.7160
3	F3	13.502	21	F21	2.6592
4	F4	13.009	22	F22	2.6144
5	F5	12.784	23	F23	2.6205
6	F6	12.763	24	F24	2.6292
7	F7	4.8577	25	F25	1.7997
8	F8	5.0682	26	F26	1.7880
9	F9	5.4802	27	F27	1.7764
10	F10	8.2529	28	F28	1.7659
11	F11	10.778	29	F29	1.7579
12	F12	11.139	30	F30	1.7543
13	F13	3.8386	31	F31	0.88561
14	F14	3.8340	32	F32	0.88272
15	F15	3.7873	33	F33	0.87969
16	F16	3.6648	34	F34	0.87663
17	F17	3.5509	35	F35	0.87355
18	F18	3.5218	36	F36	0.87150

PREDICTED VALUE, GP= 11.333

PARAMETERS FOR SAMPLE NO.   2

NO.	NAME	B	NO.	NAME	B
1	HK_1	1.4855	2	HK_2	0.88468E-01

DEPENDENT VARIABLES COMPUTED FOR SAMPLE NO.   2

NO.	OBSERVATION	FC	NO.	OBSERVATION	FC
1	F1	15.379	19	F19	2.6848
2	F2	15.251	20	F20	2.6420
3	F3	15.050	21	F21	2.5850
4	F4	14.525	22	F22	2.5389
5	F5	14.291	23	F23	2.5411

```
    6  F6             14.271        24  F24           2.5467
    7  F7             4.7170        25  F25           1.7497
    8  F8             4.9454        26  F26           1.7377
    9  F9             5.3899        27  F27           1.7256
   10  F10            8.9545        28  F28           1.7146
   11  F11            12.180        29  F29           1.7057
   12  F12            12.583        30  F30           1.7014
   13  F13            3.7388        31  F31          0.86057
   14  F14            3.7377        32  F32          0.85756
   15  F15            3.6920        33  F33          0.85437
   16  F16            3.5631        34  F34          0.85108
   17  F17            3.4369        35  F35          0.84774
   18  F18            3.3999        36  F36          0.84557


PREDICTED VALUE, GP=  12.745


*** INTERVAL NO.   3

                    PARAMETERS FOR SAMPLE NO.   1
   NO. NAME              B         NO. NAME              B
    1  HK_1         1.8340          2  HK_2       0.81992E-01

        DEPENDENT VARIABLES COMPUTED FOR SAMPLE NO.   1
   NO. OBSERVATION      FC          NO. OBSERVATION      FC
    1  F1             14.664        19  F19           2.1794
    2  F2             14.549        20  F20           2.1439
    3  F3             14.372        21  F21           2.0964
    4  F4             13.912        22  F22           2.0570
    5  F5             13.709        23  F23           2.0559
    6  F6             13.693        24  F24           2.0582
    7  F7             3.8215        25  F25           1.4191
    8  F8             4.0253        26  F26           1.4089
    9  F9             4.4201        27  F27           1.3985
   10  F10            8.3208        28  F28           1.3888
   11  F11            11.827        29  F29           1.3807
   12  F12            12.201        30  F30           1.3765
   13  F13            3.0380        31  F31          0.69779
   14  F14            3.0395        32  F32          0.69504
   15  F15            3.0022        33  F33          0.69222
   16  F16            2.8900        34  F34          0.68930
   17  F17            2.7756        35  F35          0.68633
   18  F18            2.7391        36  F36          0.68441


PREDICTED VALUE, GP=  3.6750

                    PARAMETERS FOR SAMPLE NO.   2
   NO. NAME              B         NO. NAME              B
    1  HK_1         1.1683          2  HK_2       0.12058

        DEPENDENT VARIABLES COMPUTED FOR SAMPLE NO.   2
   NO. OBSERVATION      FC          NO. OBSERVATION      FC
    1  F1             14.855        19  F19           3.3974
    2  F2             14.731        20  F20           3.3460
```

```
    3  F3             14.531        21  F21            3.2785
    4  F4             13.993        22  F22            3.2273
    5  F5             13.741        23  F23            3.2402
    6  F6             13.715        24  F24            3.2552
    7  F7             5.9958        25  F25            2.2185
    8  F8             6.2196        26  F26            2.2051
    9  F9             6.6612        27  F27            2.1918
   10  F10            9.1641        28  F28            2.1804
   11  F11            11.458        29  F29            2.1721
   12  F12            11.834        30  F30            2.1690
   13  F13            4.7209        31  F31            1.0921
   14  F14            4.7106        32  F32            1.0890
   15  F15            4.6538        33  F33            1.0857
   16  F16            4.5176        34  F34            1.0824
   17  F17            4.4001        35  F35            1.0791
   18  F18            4.3763        36  F36            1.0769


PREDICTED VALUE, GP=  5.5928


*** INTERVAL NO.   4

                    PARAMETERS FOR SAMPLE NO.   1
   NO. NAME             B          NO. NAME            B
    1  HK_1        1.8277          2  HK_2       0.81782E-01

        DEPENDENT VARIABLES COMPUTED FOR SAMPLE NO.   1
   NO. OBSERVATION      FC          NO. OBSERVATION      FC
    1  F1             14.707        19  F19            2.1869
    2  F2             14.592        20  F20            2.1513
    3  F3             14.414        21  F21            2.1036
    4  F4             13.952        22  F22            2.0641
    5  F5             13.749        23  F23            2.0630
    6  F6             13.733        24  F24            2.0653
    7  F7             3.8348        25  F25            1.4240
    8  F8             4.0392        26  F26            1.4138
    9  F9             4.4352        27  F27            1.4033
   10  F10            8.3458        28  F28            1.3936
   11  F11            11.861        29  F29            1.3855
   12  F12            12.236        30  F30            1.3813
   13  F13            3.0485        31  F31           0.70019
   14  F14            3.0500        32  F32           0.69744
   15  F15            3.0125        33  F33           0.69462
   16  F16            2.9000        34  F34           0.69169
   17  F17            2.7852        35  F35           0.68871
   18  F18            2.7486        36  F36           0.68678


PREDICTED VALUE, GP=  1.7151

                    PARAMETERS FOR SAMPLE NO.   2
   NO. NAME             B          NO. NAME            B
    1  HK_1        1.1723          2  HK_2       0.12089

        DEPENDENT VARIABLES COMPUTED FOR SAMPLE NO.   2
```

```
   NO. OBSERVATION       FC          NO. OBSERVATION       FC
    1  F1             14.810          19  F19             3.3858
    2  F2             14.686          20  F20             3.3345
    3  F3             14.487          21  F21             3.2672
    4  F4             13.950          22  F22             3.2162
    5  F5             13.700          23  F23             3.2290
    6  F6             13.673          24  F24             3.2439
    7  F7             5.9751          25  F25             2.2109
    8  F8             6.1982          26  F26             2.1975
    9  F9             6.6386          27  F27             2.1843
   10  F10            9.1353          28  F28             2.1728
   11  F11            11.424          29  F29             2.1646
   12  F12            11.798          30  F30             2.1615
   13  F13            4.7047          31  F31             1.0884
   14  F14            4.6944          32  F32             1.0853
   15  F15            4.6378          33  F33             1.0820
   16  F16            4.5021          34  F34             1.0787
   17  F17            4.3849          35  F35             1.0754
   18  F18            4.3612          36  F36             1.0732


PREDICTED VALUE, GP=  2.6723


*** INTERVAL NO.   5

                    PARAMETERS FOR SAMPLE NO.   1
   NO. NAME             B          NO. NAME             B
    1  HK_1        1.8276           2  HK_2       0.81780E-01

        DEPENDENT VARIABLES COMPUTED FOR SAMPLE NO.   1
   NO. OBSERVATION       FC          NO. OBSERVATION       FC
    1  F1             14.708          19  F19             2.1869
    2  F2             14.593          20  F20             2.1512
    3  F3             14.415          21  F21             2.1036
    4  F4             13.953          22  F22             2.0640
    5  F5             13.750          23  F23             2.0630
    6  F6             13.734          24  F24             2.0654
    7  F7             3.8349          25  F25             1.4239
    8  F8             4.0393          26  F26             1.4137
    9  F9             4.4354          27  F27             1.4033
   10  F10            8.3461          28  F28             1.3936
   11  F11            11.861          29  F29             1.3855
   12  F12            12.237          30  F30             1.3814
   13  F13            3.0485          31  F31            0.70014
   14  F14            3.0500          32  F32            0.69745
   15  F15            3.0126          33  F33            0.69463
   16  F16            2.9000          34  F34            0.69170
   17  F17            2.7852          35  F35            0.68874
   18  F18            2.7486          36  F36            0.68681


PREDICTED VALUE, GP=  1.0175

                    PARAMETERS FOR SAMPLE NO.   2
   NO. NAME             B          NO. NAME             B
```

NO.	NAME	B	NO.	NAME	B
1	HK_1	1.1724	2	HK_2	0.12090

DEPENDENT VARIABLES COMPUTED FOR SAMPLE NO. 2

NO.	OBSERVATION	FC	NO.	OBSERVATION	FC
1	F1	14.809	19	F19	3.3856
2	F2	14.686	20	F20	3.3344
3	F3	14.486	21	F21	3.2671
4	F4	13.950	22	F22	3.2161
5	F5	13.699	23	F23	3.2289
6	F6	13.673	24	F24	3.2439
7	F7	5.9750	25	F25	2.2109
8	F8	6.1981	26	F26	2.1975
9	F9	6.6384	27	F27	2.1843
10	F10	9.1351	28	F28	2.1728
11	F11	11.423	29	F29	2.1645
12	F12	11.798	30	F30	2.1614
13	F13	4.7046	31	F31	1.0884
14	F14	4.6942	32	F32	1.0852
15	F15	4.6376	33	F33	1.0820
16	F16	4.5019	34	F34	1.0786
17	F17	4.3848	35	F35	1.0753
18	F18	4.3611	36	F36	1.0731

PREDICTED VALUE, GP= 1.5862

*** INTERVAL NO. 6

PARAMETERS FOR SAMPLE NO. 1

NO.	NAME	B	NO.	NAME	B
1	HK_1	1.8294	2	HK_2	0.81832E-01

DEPENDENT VARIABLES COMPUTED FOR SAMPLE NO. 1

NO.	OBSERVATION	FC	NO.	OBSERVATION	FC
1	F1	14.696	19	F19	2.1848
2	F2	14.581	20	F20	2.1493
3	F3	14.404	21	F21	2.1017
4	F4	13.942	22	F22	2.0622
5	F5	13.739	23	F23	2.0611
6	F6	13.723	24	F24	2.0634
7	F7	3.8312	25	F25	1.4227
8	F8	4.0354	26	F26	1.4125
9	F9	4.4311	27	F27	1.4021
10	F10	8.3394	28	F28	1.3923
11	F11	11.852	29	F29	1.3842
12	F12	12.228	30	F30	1.3800
13	F13	3.0456	31	F31	0.69955
14	F14	3.0471	32	F32	0.69680
15	F15	3.0097	33	F33	0.69397
16	F16	2.8973	34	F34	0.69105
17	F17	2.7826	35	F35	0.68807
18	F18	2.7460	36	F36	0.68615

PREDICTED VALUE, GP= 2.5731

```
                   PARAMETERS FOR SAMPLE NO.   2
   NO. NAME            B         NO. NAME            B
    1  HK_1        1.1713         2  HK_2       0.12082

        DEPENDENT VARIABLES COMPUTED FOR SAMPLE NO.   2
   NO. OBSERVATION      FC          NO. OBSERVATION      FC
    1  F1             14.821        19  F19            3.3889
    2  F2             14.698        20  F20            3.3376
    3  F3             14.498        21  F21            3.2703
    4  F4             13.961        22  F22            3.2192
    5  F5             13.710        23  F23            3.2320
    6  F6             13.684        24  F24            3.2470
    7  F7             5.9806        25  F25            2.2130
    8  F8             6.2038        26  F26            2.1996
    9  F9             6.6445        27  F27            2.1863
   10  F10            9.1427        28  F28            2.1748
   11  F11            11.432        29  F29            2.1666
   12  F12            11.807        30  F30            2.1635
   13  F13            4.7090        31  F31            1.0894
   14  F14            4.6987        32  F32            1.0863
   15  F15            4.6421        33  F33            1.0830
   16  F16            4.5062        34  F34            1.0797
   17  F17            4.3890        35  F35            1.0764
   18  F18            4.3653        36  F36            1.0741


PREDICTED VALUE, GP=  3.9844


*** INTERVAL NO.   7

                   PARAMETERS FOR SAMPLE NO.   1
   NO. NAME            B         NO. NAME            B
    1  HK_1        1.1724         2  HK_2       0.12090

        DEPENDENT VARIABLES COMPUTED FOR SAMPLE NO.   1
   NO. OBSERVATION      FC          NO. OBSERVATION      FC
    1  F1             14.809        19  F19            3.3856
    2  F2             14.686        20  F20            3.3343
    3  F3             14.486        21  F21            3.2671
    4  F4             13.950        22  F22            3.2161
    5  F5             13.699        23  F23            3.2289
    6  F6             13.673        24  F24            3.2438
    7  F7             5.9749        25  F25            2.2109
    8  F8             6.1981        26  F26            2.1975
    9  F9             6.6384        27  F27            2.1842
   10  F10            9.1350        28  F28            2.1728
   11  F11            11.423        29  F29            2.1645
   12  F12            11.798        30  F30            2.1614
   13  F13            4.7046        31  F31            1.0884
   14  F14            4.6942        32  F32            1.0852
   15  F15            4.6376        33  F33            1.0819
   16  F16            4.5018        34  F34            1.0786
   17  F17            4.3847        35  F35            1.0753
   18  F18            4.3610        36  F36            1.0731
```

```
PREDICTED VALUE, GP= 0.15904

                    PARAMETERS FOR SAMPLE NO.   2
   NO. NAME             B         NO. NAME             B
    1  HK_1        1.8276          2  HK_2       0.81780E-01

        DEPENDENT VARIABLES COMPUTED FOR SAMPLE NO.   2
   NO. OBSERVATION       FC          NO. OBSERVATION      FC
    1  F1              14.708         19  F19            2.1871
    2  F2              14.593         20  F20            2.1515
    3  F3              14.415         21  F21            2.1038
    4  F4              13.953         22  F22            2.0642
    5  F5              13.750         23  F23            2.0631
    6  F6              13.734         24  F24            2.0655
    7  F7              3.8351         25  F25            1.4241
    8  F8              4.0396         26  F26            1.4138
    9  F9              4.4358         27  F27            1.4034
   10  F10             8.3465         28  F28            1.3937
   11  F11             11.861         29  F29            1.3856
   12  F12             12.237         30  F30            1.3814
   13  F13             3.0489         31  F31           0.70022
   14  F14             3.0503         32  F32           0.69747
   15  F15             3.0128         33  F33           0.69464
   16  F16             2.9003         34  F34           0.69168
   17  F17             2.7855         35  F35           0.68875
   18  F18             2.7488         36  F36           0.68681


PREDICTED VALUE, GP= 0.60300


*** INTERVAL NO.   8

                    PARAMETERS FOR SAMPLE NO.   1
   NO. NAME             B         NO. NAME             B
    1  HK_1        1.5854          2  HK_2       0.87532E-01

        DEPENDENT VARIABLES COMPUTED FOR SAMPLE NO.   1
   NO. OBSERVATION       FC          NO. OBSERVATION      FC
    1  F1              15.025         19  F19            2.5172
    2  F2              14.901         20  F20            2.4770
    3  F3              14.709         21  F21            2.4232
    4  F4              14.206         22  F22            2.3795
    5  F5              13.982         23  F23            2.3807
    6  F6              13.963         24  F24            2.3854
    7  F7              4.4208         25  F25            1.6401
    8  F8              4.6408         26  F26            1.6287
    9  F9              5.0687         27  F27            1.6173
   10  F10             8.6867         28  F28            1.6067
   11  F11             11.955         29  F29            1.5983
   12  F12             12.347         30  F30            1.5941
   13  F13             3.5065         31  F31           0.80668
   14  F14             3.5064         32  F32           0.80374
   15  F15             3.4637         33  F33           0.80067
```

```
   16  F16            3.3403        34  F34           0.79741
   17  F17            3.2183        35  F35           0.79416
   18  F18            3.1816        36  F36           0.79220


PREDICTED VALUE, GP= -2.4358

                    PARAMETERS FOR SAMPLE NO.   2
   NO. NAME             B         NO. NAME            B
    1  HK_1         1.3514         2  HK_2        0.11295

        DEPENDENT VARIABLES COMPUTED FOR SAMPLE NO.   2
   NO. OBSERVATION       FC         NO. OBSERVATION      FC
    1  F1             14.191        19  F19            2.9427
    2  F2             14.070        20  F20            2.8971
    3  F3             13.878        21  F21            2.8370
    4  F4             13.367        22  F22            2.7901
    5  F5             13.133        23  F23            2.7977
    6  F6             13.110        24  F24            2.8079
    7  F7             5.1838        25  F25            1.9200
    8  F8             5.4004        26  F26            1.9077
    9  F9             5.8252        27  F27            1.8955
   10  F10            8.5518        28  F28            1.8847
   11  F11            11.039        29  F29            1.8765
   12  F12            11.408        30  F30            1.8729
   13  F13            4.0926        31  F31           0.94490
   14  F14            4.0866        32  F32           0.94193
   15  F15            4.0371        33  F33           0.93885
   16  F16            3.9096        34  F34           0.93561
   17  F17            3.7931        35  F35           0.93241
   18  F18            3.7647        36  F36           0.93026


PREDICTED VALUE, GP= -2.1808

               COMBINED INTRINSIC NONLINEARITY
     INTERVAL NO.       BMI           INTERVAL NO.       BMI
    1  G1            0.91136E-01     5  G5            0.92165E-01
    2  G2            0.13976E-04     6  G6            0.89142E-01
    3  G3            0.80532E-01     7    HK_1        0.37137E-01
    4  G4            0.92049E-01     8    HK_2        0.22188E-01

     COMBINED INTRINSIC NONLINEARITY AS IF F WERE LINEAR
     INTERVAL NO.      BMF0           INTERVAL NO.      BMF0
    1  G1            0.12232E-01     5  G5            0.12491E-01
    2  G2            0.37404E-02     6  G6            0.11832E-01
    3  G3            0.99148E-02     7    HK_1        0.58584E-12
    4  G4            0.12468E-01     8    HK_2        0.59462E-10

     COMBINED INTRINSIC NONLINEARITY AS IF G WERE LINEAR
     INTERVAL NO.      BMG0           INTERVAL NO.      BMG0
    1  G1            0.36826E-01     5  G5            0.37051E-01
    2  G2            0.40559E-02     6  G6            0.36261E-01
    3  G3            0.34126E-01     7    HK_1        0.37137E-01
    4  G4            0.37003E-01     8    HK_2        0.22186E-01
```

```
       COMBINED INTRINSIC NONLINEARITY - MAX. SUM
 INTERVAL NO.      BMIMAX        INTERVAL NO.      BMIMAX
1  G1           0.11560         5  G5           0.11715
2  G2           0.80979E-02     6  G6           0.11280
3  G3           0.10036         7    HK_1       0.37137E-01
4  G4           0.11699         8    HK_2       0.22188E-01
```

RESAN2-2k Input Files

Modified _rs file (example._rs):

```
    2   36   36    0    0    0 1000     10059   1.2028920299866620D-02
.01    0    0    1    1
HK_1       HK_2
   1.5984446317565970D-02  -9.3897459008995630D-02
   1.2171445371320360D+00
 3.70299257E-02 3.80506031E-02 3.86905819E-02 3.78140099E-02 3.70474569E-02
3.65929864E-02 3.94278727E-02 3.87343839E-02 3.81299071E-02 3.72347161E-02
3.73285078E-02 3.69736925E-02 3.95077951E-02 3.92752253E-02 4.01894972E-02
4.05620262E-02
 3.95699181E-02 3.98577228E-02 4.27163243E-02 4.33942601E-02 4.35817763E-02
4.33828235E-02 4.27807719E-02 4.29287367E-02 4.85740304E-02 4.83402126E-02
4.82680798E-02 4.84433360E-02 4.81047295E-02 4.74082753E-02 8.08135197E-02
7.11964741E-02
 7.12072998E-02 7.03493059E-02 6.85945898E-02 7.03145191E-02
-7.04659367E+00-1.50004828E+00
-7.06339741E+00-1.48310077E+00
-7.10597181E+00-1.43996620E+00
-7.27100706E+00-1.27518404E+00
-7.40044165E+00-1.14634621E+00
-7.43134212E+00-1.11610472E+00
-6.84805489E+00-8.78273845E-02
-6.79571819E+00-1.33685842E-01
-6.68890238E+00-2.35920116E-01
-6.33737326E+00-5.86289763E-01
-6.05908632E+00-8.68575454E-01
-5.98694611E+00-9.47160363E-01
-5.29238510E+00-6.16868287E-02
-5.25664139E+00-5.80927134E-02
-5.23037148E+00-3.93029377E-02
-5.26140881E+00 1.06110601E-02
-5.35310459E+00 5.58182150E-02
-5.40344524E+00 6.14485182E-02
-3.86938190E+00-2.47615427E-02
-3.83271551E+00-1.77744813E-02
-3.78756404E+00-8.75341985E-03
-3.77330446E+00 2.30506901E-03
-3.84462976E+00 1.46126971E-02
-3.90307307E+00 2.25643124E-02
-2.55457449E+00-8.90955608E-03
-2.54985857E+00-6.12230739E-03
-2.54753423E+00-2.92208139E-03
-2.54963517E+00 7.52098567E-04
-2.55824447E+00 4.94222483E-03
-2.56872201E+00 8.00079107E-03
-1.26404727E+00-2.83111562E-03
-1.26398706E+00-1.93543814E-03
-1.26431274E+00-9.20786173E-04
-1.26529419E+00 2.35229818E-04
-1.26728976E+00 1.55798520E-03
```

```
-1.26906574E+00 2.53848336E-03
  0.66151  0.57163  0.57791  0.65444  0.70896  0.78005  0.59267  0.58384
  0.54952  0.43816  0.37298  0.38888  0.47908  0.43970  0.40578  0.41702
  0.43077  0.42120  0.32116  0.30408  0.29091  0.27985  0.28804  0.26147
  0.12901  0.15028  0.15210  0.16090  0.16435  0.17098 -.048154 -.018498
-.0080944 .0071884  .033326  .055387
729.28    667.57    615.68    586.33    557.59    534.25    584.85    598.77
591.88    569.46    549.34    541.11    477.64    485.80    477.81    474.03
490.18    486.31    326.73    325.31    323.54    332.79    344.61    339.91
208.67    221.75    226.29    225.34    240.21    245.61    68.870    101.52
103.49    110.91    118.31    98.075
667.57    690.68    654.63    620.72    586.71    561.51    589.59    601.63
595.99    577.41    559.76    549.42    478.84    483.95    474.92    467.99
483.29    478.43    321.55    318.49    315.94    322.14    333.98    331.21
214.14    224.01    227.44    222.64    233.67    236.83    72.997    106.27
108.19    114.37    119.57    96.373
615.68    654.63    668.02    651.43    618.29    587.79    577.61    590.09
588.78    576.27    558.71    553.40    467.96    471.16    460.22    452.06
465.32    460.42    308.79    303.50    300.50    304.75    314.61    312.42
202.47    210.94    215.14    210.02    220.51    221.90    72.489    104.27
105.26    110.19    114.24    92.439
586.33    620.72    651.43    699.35    686.13    649.67    562.03    574.93
574.79    566.42    550.59    553.37    452.96    452.53    440.17    430.63
441.05    439.34    293.55    290.00    287.19    289.52    297.87    293.66
193.48    201.20    204.83    198.65    206.20    206.93    69.506    99.734
99.477    103.72    107.11    87.286
557.59    586.71    618.29    686.13    728.59    707.08    543.25    559.94
561.06    555.06    538.05    538.75    443.24    442.05    428.49    417.27
424.38    421.98    288.46    285.79    281.38    283.14    288.82    282.64
192.57    200.60    204.67    197.13    203.52    203.09    69.115    99.001
98.459    104.13    107.79    87.132
534.25    561.51    587.79    649.67    707.08    746.80    525.38    543.55
547.06    545.23    529.14    527.88    437.16    436.68    423.31    411.63
418.82    415.31    289.42    286.38    280.51    281.62    286.86    279.57
191.49    200.05    202.37    193.86    198.61    197.71    65.800    95.801
95.834    100.16    103.22    82.084
584.85    589.59    577.61    562.03    543.25    525.38    643.27    632.46
614.20    600.57    577.59    562.10    507.35    507.86    491.01    477.72
483.99    476.30    331.83    326.31    325.01    329.89    338.91    334.53
216.78    225.84    232.23    227.82    238.01    242.82    71.272    107.29
108.79    114.71    123.51    104.54
598.77    601.63    590.09    574.93    559.94    543.55    632.46    666.51
657.18    644.11    618.41    599.20    524.83    525.59    509.64    499.58
510.39    501.63    346.45    338.31    333.05    337.30    349.23    345.68
221.67    230.89    237.21    232.60    242.72    247.01    73.206    109.94
110.31    115.26    124.50    105.37
591.88    595.99    588.78    574.79    561.06    547.06    614.20    657.18
687.81    686.21    659.29    637.88    537.68    541.81    526.18    517.05
531.07    522.43    362.45    354.14    347.07    349.82    361.59    358.58
232.67    240.53    246.07    242.48    250.68    254.24    78.717    114.03
114.30    119.04    127.26    106.76
569.46    577.41    576.27    566.42    555.06    545.23    600.57    644.11
686.21    721.28    701.42    676.61    554.47    562.74    551.08    543.76
558.91    552.38    379.87    372.12    363.43    363.69    375.96    372.75
242.19    249.08    254.99    254.22    261.06    263.36    84.298    120.19
120.19    124.31    131.48    110.02
```

```
549.34    559.76    558.71    550.59    538.05    529.14    577.59    618.41
659.29    701.42    717.66    702.17    553.51    566.83    558.53    551.51
566.99    560.49    382.08    375.64    366.97    367.21    378.36    374.44
245.30    252.08    257.29    255.75    261.15    262.41    88.611    121.30
120.89    124.28    131.52    112.32
541.11    549.42    553.40    553.37    538.75    527.88    562.10    599.20
637.88    676.61    702.17    731.50    549.20    564.90    560.42    557.96
574.98    566.97    382.48    378.58    371.67    371.59    381.56    374.77
248.91    256.43    261.51    258.12    261.74    261.68    91.934    123.40
123.28    127.11    134.16    113.32
477.64    478.84    467.96    452.96    443.24    437.16    507.35    524.83
537.68    554.47    553.51    549.20    640.67    626.22    591.51    563.61
555.08    535.82    453.45    447.14    440.73    438.31    441.10    423.05
295.30    305.66    312.49    311.97    316.94    320.88    105.64    144.94
148.93    153.49    165.66    142.97
485.80    483.95    471.16    452.53    442.05    436.68    507.86    525.59
541.81    562.74    566.83    564.90    626.22    648.28    618.24    588.02
580.79    558.88    460.96    454.52    448.96    446.67    449.88    432.98
303.50    313.53    320.28    319.66    325.02    328.34    111.31    149.19
151.82    155.30    165.42    142.83
477.81    474.92    460.22    440.17    428.49    423.31    491.01    509.64
526.18    551.08    558.53    560.42    591.51    618.24    619.12    597.36
588.69    566.62    452.11    449.96    444.33    443.98    453.68    439.92
300.25    308.91    315.03    313.82    319.76    324.34    108.06    145.56
148.64    152.55    161.93    139.60
474.03    467.99    452.06    430.63    417.27    411.63    477.72    499.58
517.05    543.76    551.51    557.96    563.61    588.02    597.36    607.80
599.81    577.83    445.39    443.84    438.99    440.63    456.72    446.56
296.70    305.68    312.57    310.46    316.16    321.64    106.61    144.37
146.88    150.81    159.16    137.11
490.18    483.29    465.32    441.05    424.38    418.82    483.99    510.39
531.07    558.91    566.99    574.98    555.08    580.79    588.69    599.81
638.66    617.67    438.33    438.82    437.99    440.62    458.55    449.80
292.93    303.57    309.94    308.99    313.48    315.66    105.79    143.49
145.72    148.31    155.68    131.83
486.31    478.43    460.42    439.34    421.98    415.31    476.30    501.63
522.43    552.38    560.49    566.97    535.82    558.88    566.62    577.83
617.67    629.47    428.62    428.57    430.59    437.01    456.18    447.76
288.83    299.85    307.41    307.76    311.41    313.08    105.58    143.63
146.56    150.52    156.68    132.63
326.73    321.55    308.79    293.55    288.46    289.42    331.83    346.45
362.45    379.87    382.08    382.48    453.45    460.96    452.11    445.39
438.33    428.62    548.04    522.35    500.04    484.78    471.74    454.53
379.15    390.62    392.18    383.88    378.94    379.17    137.98    179.29
184.21    190.21    201.84    174.92
325.31    318.49    303.50    290.00    285.79    286.38    326.31    338.31
354.14    372.12    375.64    378.58    447.14    454.52    449.96    443.84
438.82    428.57    522.35    531.05    515.27    499.46    486.02    465.12
377.99    389.36    391.95    384.08    380.66    379.82    139.14    177.36
182.01    187.59    198.06    171.04
323.54    315.94    300.50    287.19    281.38    280.51    325.01    333.05
347.07    363.43    366.97    371.67    440.73    448.96    444.33    438.99
437.99    430.59    500.04    515.27    526.49    517.52    502.76    477.30
381.07    395.46    399.39    394.44    392.14    390.23    145.44    183.03
188.11    193.42    204.07    177.28
332.79    322.14    304.75    289.52    283.14    281.62    329.89    337.30
```

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349.82    363.69    367.21    371.59    438.31    446.67    443.98    440.63
440.62    437.01    484.78    499.46    517.52    531.33    522.51    497.03
371.13    389.59    396.26    394.86    398.34    402.69    143.86    182.63
188.43    193.53    205.17    179.10
344.61    333.98    314.61    297.87    288.82    286.86    338.91    349.23
361.59    375.96    378.36    381.56    441.10    449.88    453.68    456.72
458.55    456.18    471.74    486.02    502.76    522.51    546.39    526.83
360.58    381.27    390.93    393.82    401.50    409.36    141.58    181.57
187.82    192.83    203.97    177.63
339.91    331.21    312.42    293.66    282.64    279.57    334.53    345.68
358.58    372.75    374.44    374.77    423.05    432.98    439.92    446.56
449.80    447.76    454.53    465.12    477.30    497.03    526.83    542.63
346.27    367.35    378.05    383.54    394.49    404.22    134.42    174.09
180.86    186.84    198.00    171.15
208.67    214.14    202.47    193.48    192.57    191.49    216.78    221.67
232.67    242.19    245.30    248.91    295.30    303.50    300.25    296.70
292.93    288.83    379.15    377.99    381.07    371.13    360.58    346.27
423.83    409.60    393.71    366.08    338.05    324.23    170.89    210.96
207.57    202.51    198.52    162.88
221.75    224.01    210.94    201.20    200.60    200.05    225.84    230.89
240.53    249.08    252.08    256.43    305.66    313.53    308.91    305.68
303.57    299.85    390.62    389.36    395.46    389.59    381.27    367.35
409.60    427.94    417.14    392.68    365.92    350.74    173.99    216.39
216.19    214.18    214.04    179.48
226.29    227.44    215.14    204.83    204.67    202.37    232.23    237.21
246.07    254.99    257.29    261.51    312.49    320.28    315.03    312.57
309.94    307.41    392.18    391.95    399.39    396.26    390.93    378.05
393.71    417.14    429.22    411.90    388.36    372.38    172.20    216.59
217.49    217.96    221.48    188.33
225.34    222.64    210.02    198.65    197.13    193.86    227.82    232.60
242.48    254.22    255.75    258.12    311.97    319.66    313.82    310.46
308.99    307.76    383.88    384.08    394.44    394.86    393.82    383.54
366.08    392.68    411.90    426.12    411.10    395.28    165.65    211.41
215.82    218.80    226.66    197.82
240.21    233.67    220.51    206.20    203.52    198.61    238.01    242.72
250.68    261.06    261.15    261.74    316.94    325.02    319.76    316.16
313.48    311.41    378.94    380.66    392.14    398.34    401.50    394.49
338.05    365.92    388.36    411.10    432.14    425.39    160.29    207.36
214.39    219.04    231.88    204.96
245.61    236.83    221.90    206.93    203.09    197.71    242.82    247.01
254.24    263.36    262.41    261.68    320.88    328.34    324.34    321.64
315.66    313.08    379.17    379.82    390.23    402.69    409.36    404.22
324.23    350.74    372.38    395.28    425.39    444.93    153.77    201.63
210.36    217.26    232.57    206.41
68.870    72.997    72.489    69.506    69.115    65.800    71.272    73.206
78.717    84.298    88.611    91.934    105.64    111.31    108.06    106.61
105.79    105.58    137.98    139.14    145.44    143.86    141.58    134.42
170.89    173.99    172.20    165.65    160.29    153.77    153.12    155.86
140.83    128.13    111.47    93.066
101.52    106.27    104.27    99.734    99.001    95.801    107.29    109.94
114.03    120.19    121.30    123.40    144.94    149.19    145.56    144.37
143.49    143.63    179.29    177.36    183.03    182.63    181.57    174.09
210.96    216.39    216.59    211.41    207.36    201.63    155.86    197.28
185.59    173.70    156.95    128.51
103.49    108.19    105.26    99.477    98.459    95.834    108.79    110.31
114.30    120.19    120.89    123.28    148.93    151.82    148.64    146.88
```

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145.72    146.56    184.21    182.01    188.11    188.43    187.82    180.86
207.57    216.19    217.49    215.82    214.39    210.36    140.83    185.59
197.22    190.73    175.32    147.00
110.91    114.37    110.19    103.72    104.13    100.16    114.71    115.26
119.04    124.31    124.28    127.11    153.49    155.30    152.55    150.81
148.31    150.52    190.21    187.59    193.42    193.53    192.83    186.84
202.51    214.18    217.96    218.80    219.04    217.26    128.13    173.70
190.73    202.06    192.15    162.93
118.31    119.57    114.24    107.11    107.79    103.22    123.51    124.50
127.26    131.48    131.52    134.16    165.66    165.42    161.93    159.16
155.68    156.68    201.84    198.06    204.07    205.17    203.97    198.00
198.52    214.04    221.48    226.66    231.88    232.57    111.47    156.95
175.32    192.15    212.53    188.12
98.075    96.373    92.439    87.286    87.132    82.084    104.54    105.37
106.76    110.02    112.32    113.32    142.97    142.83    139.60    137.11
131.83    132.63    174.92    171.04    177.28    179.10    177.63    171.15
162.88    179.48    188.33    197.82    204.96    206.41    93.066    128.51
147.00    162.93    188.12    202.26
```

_ws file (example._ws):

```
  0.5387840       0.1222136E-01     1  F1
  0.5489494       0.1343849E-01     1  F2
  0.5506946       0.2424740E-01     1  F3
  0.5189314       0.5548934E-02     1  F4
  0.4998959      -0.1790851E-01     1  F5
  0.4930008      -0.1838977E-01     1  F6
  0.1887295       0.3246087E-01     1  F7
  0.1939302       0.2414436E-01     1  F8
  0.2072599       0.1923179E-01     1  F9
  0.3195286       0.9253923E-02     1  F10
  0.4269593      -0.1335947E-01     1  F11
  0.4369872      -0.1733579E-01     1  F12
  0.1496757      -0.3496893E-02     1  F13
  0.1486864      -0.1404292E-02     1  F14
  0.1502898      -0.8822737E-02     1  F15
  0.1465700      -0.1068726E-01     1  F16
  0.1382196      -0.2890517E-02     1  F17
  0.1379032       0.9968983E-02     1  F18
  0.1162644      -0.1502673E-01     1  F19
  0.1162447      -0.3336162E-01     1  F20
  0.1142654      -0.3756152E-01     1  F21
  0.1117733      -0.2674299E-01     1  F22
  0.1103901      -0.3252914E-01     1  F23
  0.1110804      -0.2264722E-01     1  F24
  0.8620078E-01  -0.1139677E-01     1  F25
  0.8520906E-01  -0.4964315E-02     1  F26
  0.8450945E-01   0.1407734E-02     1  F27
  0.8429423E-01  -0.9691494E-02     1  F28
  0.8329535E-01  -0.1517311E-02     1  F29
  0.8189733E-01  -0.8414512E-02     1  F30
  0.7055598E-01   0.5408723E-02     1  F31
  0.6194711E-01   0.3843991E-01     1  F32
  0.6173658E-01   0.2513633E-01     1  F33
```

```
0.6075818E-01   0.4265530E-01     1  F34
0.5902952E-01   0.1505264E-01     1  F35
0.6035101E-01   0.1525764E-02     1  F36
```

RESAN2-2k Output Files

#nr file (example.#nr):

```
                                  RESAN2-2k

                       MODFLOW-2000 POST-PROCESSING PROGRAM
                TO PERFORM ANALYSIS OF NON-LINEARITY AND RESIDUALS
                            Version 1.0.0 25/06/2003

 WEIGHTED RESIDUALS WILL BE READ FROM FILE Example._ws


 NUMBER OF ESTIMATED PARAMETERS.............      2
 NUMBER OF OBSERVATIONS ....................     36
 NUMBER OF HEADS ...........................     36
 NUMBER OF OBSERVATIONS OTHER THAN HEADS ....     0
 NUMBER OF PRIOR EQUATIONS..................      0
 NUMBER OF PRIOR WITH FULL WEIGHT MATRIX.....     0
 NUMBER OF SETS OF RANDOM DEVIATES ..........   1000
 NUMBER FOR RANDOM NUMBER GENERATOR .........      -10059
 CALCULATED ERROR VARIANCE .................  0.120289E-01
 THEORETICAL ERROR VARIANCE ................  0.100000E-01
 PRINT (I-R) MATRIX.........................      0
 PRINT SIMULATED RESIDUALS..................      0
 READ MEAN TRUE ERRORS......................      1
 READ OBSERVATION ERROR COVARIANCE MATRIX....     1


 COVARIANCE MATRIX FOR ESTIMATED PARAMETERS

             HK_1         HK_2
 ....................................
 HK_1        1.59844E-02 -9.38975E-02
 HK_2       -9.38975E-02   1.2171

              RELIABILITY WEIGHTS FOR SAMPLE INFORMATION
        OBSERVATION                       OBSERVATION
  OBS#     NAME        W**.5       OBS#      NAME        W**.5
    1   F1           0.37030E-01    19   F19           0.42716E-01
    2   F2           0.38051E-01    20   F20           0.43394E-01
    3   F3           0.38691E-01    21   F21           0.43582E-01
    4   F4           0.37814E-01    22   F22           0.43383E-01
    5   F5           0.37047E-01    23   F23           0.42781E-01
    6   F6           0.36593E-01    24   F24           0.42929E-01
    7   F7           0.39428E-01    25   F25           0.48574E-01
    8   F8           0.38734E-01    26   F26           0.48340E-01
    9   F9           0.38130E-01    27   F27           0.48268E-01
   10   F10          0.37235E-01    28   F28           0.48443E-01
   11   F11          0.37329E-01    29   F29           0.48105E-01
   12   F12          0.36974E-01    30   F30           0.47408E-01
   13   F13          0.39508E-01    31   F31           0.80814E-01
   14   F14          0.39275E-01    32   F32           0.71196E-01
```

```
   15  F15          0.40189E-01    33  F33          0.71207E-01
   16  F16          0.40562E-01    34  F34          0.70349E-01
   17  F17          0.39570E-01    35  F35          0.68595E-01
   18  F18          0.39858E-01    36  F36          0.70315E-01

SENSITIVITIES FOR OPTIMUM PARAMETERS

PARAMETER   F1           F2           F3           F4           F5
----------  ------------ ------------ ------------ ------------ ------------
HK_1         -7.0466      -7.0634      -7.1060      -7.2710      -7.4004
HK_2         -1.5000      -1.4831      -1.4400      -1.2752      -1.1463

PARAMETER   F6           F7           F8           F9           F10
----------  ------------ ------------ ------------ ------------ ------------
HK_1         -7.4313      -6.8481      -6.7957      -6.6889      -6.3374
HK_2         -1.1161     -0.87827E-01 -0.13369     -0.23592     -0.58629

PARAMETER   F11          F12          F13          F14          F15
----------  ------------ ------------ ------------ ------------ ------------
HK_1         -6.0591      -5.9869      -5.2924      -5.2566      -5.2304
HK_2        -0.86858     -0.94716     -0.61687E-01 -0.58093E-01 -0.39303E-01

PARAMETER   F16          F17          F18          F19          F20
----------  ------------ ------------ ------------ ------------ ------------
HK_1         -5.2614      -5.3531      -5.4034      -3.8694      -3.8327
HK_2         0.10611E-01  0.55818E-01  0.61449E-01 -0.24762E-01 -0.17774E-01

PARAMETER   F21          F22          F23          F24          F25
----------  ------------ ------------ ------------ ------------ ------------
HK_1         -3.7876      -3.7733      -3.8446      -3.9031      -2.5546
HK_2        -0.87534E-02  0.23051E-02  0.14613E-01  0.22564E-01 -0.89096E-02

PARAMETER   F26          F27          F28          F29          F30
----------  ------------ ------------ ------------ ------------ ------------
HK_1         -2.5499      -2.5475      -2.5496      -2.5582      -2.5687
HK_2        -0.61223E-02 -0.29221E-02  0.75210E-03  0.49422E-02  0.80008E-02

PARAMETER   F31          F32          F33          F34          F35
----------  ------------ ------------ ------------ ------------ ------------
HK_1         -1.2640      -1.2640      -1.2643      -1.2653      -1.2673
HK_2        -0.28311E-02 -0.19354E-02 -0.92079E-03  0.23523E-03  0.15580E-02

PARAMETER   F36
----------  ------------
HK_1         -1.2691
HK_2         0.25385E-02

MEAN WEIGHTED RESIDUAL (EM) --------- = -.50018E-03
SLOPE OF WEIGHTED RESIDUAL PLOT (SLP) = 0.35753E-02
INTRINSIC NONLINEARITY MEASURE (QINT) = 0.19544E-03 (SHOULD BE <<0.14039E-01)

         ORDERED, WEIGHTED RESIDUALS
          OBSERVATION
    NO.      NAME            E          FRQ. (%)
      1   F21            -.37562E-01    1.3889
      2   F20            -.33362E-01    4.1667
```

3	F23	-.32529E-01	6.9444
4	F22	-.26743E-01	9.7222
5	F24	-.22647E-01	12.500
6	F6	-.18390E-01	15.278
7	F5	-.17909E-01	18.056
8	F12	-.17336E-01	20.833
9	F19	-.15027E-01	23.611
10	F11	-.13359E-01	26.389
11	F25	-.11397E-01	29.167
12	F16	-.10687E-01	31.944
13	F28	-.96915E-02	34.722
14	F15	-.88227E-02	37.500
15	F30	-.84145E-02	40.278
16	F26	-.49643E-02	43.056
17	F13	-.34969E-02	45.833
18	F17	-.28905E-02	48.611
19	F29	-.15173E-02	51.389
20	F14	-.14043E-02	54.167
21	F27	0.14077E-02	56.944
22	F36	0.15258E-02	59.722
23	F31	0.54087E-02	62.500
24	F4	0.55489E-02	65.278
25	F10	0.92539E-02	68.056
26	F18	0.99690E-02	70.833
27	F1	0.12221E-01	73.611
28	F2	0.13438E-01	76.389
29	F35	0.15053E-01	79.167
30	F9	0.19232E-01	81.944
31	F8	0.24144E-01	84.722
32	F3	0.24247E-01	87.500
33	F33	0.25136E-01	90.278
34	F7	0.32461E-01	93.056
35	F32	0.38440E-01	95.833
36	F34	0.42655E-01	98.611

MEAN ORDERED, SIMULATED WEIGHTED RESIDUALS

NO.	OBSERVATION NAME	D	FRQ. (%)
1	F21	-.10938	1.3889
2	F20	-.92706E-01	4.1667
3	F23	-.81207E-01	6.9444
4	F22	-.71524E-01	9.7222
5	F24	-.63615E-01	12.500
6	F6	-.57005E-01	15.278
7	F5	-.50915E-01	18.056
8	F12	-.45545E-01	20.833
9	F19	-.40679E-01	23.611
10	F11	-.35812E-01	26.389
11	F25	-.31282E-01	29.167
12	F16	-.26841E-01	31.944
13	F28	-.22280E-01	34.722
14	F15	-.18282E-01	37.500
15	F30	-.14528E-01	40.278
16	F26	-.10723E-01	43.056
17	F13	-.67828E-02	45.833
18	F17	-.30485E-02	48.611

19	F29	0.91987E-03	51.389
20	F14	0.45571E-02	54.167
21	F27	0.85930E-02	56.944
22	F36	0.12630E-01	59.722
23	F31	0.16606E-01	62.500
24	F4	0.20888E-01	65.278
25	F10	0.25444E-01	68.056
26	F18	0.30108E-01	70.833
27	F1	0.34861E-01	73.611
28	F2	0.39605E-01	76.389
29	F35	0.44706E-01	79.167
30	F9	0.50015E-01	81.944
31	F8	0.56072E-01	84.722
32	F3	0.62882E-01	87.500
33	F33	0.70577E-01	90.278
34	F7	0.80583E-01	93.056
35	F32	0.92808E-01	95.833
36	F34	0.10747	98.611

STD. DVS. OF ORDERED, SIMULATED WEIGHTED RESIDUALS

NO.	OBSERVATION NAME	D	FRQ. (%)
1	F21	0.37500E-01	1.3889
2	F20	0.33337E-01	4.1667
3	F23	0.30846E-01	6.9444
4	F22	0.27941E-01	9.7222
5	F24	0.25728E-01	12.500
6	F6	0.24604E-01	15.278
7	F5	0.23011E-01	18.056
8	F12	0.22052E-01	20.833
9	F19	0.21242E-01	23.611
10	F11	0.20091E-01	26.389
11	F25	0.19207E-01	29.167
12	F16	0.17644E-01	31.944
13	F28	0.16257E-01	34.722
14	F15	0.15356E-01	37.500
15	F30	0.14826E-01	40.278
16	F26	0.14434E-01	43.056
17	F13	0.14270E-01	45.833
18	F17	0.14161E-01	48.611
19	F29	0.14106E-01	51.389
20	F14	0.14000E-01	54.167
21	F27	0.14133E-01	56.944
22	F36	0.14548E-01	59.722
23	F31	0.14758E-01	62.500
24	F4	0.14946E-01	65.278
25	F10	0.15909E-01	68.056
26	F18	0.16967E-01	70.833
27	F1	0.17980E-01	73.611
28	F2	0.19061E-01	76.389
29	F35	0.20546E-01	79.167
30	F9	0.21745E-01	81.944
31	F8	0.23228E-01	84.722
32	F3	0.24758E-01	87.500
33	F33	0.26490E-01	90.278
34	F7	0.30245E-01	93.056

```
     35   F32            0.34256E-01    95.833
     36   F34            0.37263E-01    98.611

CORRELATION (CED) --------------- = 0.99559
PROBABILITY OF CORRELATION (PROB) = 0.98800
99% CONFIDENCE LIMIT (CL99) ----- = 0.99571
95% CONFIDENCE LIMIT (CL95) ----- = 0.99380
90% CONFIDENCE LIMIT (CL90) ----- = 0.99229
```

_md file (example._md):

```
  "ORD.WEIGHT.RES."  "ORD.SIM.WT.RES."  "STDVS.O.S.W.RS."  "2*STDV.O.S.W.R."  "FREQUENCY/PROB."
"PROB.PLOT.POSI."  "OBSERVATION"   "PLOT-SYMBOL"
       -0.37562E-01       -0.10938            0.37500E-01        0.75001E-01         1.3889
-2.2003      F21               1
       -0.33362E-01       -0.92706E-01        0.33337E-01        0.66674E-01         4.1667
-1.7322      F20               1
       -0.32529E-01       -0.81207E-01        0.30846E-01        0.61693E-01         6.9444
-1.4804      F23               1
       -0.26743E-01       -0.71524E-01        0.27941E-01        0.55881E-01         9.7222
-1.2976      F22               1
       -0.22647E-01       -0.63615E-01        0.25728E-01        0.51455E-01         12.500
-1.1505      F24               1
       -0.18390E-01       -0.57005E-01        0.24604E-01        0.49208E-01         15.278
-1.0251      F6                1
       -0.17909E-01       -0.50915E-01        0.23011E-01        0.46023E-01         18.056
-0.91363      F5                1
       -0.17336E-01       -0.45545E-01        0.22052E-01        0.44103E-01         20.833
-0.81256      F12               1
       -0.15027E-01       -0.40679E-01        0.21242E-01        0.42484E-01         23.611
-0.71912      F19               1
       -0.13359E-01       -0.35812E-01        0.20091E-01        0.40183E-01         26.389
-0.63155      F11               1
       -0.11397E-01       -0.31282E-01        0.19207E-01        0.38414E-01         29.167
-0.54865      F25               1
       -0.10687E-01       -0.26841E-01        0.17644E-01        0.35289E-01         31.944
-0.46943      F16               1
       -0.96915E-02       -0.22280E-01        0.16257E-01        0.32514E-01         34.722
-0.39295      F28               1
       -0.88227E-02       -0.18282E-01        0.15356E-01        0.30712E-01         37.500
-0.31878      F15               1
       -0.84145E-02       -0.14528E-01        0.14826E-01        0.29652E-01         40.278
-0.24619      F30               1
       -0.49643E-02       -0.10723E-01        0.14434E-01        0.28868E-01         43.056
-0.17499      F26               1
       -0.34969E-02       -0.67828E-02        0.14270E-01        0.28540E-01         45.833
-0.10487      F13               1
       -0.28905E-02       -0.30485E-02        0.14161E-01        0.28322E-01         48.611
-0.34955E-01  F17               1
       -0.15173E-02        0.91987E-03        0.14106E-01        0.28213E-01         51.389
0.34955E-01  F29               1
       -0.14043E-02        0.45571E-02        0.14000E-01        0.28000E-01         54.167
0.10487      F14               1
```

```
        0.14077E-02       0.85930E-02       0.14133E-01       0.28266E-01        56.944
0.17499     F27              1
        0.15258E-02       0.12630E-01       0.14548E-01       0.29096E-01        59.722
0.24619     F36              1
        0.54087E-02       0.16606E-01       0.14758E-01       0.29516E-01        62.500
0.31878     F31              1
        0.55489E-02       0.20888E-01       0.14946E-01       0.29892E-01        65.278
0.39295     F4               1
        0.92539E-02       0.25444E-01       0.15909E-01       0.31818E-01        68.056
0.46943     F10              1
        0.99690E-02       0.30108E-01       0.16967E-01       0.33933E-01        70.833
0.54865     F18              1
        0.12221E-01       0.34861E-01       0.17980E-01       0.35960E-01        73.611
0.63155     F1               1
        0.13438E-01       0.39605E-01       0.19061E-01       0.38123E-01        76.389
0.71912     F2               1
        0.15053E-01       0.44706E-01       0.20546E-01       0.41093E-01        79.167
0.81256     F35              1
        0.19232E-01       0.50015E-01       0.21745E-01       0.43490E-01        81.944
0.91363     F9               1
        0.24144E-01       0.56072E-01       0.23228E-01       0.46457E-01        84.722
1.0251     F8               1
        0.24247E-01       0.62882E-01       0.24758E-01       0.49517E-01        87.500
1.1505     F3               1
        0.25136E-01       0.70577E-01       0.26490E-01       0.52980E-01        90.278
1.2976     F33              1
        0.32461E-01       0.80583E-01       0.30245E-01       0.60491E-01        93.056
1.4804     F7               1
        0.38440E-01       0.92808E-01       0.34256E-01       0.68513E-01        95.833
1.7322     F32              1
        0.42655E-01       0.10747           0.37263E-01       0.74526E-01        98.611
2.2003     F34              1
```

MODFLOW-2000 Input Files For Confidence Interval Calculation

Name File (example.nam):

```
GLOBAL          4 mf2k.global_listing
LIST            3 output.dat
DIS            95 discret.dat
BAS6            1 bas6.dat
ZONE           93 zone.dat
MULT           94 multiple.dat
LPF            31 lpf6.dat
RCH            11 rech6.dat
WEL            12 wel6.dat
PCG            23 pcg2.dat
OC             22 oc.dat
DATA           10 inithead.dat
OBS            40 obs.dat
HOB            41 hob.dat
PES            47 pes.dat
SEN            46 sen.dat
UNC            60 unc.dat
DATAGLO        61 confint.dat
DATAGLO        62 weight-res.dat
```

UNC File (unc.dat):

```
    0    2    0   00    1    0   61  1    1    0    62    0
.001 .0 .0
  .0919  .0413  .0941  .0916  .0916  .0923  .0916  .0323
HK_1 .0
HK_2 .0
```

SEN File (sen.dat):

```
# SEN file for MODFLOW-2000, UNC1NLI1 Report Example
#
 2  0  0  2                          Item 1
 1  0   0  0                         Item 2
HK_1 1  1   1.46378  .01  100  1E-10  Item 3
HK_2 1  1   .099433  .01  100  1E-10  Item 3
```

HOB File (hob.dat):

```
# HOBS file for MODFLOW-2000, UNC1NLI1 Report Example
 42  0  0  6
 1  1
F1   1  37  13  1  0  0  0  14.88  729.28  0  1
F2   1  30  13  1  0  0  0  14.78  690.68  0  1
F3   1  25  13  1  0  0  0  14.86  668.02  0  1
```

```
F4   1  20  13  1  0  0  0  13.87  699.35  0  1
F5   1  14  13  1  0  0  0  13.01  728.59  0  1
F6   1   8  13  1  0  0  0  12.97  746.80  0  1
F7   1  37  26  1  0  0  0   5.61  643.27  0  1
F8   1  30  26  1  0  0  0   5.63  666.51  0  1
F9   1  25  26  1  0  0  0   5.94  687.81  0  1
F10  1  20  26  1  0  0  0   8.83  721.28  0  1
F11  1  14  26  1  0  0  0  11.08  717.66  0  1
F12  1   8  26  1  0  0  0  11.35  731.50  0  1
F13  1  37  39  1  0  0  0    3.7  640.67  0  1
F14  1  30  39  1  0  0  0   3.75  648.28  0  1
F15  1  25  39  1  0  0  0   3.52  619.12  0  1
F16  1  20  39  1  0  0  0   3.35  607.80  0  1
F17  1  14  39  1  0  0  0   3.42  638.66  0  1
F18  1   8  39  1  0  0  0   3.71  629.47  0  1
F19  1  37  52  1  0  0  0   2.37  548.04  0  1
F20  1  30  52  1  0  0  0   1.91  531.05  0  1
F21  1  25  52  1  0  0  0   1.76  526.49  0  1
F22  1  20  52  1  0  0  0   1.96  531.33  0  1
F23  1  14  52  1  0  0  0   1.82  546.39  0  1
F24  1   8  52  1  0  0  0   2.06  542.63  0  1
F25  1  37  65  1  0  0  0   1.54  423.83  0  1
F26  1  30  65  1  0  0  0   1.66  427.94  0  1
F27  1  25  65  1  0  0  0   1.78  429.22  0  1
F28  1  20  65  1  0  0  0   1.54  426.12  0  1
F29  1  14  65  1  0  0  0    1.7  432.14  0  1
F30  1   8  65  1  0  0  0   1.55  444.93  0  1
F31  1  37  78  1  0  0  0    .94  153.12  0  1
F32  1  30  78  1  0  0  0   1.41  197.28  0  1
F33  1  25  78  1  0  0  0   1.22  197.22  0  1
F34  1  20  78  1  0  0  0   1.47  202.06  0  1
F35  1  14  78  1  0  0  0   1.08  212.53  0  1
F36  1   8  78  1  0  0  0    .88  202.26  0  1
G1   1  22  46  1  0  0  0      0  1037.4  0  1
G2   1  21  20  1  0  0  0      0  723.55  0  1
G3   1  21  33  1  0  0  0      0  620.74  0  1
G4   1  21  59  1  0  0  0      0  488.07  0  1
G5   1  21  72  1  0  0  0      0  329.80  0  1
G6   1  40  46  1  0  0  0      0  597.63  0  1
```

GLOBAL Output File For Confidence Interval Calculation

GLOBAL Output File (mf2k.global_listing):

```
     U.S. GEOLOGICAL SURVEY MODULAR FINITE-DIFFERENCE GROUND-WATER FLOW MODEL
                          VERSION 1.6SC1 ¨25/02/2003


 This model run produced both GLOBAL and LIST files.  This is the GLOBAL file.

 GLOBAL LISTING FILE: mf2k.global_listing
                         UNIT   4

 OPENING output.dat
 FILE TYPE:LIST   UNIT   3   STATUS:REPLACE
 FORMAT:FORMATTED              ACCESS:SEQUENTIAL

 OPENING discret.dat
 FILE TYPE:DIS   UNIT  95   STATUS:OLD
 FORMAT:FORMATTED              ACCESS:SEQUENTIAL

 OPENING bas6.dat
 FILE TYPE:BAS6   UNIT   1   STATUS:OLD
 FORMAT:FORMATTED              ACCESS:SEQUENTIAL

 OPENING zone.dat
 FILE TYPE:ZONE   UNIT  93   STATUS:OLD
 FORMAT:FORMATTED              ACCESS:SEQUENTIAL

 OPENING multiple.dat
 FILE TYPE:MULT   UNIT  94   STATUS:OLD
 FORMAT:FORMATTED              ACCESS:SEQUENTIAL

 OPENING lpf6.dat
 FILE TYPE:LPF   UNIT  31   STATUS:OLD
 FORMAT:FORMATTED              ACCESS:SEQUENTIAL

 OPENING rech6.dat
 FILE TYPE:RCH   UNIT  11   STATUS:OLD
 FORMAT:FORMATTED              ACCESS:SEQUENTIAL

 OPENING wel6.dat
 FILE TYPE:WEL   UNIT  12   STATUS:OLD
 FORMAT:FORMATTED              ACCESS:SEQUENTIAL

 OPENING pcg2.dat
 FILE TYPE:PCG   UNIT  23   STATUS:OLD
 FORMAT:FORMATTED              ACCESS:SEQUENTIAL

 OPENING oc.dat
 FILE TYPE:OC   UNIT  22   STATUS:OLD
 FORMAT:FORMATTED              ACCESS:SEQUENTIAL
```

```
OPENING inithead.dat
FILE TYPE:DATA   UNIT  10   STATUS:UNKNOWN
FORMAT:FORMATTED              ACCESS:SEQUENTIAL

OPENING obs.dat
FILE TYPE:OBS   UNIT  40   STATUS:OLD
FORMAT:FORMATTED              ACCESS:SEQUENTIAL

OPENING hob.dat
FILE TYPE:HOB   UNIT  41   STATUS:OLD
FORMAT:FORMATTED              ACCESS:SEQUENTIAL

OPENING pes.dat
FILE TYPE:PES   UNIT  47   STATUS:OLD
FORMAT:FORMATTED              ACCESS:SEQUENTIAL

OPENING sen.dat
FILE TYPE:SEN   UNIT  46   STATUS:OLD
FORMAT:FORMATTED              ACCESS:SEQUENTIAL

OPENING unc.dat
FILE TYPE:UNC   UNIT  60   STATUS:OLD
FORMAT:FORMATTED              ACCESS:SEQUENTIAL

OPENING confint.dat
FILE TYPE:DATAGLO   UNIT  61   STATUS:UNKNOWN
FORMAT:FORMATTED              ACCESS:SEQUENTIAL

OPENING weight-res.dat
FILE TYPE:DATAGLO   UNIT  62   STATUS:UNKNOWN
FORMAT:FORMATTED              ACCESS:SEQUENTIAL
THE FREE FORMAT OPTION HAS BEEN SELECTED

DISCRETIZATION INPUT DATA READ FROM UNIT 95
# Discretization file for MODFLOW-2000, UNC1NLI1 Report Example
   1 LAYERS        41 ROWS        91 COLUMNS
  1 STRESS PERIOD(S) IN SIMULATION
MODEL TIME UNIT IS SECONDS
MODEL LENGTH UNIT IS UNDEFINED
THE GROUND-WATER TRANSPORT PROCESS IS INACTIVE

THE OBSERVATION PROCESS IS ACTIVE
THE SENSITIVITY PROCESS IS ACTIVE
THE PARAMETER-ESTIMATION PROCESS IS ACTIVE

MODE: PARAMETER ESTIMATION


ZONE OPTION, INPUT READ FROM UNIT 93
# Zone file for MODFLOW-2000, UNC1NLI1 Report Example
    2 ZONE ARRAYS

MULTIPLIER OPTION, INPUT READ FROM UNIT 94
# Multiplier file for MODFLOW-2000, UNC1NLI1 Report Example
  2 MULTIPLIER ARRAYS
 Confining bed flag for each layer:
```

```
  0

     41173  ELEMENTS OF GX ARRAY USED OUT OF      41173
      3731  ELEMENTS OF GZ ARRAY USED OUT OF       3731
     11193  ELEMENTS OF IG ARRAY USED OUT OF      11193



                              DELR
READING ON UNIT  95 WITH FORMAT: (16G5.0)



                              DELC
READING ON UNIT  95 WITH FORMAT: (16G5.0)

TOP ELEVATION OF LAYER 1 =   1.00000

  MODEL LAYER BOTTOM EL. =   0.00000     FOR LAYER   1


STRESS PERIOD     LENGTH       TIME STEPS     MULTIPLIER FOR DELT    SS FLAG
----------------------------------------------------------------------------
       1         1.000000          1                    1.000         SS

STEADY-STATE SIMULATION




 MULT. ARRAY: HK1        =   1.00000

 MULT. ARRAY: VK1        =   1.00000



            ZONE ARRAY: ZHK1
READING ON UNIT  93 WITH FORMAT: (91I1)

  ZONE ARRAY: ZVK1       =            999

LPF1 -- LAYER PROPERTY FLOW PACKAGE, VERSION 1, 1/11/2000
        INPUT READ FROM UNIT 31
# Layer-Property Flow file for MODFLOW-2000, UNC1NLI1 Report Example
HEAD AT CELLS THAT CONVERT TO DRY=   999.00
    3 Named Parameters

  LAYER FLAGS:
LAYER       LAYTYP        LAYAVG         CHANI        LAYVKA        LAYWET
---------------------------------------------------------------------------
   1             0             0     1.000E+00             0             0

  INTERPRETATION OF LAYER FLAGS:
                     INTERBLOCK     HORIZONTAL    DATA IN
        LAYER TYPE   TRANSMISSIVITY   ANISOTROPY   ARRAY VKA   WETTABILITY
LAYER      (LAYTYP)      (LAYAVG)       (CHANI)      (LAYVKA)      (LAYWET)
```

```
----------------------------------------------------------------------------
   1      CONFINED      HARMONIC     1.000E+00    VERTICAL K  NON-WETTABLE

      7462 ELEMENTS IN X ARRAY ARE USED BY LPF
         6 ELEMENTS IN IX ARRAY ARE USED BY LPF

PCG2 -- CONJUGATE GRADIENT SOLUTION PACKAGE, VERSION 2.4, 12/29/98
MAXIMUM OF     50 CALLS OF SOLUTION ROUTINE
MAXIMUM OF     30 INTERNAL ITERATIONS PER CALL TO SOLUTION ROUTINE
MATRIX PRECONDITIONING TYPE :    1
     14193 ELEMENTS IN X ARRAY ARE USED BY PCG
     10500 ELEMENTS IN IX ARRAY ARE USED BY PCG
      7462 ELEMENTS IN Z ARRAY ARE USED BY PCG

SEN1BAS6 -- SENSITIVITY PROCESS, VERSION 1.0, 10/15/98
INPUT READ FROM UNIT  46
# SEN file for MODFLOW-2000, UNC1NLI1 Report Example
#

NUMBER OF PARAMETER VALUES TO BE READ FROM SEN FILE:    2
ISENALL.............................................:    0
SENSITIVITIES WILL BE STORED IN MEMORY
FOR UP TO   2 PARAMETERS

      3745 ELEMENTS IN X ARRAY ARE USED FOR SENSITIVITIES
      3731 ELEMENTS IN Z ARRAY ARE USED FOR SENSITIVITIES
         4 ELEMENTS IN IX ARRAY ARE USED FOR SENSITIVITIES

PES1BAS6 -- PARAMETER-ESTIMATION PROCESS, VERSION 1.0, 07/22/99
INPUT READ FROM UNIT  47
# PES file for MODFLOW-2000, UNC1NLI1 Report Example
#

MAXIMUM NUMBER OF PARAMETER-ESTIMATION ITERATIONS (MAX-ITER)  =    50
MAXIMUM PARAMETER CORRECTION (MAX-CHANGE) ------------------- =  2.0000
CLOSURE CRITERION (TOL) ------------------------------------- = 0.10000E-01
SUM OF SQUARES CLOSURE CRITERION (SOSC) --------------------- =  0.0000

FLAG TO GENERATE INPUT NEEDED BY BEALE-2000 (IBEFLG) -------- =     0
FLAG TO GENERATE INPUT NEEDED BY YCINT-2000 (IYCFLG) -------- =     0
OMIT PRINTING TO SCREEN (IF = 1) (IOSTAR) ------------------ =     0
ADJUST GAUSS-NEWTON MATRIX WITH NEWTON UPDATES (IF = 1)(NOPT) =     0
NUMBER OF FLETCHER-REEVES ITERATIONS (NFIT) ----------------- =     0
CRITERION FOR ADDING MATRIX R (SOSR) ----------------------- =  0.0000
VALUE USED TO INCREMENT MARQUARDT PARAMETER (RMAR) ---------- = 0.10000E-02
MARQUARDT PARAMETER MULTIPLIER (RMARM) ---------------------- =  1.5000
APPLY MAX-CHANGE IN REGRESSION SPACE (IF = 1) (IAP) --------- =     0

FORMAT CODE FOR COVARIANCE AND CORRELATION MATRICES (IPRCOV)  =     1
PRINT PARAMETER-ESTIMATION STATISTICS
    EACH ITERATION (IF > 0)  (IPRINT) ----------------------- =     0
PRINT EIGENVALUES AND EIGENVECTORS OF
    COVARIANCE MATRIX (IF > 0)  (LPRINT) -------------------- =     0

SEARCH DIRECTION ADJUSTMENT PARAMETER (CSA) ----------------- = 0.80000E-01
MODIFY CONVERGENCE CRITERIA (IF > 0) (FCONV) ---------------- =  0.0000
```

```
CALCULATE SENSITIVITIES USING FINAL
    PARAMETER ESTIMATES (IF > 0) (LASTX) ------------------- =     1

NUMBER OF USUALLY POS. PARAMETERS THAT MAY BE NEGATIVE (NPNG) =     0
NUMBER OF PARAMETERS WITH CORRELATED PRIOR INFORMATION (IPR)  =     0
NUMBER OF PRIOR-INFORMATION EQUATIONS (MPR) ---------------- =     0

   479 ELEMENTS IN X ARRAY ARE USED FOR PARAMETER ESTIMATION
    81 ELEMENTS IN Z ARRAY ARE USED FOR PARAMETER ESTIMATION
    52 ELEMENTS IN IX ARRAY ARE USED FOR PARAMETER ESTIMATION

OBS1BAS6 -- OBSERVATION PROCESS, VERSION 1.0, 4/27/99
INPUT READ FROM UNIT  40
# OBS file for MODFLOW-2000, UNC1NLI1 Report Example
OBSERVATION GRAPH-DATA OUTPUT FILES
WILL BE PRINTED AND NAMED USING THE BASE: Example
DIMENSIONLESS SCALED OBSERVATION SENSITIVITIES WILL BE PRINTED

HEAD OBSERVATIONS -- INPUT READ FROM UNIT  41
# HOBS file for MODFLOW-2000, UNC1NLI1 Report Example

NUMBER OF HEADS....................................:   42
  NUMBER OF MULTILAYER HEADS.......................:    0
  MAXIMUM NUMBER OF LAYERS FOR MULTILAYER HEADS....:    0
NUMBER OF HEADS USED FOR INTERVAL CALCULATION......:    6

    826 ELEMENTS IN X ARRAY ARE USED FOR OBSERVATIONS
      2 ELEMENTS IN Z ARRAY ARE USED FOR OBSERVATIONS
    423 ELEMENTS IN IX ARRAY ARE USED FOR OBSERVATIONS

COMMON ERROR VARIANCE FOR ALL OBSERVATIONS SET TO:       1.000

UNC1NLI1 -- UNCERTAINTY-ESTIMATION PROCESS, VERSION 1.0, 03/08/02
INPUT READ FROM UNIT  60
IACT=0: COMPUTE CONFIDENCE OR PREDICTION INTERVALS
NUMBER OF HEAD INTERVALS...............................:    6
NUMBER OF PARAMETER INTERVALS..........................:    2
TOTAL NUMBER OF INTERVALS..............................:    8
HEAD AND FLOW INTERVALS ON DIFFERENCES (0,1)=(NO,YES)..:    0
INTERVAL LIMITS? (1=UPPER,-1=LOWER,O=UPPER & LOWER)....:    0
INTERVAL TYPE (1=CONFIDENCE,2=PREDICTION)..............:    1
NUMBER OF INITIAL PARAMETER SETS (0=USE DATASET 8).....:    0
RESULT SUMMARY IS WRITTEN TO UNIT NO (1=NOT WRITTEN)...:   61
CRITICAL VALUE CONST./VAR. (IDSQ=0/1)..................:    1
PRINT ITERATION LOG (1=YES,ELSE=NO)....................:    1
USE APPROXIMATE INCREMENTAL ADJUSTMENT? (1=YES,0=NO)...:    0
WEIGHTED RESIDUALS ARE WRITTEN TO UNIT NO (O=NOT WRIT.):   62
SCALING VALUES BS (1=READ VALUES, 0=COPY START. VAL.)..:    0
TOLP (CONVERGENCE CRITERIA FOR PARAMETER CHANGE).......: 0.100000E-02
TOLS (CONV. CRIT. FOR CHANGE OF OBJECTIVE FUNCTION)....:  0.00000
TOLY (CONV. CRIT. FOR CHANGE OF COMPUTED LIMIT VALUE)..:  0.00000

    24 ELEMENTS IN X ARRAY ARE USED FOR PARAMETER ESTIMATION
     6 ELEMENTS IN Z ARRAY ARE USED FOR PARAMETER ESTIMATION
    48 ELEMENTS IN IX ARRAY ARE USED FOR PARAMETER ESTIMATION
```

```
     26729  ELEMENTS OF X ARRAY USED OUT OF      26729
     11282  ELEMENTS OF Z ARRAY USED OUT OF      11282
     11033  ELEMENTS OF IX ARRAY USED OUT OF      11033
      7462  ELEMENTS OF XHS ARRAY USED OUT OF       7462

INFORMATION ON PARAMETERS LISTED IN SEN FILE
                                         LOWER         UPPER       ALTERNATE
                       VALUE IN SEN   REASONABLE    REASONABLE     SCALING
   NAME     ISENS  LN   INPUT FILE      LIMIT         LIMIT         FACTOR
----------  -----  --  ------------  ------------  ------------  ------------
HK_1          1     1    1.4638       0.10000E-01    100.00       0.10000E-09
HK_2          1     1   0.99433E-01   0.10000E-01    100.00       0.10000E-09
-----------------------------------------------------------------------------
FOR THE PARAMETERS LISTED IN THE TABLE ABOVE, PARAMETER VALUES IN INDIVIDUAL
PACKAGE INPUT FILES ARE REPLACED BY THE VALUES FROM THE SEN INPUT FILE.  THE
ALTERNATE SCALING FACTOR IS USED TO SCALE SENSITIVITIES IF IT IS LARGER THAN
THE PARAMETER VALUE IN ABSOLUTE VALUE AND THE PARAMETER IS NOT LOG-TRANSFORMED.

ISENS IS GREATER THAN ZERO FOR    2 PARAMETERS

HEAD OBSERVATION VARIANCES ARE MULTIPLIED BY:       1.000

OBSERVED HEAD DATA -- TIME OFFSETS ARE MULTIPLIED BY:   1.0000


                  REFER.
      OBSERVATION  STRESS    TIME                                  STATISTIC   PLOT
 OBS#    NAME      PERIOD   OFFSET    OBSERVATION  STATISTIC         TYPE      SYM.
    1 F1              1    0.000       14.88        729.3       VARIANCE       1
    2 F2              1    0.000       14.78        690.7       VARIANCE       1
    3 F3              1    0.000       14.86        668.0       VARIANCE       1
    4 F4              1    0.000       13.87        699.3       VARIANCE       1
    5 F5              1    0.000       13.01        728.6       VARIANCE       1
    6 F6              1    0.000       12.97        746.8       VARIANCE       1
    7 F7              1    0.000       5.610        643.3       VARIANCE       1
    8 F8              1    0.000       5.630        666.5       VARIANCE       1
    9 F9              1    0.000       5.940        687.8       VARIANCE       1
   10 F10             1    0.000       8.830        721.3       VARIANCE       1
   11 F11             1    0.000       11.08        717.7       VARIANCE       1
   12 F12             1    0.000       11.35        731.5       VARIANCE       1
   13 F13             1    0.000       3.700        640.7       VARIANCE       1
   14 F14             1    0.000       3.750        648.3       VARIANCE       1
   15 F15             1    0.000       3.520        619.1       VARIANCE       1
   16 F16             1    0.000       3.350        607.8       VARIANCE       1
   17 F17             1    0.000       3.420        638.7       VARIANCE       1
   18 F18             1    0.000       3.710        629.5       VARIANCE       1
   19 F19             1    0.000       2.370        548.0       VARIANCE       1
   20 F20             1    0.000       1.910        531.0       VARIANCE       1
   21 F21             1    0.000       1.760        526.5       VARIANCE       1
   22 F22             1    0.000       1.960        531.3       VARIANCE       1
   23 F23             1    0.000       1.820        546.4       VARIANCE       1
   24 F24             1    0.000       2.060        542.6       VARIANCE       1
   25 F25             1    0.000       1.540        423.8       VARIANCE       1
   26 F26             1    0.000       1.660        427.9       VARIANCE       1
   27 F27             1    0.000       1.780        429.2       VARIANCE       1
   28 F28             1    0.000       1.540        426.1       VARIANCE       1
   29 F29             1    0.000       1.700        432.1       VARIANCE       1
```

30	F30	1	0.000	1.550	444.9	VARIANCE	1
31	F31	1	0.000	0.9400	153.1	VARIANCE	1
32	F32	1	0.000	1.410	197.3	VARIANCE	1
33	F33	1	0.000	1.220	197.2	VARIANCE	1
34	F34	1	0.000	1.470	202.1	VARIANCE	1
35	F35	1	0.000	1.080	212.5	VARIANCE	1
36	F36	1	0.000	0.8800	202.3	VARIANCE	1
37	G1	1	0.000	0.000	1037.	VARIANCE	1
38	G2	1	0.000	0.000	723.5	VARIANCE	1
39	G3	1	0.000	0.000	620.7	VARIANCE	1
40	G4	1	0.000	0.000	488.1	VARIANCE	1
41	G5	1	0.000	0.000	329.8	VARIANCE	1
42	G6	1	0.000	0.000	597.6	VARIANCE	1

OBS#	OBSERVATION NAME	LAY	ROW	COL	ROW OFFSET	COL OFFSET	HEAD CHANGE REFERENCE OBSERVATION (IF > 0)
1	F1	1	37	13	0.000	0.000	0
2	F2	1	30	13	0.000	0.000	0
3	F3	1	25	13	0.000	0.000	0
4	F4	1	20	13	0.000	0.000	0
5	F5	1	14	13	0.000	0.000	0
6	F6	1	8	13	0.000	0.000	0
7	F7	1	37	26	0.000	0.000	0
8	F8	1	30	26	0.000	0.000	0
9	F9	1	25	26	0.000	0.000	0
10	F10	1	20	26	0.000	0.000	0
11	F11	1	14	26	0.000	0.000	0
12	F12	1	8	26	0.000	0.000	0
13	F13	1	37	39	0.000	0.000	0
14	F14	1	30	39	0.000	0.000	0
15	F15	1	25	39	0.000	0.000	0
16	F16	1	20	39	0.000	0.000	0
17	F17	1	14	39	0.000	0.000	0
18	F18	1	8	39	0.000	0.000	0
19	F19	1	37	52	0.000	0.000	0
20	F20	1	30	52	0.000	0.000	0
21	F21	1	25	52	0.000	0.000	0
22	F22	1	20	52	0.000	0.000	0
23	F23	1	14	52	0.000	0.000	0
24	F24	1	8	52	0.000	0.000	0
25	F25	1	37	65	0.000	0.000	0
26	F26	1	30	65	0.000	0.000	0
27	F27	1	25	65	0.000	0.000	0
28	F28	1	20	65	0.000	0.000	0
29	F29	1	14	65	0.000	0.000	0
30	F30	1	8	65	0.000	0.000	0
31	F31	1	37	78	0.000	0.000	0
32	F32	1	30	78	0.000	0.000	0
33	F33	1	25	78	0.000	0.000	0
34	F34	1	20	78	0.000	0.000	0
35	F35	1	14	78	0.000	0.000	0
36	F36	1	8	78	0.000	0.000	0
37	G1	1	22	46	0.000	0.000	0
38	G2	1	21	20	0.000	0.000	0

```
   39  G3              1   21   33   0.000   0.000        0
   40  G4              1   21   59   0.000   0.000        0
   41  G5              1   21   72   0.000   0.000        0
   42  G6              1   40   46   0.000   0.000        0


CRITICAL VALUE (DSQ) FOR INTERVALS
   0.0919    0.0413    0.0941    0.0916    0.0916    0.0923    0.0916    0.0323


CONFIDENCE INTERVAL TO BE CALCULATED FOR THE FOLLOWING PARAMETERS
PAR. NO
  HK_1
  HK_2
SCALING VALUES FOR DAMPING PARAMETER CHANGES:
1.4638      0.99433E-01



                                   SOLUTION BY THE CONJUGATE-GRADIENT METHOD
                                  ------------------------------------------
                   MAXIMUM NUMBER OF CALLS TO PCG ROUTINE =       50
                       MAXIMUM ITERATIONS PER CALL TO PCG =       30
                              MATRIX PRECONDITIONING TYPE =        1
       RELAXATION FACTOR (ONLY USED WITH PRECOND. TYPE 1) =    0.10000E+01
PARAMETER OF POLYNOMIAL PRECOND. = 2 (2) OR IS CALCULATED :        1
                        HEAD CHANGE CRITERION FOR CLOSURE =    0.10000E-02
                    RESIDUAL CHANGE CRITERION FOR CLOSURE =    0.10000E-02
           PCG HEAD AND RESIDUAL CHANGE PRINTOUT INTERVAL =        1
    PRINTING FROM SOLVER IS LIMITED(1) OR SUPPRESSED (>1) =        0
                                        DAMPING PARAMETER =    0.10000E+01

CONVERGENCE CRITERIA FOR SENSITIVITIES
PARAMETER      HCLOSE        RCLOSE
----------  ------------  ------------
HK_1         0.68316E-05   0.68316E-05
HK_2         0.10057E-03   0.10057E-03
--------------------------------------

WETTING CAPABILITY IS NOT ACTIVE IN ANY LAYER

PARAMETERS DEFINED IN THE LPF PACKAGE

PARAMETER NAME:HK_1         TYPE:HK     CLUSTERS:   1
Parameter value from package file is:    1.0000
This value has been changed to:          1.4638    , as read from
the Sensitivity Process file
               LAYER:  1    MULTIPLIER ARRAY: HK1    ZONE ARRAY: ZHK1
               ZONE VALUES:    1

PARAMETER NAME:HK_2         TYPE:HK     CLUSTERS:   1
Parameter value from package file is:    1.0000
This value has been changed to:         9.94330E-02, as read from
the Sensitivity Process file
               LAYER:  1    MULTIPLIER ARRAY: HK1    ZONE ARRAY: ZHK1
               ZONE VALUES:    2
```

```
PARAMETER NAME:VK_0         TYPE:VK     CLUSTERS:   1
Parameter value from package file is:    1.0000
               LAYER:  1    MULTIPLIER ARRAY: VK1    ZONE ARRAY: ZVK1
               ZONE VALUES:  999

   HYD. COND. ALONG ROWS FOR LAYER   1 WILL BE DEFINED BY PARAMETERS
(PRINT FLAG=  31)

     VERTICAL HYD. COND. FOR LAYER   1 WILL BE DEFINED BY PARAMETERS
(PRINT FLAG=  31)


********************************************************************************


CALCULATION OF CONFIDENCE INTERVAL NO.    1
  STARTING PARAMETER SET NO.  1
OBSNAM: G1


    1 Well parameters

PARAMETER NAME:WEL_0_1      TYPE:Q
Parameter value from package file is:    1.0000
  NUMBER OF ENTRIES:      1

WELL NO.  LAYER   ROW   COL   STRESS FACTOR
----------------------------------------------
     1      1     21     46      -1.000


    0 Recharge parameters

  4 PARAMETERS HAVE BEEN DEFINED IN ALL PACKAGES.
(SPACE IS ALLOCATED FOR  500 PARAMETERS.)

C.I. LIMIT FOR INTERVAL    1: FL=   4.1361

********************************************************************************




CALCULATION OF CONFIDENCE INTERVAL NO.    2
  STARTING PARAMETER SET NO.  1
OBSNAM: G2


    1 Well parameters

PARAMETER NAME:WEL_0_1      TYPE:Q
Parameter value from package file is:    1.0000
  NUMBER OF ENTRIES:      1

WELL NO.  LAYER   ROW   COL   STRESS FACTOR
```

```
----------------------------------------------
     1      1     21     46      -1.000


    0 Recharge parameters

  4 PARAMETERS HAVE BEEN DEFINED IN ALL PACKAGES.
(SPACE IS ALLOCATED FOR  500 PARAMETERS.)

C.I. LIMIT FOR INTERVAL    2: FL=   13.439

********************************************************************************




CALCULATION OF CONFIDENCE INTERVAL NO.    3
  STARTING PARAMETER SET NO.  1
OBSNAM: G3


    1 Well parameters

PARAMETER NAME:WEL_0_1      TYPE:Q
Parameter value from package file is:    1.0000
  NUMBER OF ENTRIES:      1

WELL NO.  LAYER   ROW   COL   STRESS FACTOR
----------------------------------------------
     1      1     21     46      -1.000


    0 Recharge parameters

  4 PARAMETERS HAVE BEEN DEFINED IN ALL PACKAGES.
(SPACE IS ALLOCATED FOR  500 PARAMETERS.)

C.I. LIMIT FOR INTERVAL    3: FL=   6.4088

********************************************************************************




CALCULATION OF CONFIDENCE INTERVAL NO.    4
  STARTING PARAMETER SET NO.  1
OBSNAM: G4


    1 Well parameters

PARAMETER NAME:WEL_0_1      TYPE:Q
Parameter value from package file is:    1.0000
  NUMBER OF ENTRIES:      1

WELL NO.  LAYER   ROW   COL   STRESS FACTOR
```

```
 ---------------------------------------------
      1      1     21     46      -1.000


     0 Recharge parameters

   4 PARAMETERS HAVE BEEN DEFINED IN ALL PACKAGES.
 (SPACE IS ALLOCATED FOR  500 PARAMETERS.)

 C.I. LIMIT FOR INTERVAL    4: FL=   3.1090

********************************************************************************




 CALCULATION OF CONFIDENCE INTERVAL NO.    5
   STARTING PARAMETER SET NO.  1
 OBSNAM: G5


     1 Well parameters

 PARAMETER NAME:WEL_0_1      TYPE:Q
 Parameter value from package file is:    1.0000
   NUMBER OF ENTRIES:      1

 WELL NO.  LAYER   ROW   COL   STRESS FACTOR
 ---------------------------------------------
      1      1     21     46      -1.000


     0 Recharge parameters

   4 PARAMETERS HAVE BEEN DEFINED IN ALL PACKAGES.
 (SPACE IS ALLOCATED FOR  500 PARAMETERS.)

 C.I. LIMIT FOR INTERVAL    5: FL=   1.8458

********************************************************************************




 CALCULATION OF CONFIDENCE INTERVAL NO.    6
   STARTING PARAMETER SET NO.  1
 OBSNAM: G6


     1 Well parameters

 PARAMETER NAME:WEL_0_1      TYPE:Q
 Parameter value from package file is:    1.0000
   NUMBER OF ENTRIES:      1

 WELL NO.  LAYER   ROW   COL   STRESS FACTOR
```

```
 ---------------------------------------------
      1      1     21     46      -1.000


     0 Recharge parameters

   4 PARAMETERS HAVE BEEN DEFINED IN ALL PACKAGES.
 (SPACE IS ALLOCATED FOR  500 PARAMETERS.)

 C.I. LIMIT FOR INTERVAL    6: FL=   4.6167

********************************************************************************




 CALCULATION OF CONFIDENCE INTERVAL NO.    7
   STARTING PARAMETER SET NO.  1
 PARNAM: HK_1


     1 Well parameters

 PARAMETER NAME:WEL_0_1      TYPE:Q
 Parameter value from package file is:    1.0000
   NUMBER OF ENTRIES:      1

 WELL NO.  LAYER   ROW   COL   STRESS FACTOR
 ---------------------------------------------
      1      1     21     46      -1.000


     0 Recharge parameters

   4 PARAMETERS HAVE BEEN DEFINED IN ALL PACKAGES.
 (SPACE IS ALLOCATED FOR  500 PARAMETERS.)

 C.I. LIMIT FOR INTERVAL    7: FL=  0.42100

********************************************************************************




 CALCULATION OF CONFIDENCE INTERVAL NO.    8
   STARTING PARAMETER SET NO.  1
 PARNAM: HK_2


     1 Well parameters

 PARAMETER NAME:WEL_0_1      TYPE:Q
 Parameter value from package file is:    1.0000
   NUMBER OF ENTRIES:      1

 WELL NO.  LAYER   ROW   COL   STRESS FACTOR
```

```
 ----------------------------------------------
      1      1     21     46      -1.000


     0 Recharge parameters

   4 PARAMETERS HAVE BEEN DEFINED IN ALL PACKAGES.
 (SPACE IS ALLOCATED FOR  500 PARAMETERS.)

 C.I. LIMIT FOR INTERVAL    8: FL= -0.87902

********************************************************************************




 CALCULATION OF CONFIDENCE INTERVAL NO.   -1
   STARTING PARAMETER SET NO.  1
 OBSNAM: G1


     1 Well parameters

 PARAMETER NAME:WEL_0_1      TYPE:Q
 Parameter value from package file is:    1.0000
   NUMBER OF ENTRIES:      1

 WELL NO.  LAYER   ROW   COL   STRESS FACTOR
 ----------------------------------------------
      1      1     21     46      -1.000


     0 Recharge parameters

   4 PARAMETERS HAVE BEEN DEFINED IN ALL PACKAGES.
 (SPACE IS ALLOCATED FOR  500 PARAMETERS.)

 C.I. LIMIT FOR INTERVAL   -1: FL=   1.5895

********************************************************************************




 CALCULATION OF CONFIDENCE INTERVAL NO.   -2
   STARTING PARAMETER SET NO.  1
 OBSNAM: G2


     1 Well parameters

 PARAMETER NAME:WEL_0_1      TYPE:Q
 Parameter value from package file is:    1.0000
   NUMBER OF ENTRIES:      1

 WELL NO.  LAYER   ROW   COL   STRESS FACTOR
```

```
 ----------------------------------------------
      1      1     21     46      -1.000


     0 Recharge parameters

   4 PARAMETERS HAVE BEEN DEFINED IN ALL PACKAGES.
 (SPACE IS ALLOCATED FOR  500 PARAMETERS.)

 C.I. LIMIT FOR INTERVAL   -2: FL=   10.581

********************************************************************************




 CALCULATION OF CONFIDENCE INTERVAL NO.   -3
   STARTING PARAMETER SET NO.  1
 OBSNAM: G3


     1 Well parameters

 PARAMETER NAME:WEL_0_1      TYPE:Q
 Parameter value from package file is:    1.0000
   NUMBER OF ENTRIES:      1

 WELL NO.  LAYER   ROW   COL   STRESS FACTOR
 ----------------------------------------------
      1      1     21     46      -1.000


     0 Recharge parameters

   4 PARAMETERS HAVE BEEN DEFINED IN ALL PACKAGES.
 (SPACE IS ALLOCATED FOR  500 PARAMETERS.)

 C.I. LIMIT FOR INTERVAL   -3: FL=   2.5599

********************************************************************************




 CALCULATION OF CONFIDENCE INTERVAL NO.   -4
   STARTING PARAMETER SET NO.  1
 OBSNAM: G4


     1 Well parameters

 PARAMETER NAME:WEL_0_1      TYPE:Q
 Parameter value from package file is:    1.0000
   NUMBER OF ENTRIES:      1

 WELL NO.  LAYER   ROW   COL   STRESS FACTOR
```

```
 ----------------------------------------------
      1      1     21     46      -1.000


     0 Recharge parameters

   4 PARAMETERS HAVE BEEN DEFINED IN ALL PACKAGES.
 (SPACE IS ALLOCATED FOR  500 PARAMETERS.)

 C.I. LIMIT FOR INTERVAL   -4: FL=   1.1892

********************************************************************************




 CALCULATION OF CONFIDENCE INTERVAL NO.   -5
   STARTING PARAMETER SET NO.  1
 OBSNAM: G5


     1 Well parameters

 PARAMETER NAME:WEL_0_1      TYPE:Q
 Parameter value from package file is:    1.0000
   NUMBER OF ENTRIES:      1

 WELL NO.  LAYER   ROW   COL   STRESS FACTOR
 ----------------------------------------------
      1      1     21     46      -1.000


     0 Recharge parameters

   4 PARAMETERS HAVE BEEN DEFINED IN ALL PACKAGES.
 (SPACE IS ALLOCATED FOR  500 PARAMETERS.)

 C.I. LIMIT FOR INTERVAL   -5: FL=  0.70517

********************************************************************************




 CALCULATION OF CONFIDENCE INTERVAL NO.   -6
   STARTING PARAMETER SET NO.  1
 OBSNAM: G6


     1 Well parameters

 PARAMETER NAME:WEL_0_1      TYPE:Q
 Parameter value from package file is:    1.0000
   NUMBER OF ENTRIES:      1

 WELL NO.  LAYER   ROW   COL   STRESS FACTOR
```

```
 ---------------------------------------------
      1      1     21     46      -1.000


     0 Recharge parameters

   4 PARAMETERS HAVE BEEN DEFINED IN ALL PACKAGES.
 (SPACE IS ALLOCATED FOR  500 PARAMETERS.)

 C.I. LIMIT FOR INTERVAL   -6: FL=   1.7864

********************************************************************************




 CALCULATION OF CONFIDENCE INTERVAL NO.   -7
   STARTING PARAMETER SET NO.  1
 PARNAM: HK_1


     1 Well parameters

 PARAMETER NAME:WEL_0_1      TYPE:Q
 Parameter value from package file is:    1.0000
   NUMBER OF ENTRIES:      1

 WELL NO.  LAYER   ROW   COL   STRESS FACTOR
 ---------------------------------------------
      1      1     21     46      -1.000


     0 Recharge parameters

   4 PARAMETERS HAVE BEEN DEFINED IN ALL PACKAGES.
 (SPACE IS ALLOCATED FOR  500 PARAMETERS.)

 C.I. LIMIT FOR INTERVAL   -7: FL=  0.32539E-02

********************************************************************************




 CALCULATION OF CONFIDENCE INTERVAL NO.   -8
   STARTING PARAMETER SET NO.  1
 PARNAM: HK_2


     1 Well parameters

 PARAMETER NAME:WEL_0_1      TYPE:Q
 Parameter value from package file is:    1.0000
   NUMBER OF ENTRIES:      1

 WELL NO.  LAYER   ROW   COL   STRESS FACTOR
```

```
 ---------------------------------------------
      1      1     21     46      -1.000


    0 Recharge parameters

  4 PARAMETERS HAVE BEEN DEFINED IN ALL PACKAGES.
(SPACE IS ALLOCATED FOR  500 PARAMETERS.)

C.I. LIMIT FOR INTERVAL   -8: FL=  -1.1052

*******************************************************************************


PROCESS STARTED: 20040305  124557.200
PROCESS STOPPED: 20040305  124657.840
```

Summary And Weighted Residuals Output Files

Summary Output File (confint.dat):

```
C.I.    1: FL=   4.1361    ;  SSE=0.91894E-01; ITER=  4;  PAR:    1.007     0.1538
C.I.    2: FL=   13.439    ;  SSE=0.41351E-01; ITER=  3;  PAR:    1.519     0.7981E-01
C.I.    3: FL=   6.4088    ;  SSE=0.94127E-01; ITER=  4;  PAR:    1.003     0.1496
C.I.    4: FL=   3.1090    ;  SSE=0.91639E-01; ITER=  4;  PAR:    1.008     0.1541
C.I.    5: FL=   1.8458    ;  SSE=0.91618E-01; ITER=  4;  PAR:    1.007     0.1542
C.I.    6: FL=   4.6167    ;  SSE=0.92338E-01; ITER=  4;  PAR:    1.006     0.1531
C.I.    7: FL=  0.42100    ;  SSE=0.91608E-01; ITER=  4;  PAR:    2.636     0.6966E-01
C.I.    8: FL= -0.87902    ;  SSE=0.32298E-01; ITER=  4;  PAR:    1.264     0.1321
C.I.   -1: FL=   1.5895    ;  SSE=0.91861E-01; ITER=  4;  PAR:    2.641     0.6964E-01
C.I.   -2: FL=   10.581    ;  SSE=0.41295E-01; ITER=  4;  PAR:    1.436     0.1282
C.I.   -3: FL=   2.5599    ;  SSE=0.94083E-01; ITER=  4;  PAR:    2.671     0.6945E-01
C.I.   -4: FL=   1.1892    ;  SSE=0.91594E-01; ITER=  4;  PAR:    2.636     0.6967E-01
C.I.   -5: FL=  0.70517    ;  SSE=0.91630E-01; ITER=  4;  PAR:    2.636     0.6967E-01
C.I.   -6: FL=   1.7864    ;  SSE=0.92292E-01; ITER=  4;  PAR:    2.646     0.6961E-01
C.I.   -7: FL=  0.32539E-02;  SSE=0.91624E-01; ITER=  4;  PAR:    1.008     0.1542
C.I.   -8: FL=  -1.1052    ;  SSE=0.32343E-01; ITER=  3;  PAR:    1.750     0.7849E-01
```

Weighted Residuals Output File (weight-res.dat):

```
WEIGHTED RESIDUALS AT LIMIT FOR INTERVAL     1; STARTING VALUES  1
 OBSNO    OBS. NAME  WEIGHT. RES.
     1 F1             0.167E-01
     2 F2             0.171E-01
     3 F3             0.266E-01
     4 F4             0.460E-02
     5 F5            -0.201E-01
     6 F6            -0.206E-01
     7 F7             0.316E-01
     8 F8             0.250E-01
     9 F9             0.230E-01
    10 F10            0.808E-02
    11 F11           -0.178E-01
    12 F12           -0.198E-01
    13 F13           -0.336E-02
    14 F14           -0.103E-02
    15 F15           -0.847E-02
    16 F16           -0.110E-01
    17 F17           -0.428E-02
    18 F18            0.805E-02
    19 F19           -0.151E-01
    20 F20           -0.335E-01
    21 F21           -0.378E-01
    22 F22           -0.272E-01
    23 F23           -0.333E-01
    24 F24           -0.236E-01
    25 F25           -0.116E-01
    26 F26           -0.521E-02
    27 F27            0.110E-02
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   28 F28           -0.101E-01
   29 F29           -0.198E-02
   30 F30           -0.895E-02
   31 F31            0.521E-02
   32 F32            0.382E-01
   33 F33            0.249E-01
   34 F34            0.423E-01
   35 F35            0.147E-01
   36 F36            0.117E-02


WEIGHTED RESIDUALS AT LIMIT FOR INTERVAL     2; STARTING VALUES  1
OBSNO    OBS. NAME  WEIGHT. RES.
    1 F1             0.129E-01
    2 F2             0.140E-01
    3 F3             0.247E-01
    4 F4             0.564E-02
    5 F5            -0.180E-01
    6 F6            -0.184E-01
    7 F7             0.337E-01
    8 F8             0.255E-01
    9 F9             0.209E-01
   10 F10            0.968E-02
   11 F11           -0.138E-01
   12 F12           -0.176E-01
   13 F13           -0.248E-02
   14 F14           -0.381E-03
   15 F15           -0.780E-02
   16 F16           -0.974E-02
   17 F17           -0.208E-02
   18 F18            0.108E-01
   19 F19           -0.143E-01
   20 F20           -0.326E-01
   21 F21           -0.368E-01
   22 F22           -0.260E-01
   23 F23           -0.319E-01
   24 F24           -0.220E-01
   25 F25           -0.108E-01
   26 F26           -0.441E-02
   27 F27            0.195E-02
   28 F28           -0.916E-02
   29 F29           -0.100E-02
   30 F30           -0.791E-02
   31 F31            0.587E-02
   32 F32            0.388E-01
   33 F33            0.255E-01
   34 F34            0.430E-01
   35 F35            0.154E-01
   36 F36            0.189E-02


WEIGHTED RESIDUALS AT LIMIT FOR INTERVAL     3; STARTING VALUES  1
OBSNO    OBS. NAME  WEIGHT. RES.
    1 F1             0.124E-01
    2 F2             0.128E-01
    3 F3             0.223E-01
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    4 F4              0.618E-03
    5 F5             -0.239E-01
    6 F6             -0.243E-01
    7 F7              0.318E-01
    8 F8              0.250E-01
    9 F9              0.228E-01
   10 F10             0.622E-02
   11 F11            -0.211E-01
   12 F12            -0.234E-01
   13 F13            -0.329E-02
   14 F14            -0.987E-03
   15 F15            -0.843E-02
   16 F16            -0.110E-01
   17 F17            -0.412E-02
   18 F18             0.826E-02
   19 F19            -0.151E-01
   20 F20            -0.335E-01
   21 F21            -0.378E-01
   22 F22            -0.271E-01
   23 F23            -0.332E-01
   24 F24            -0.235E-01
   25 F25            -0.115E-01
   26 F26            -0.516E-02
   27 F27             0.116E-02
   28 F28            -0.100E-01
   29 F29            -0.191E-02
   30 F30            -0.887E-02
   31 F31             0.525E-02
   32 F32             0.383E-01
   33 F33             0.249E-01
   34 F34             0.424E-01
   35 F35             0.148E-01
   36 F36             0.123E-02


WEIGHTED RESIDUALS AT LIMIT FOR INTERVAL     4; STARTING VALUES  1
OBSNO    OBS. NAME  WEIGHT. RES.
    1 F1              0.170E-01
    2 F2              0.175E-01
    3 F3              0.270E-01
    4 F4              0.490E-02
    5 F5             -0.198E-01
    6 F6             -0.203E-01
    7 F7              0.317E-01
    8 F8              0.250E-01
    9 F9              0.230E-01
   10 F10             0.824E-02
   11 F11            -0.175E-01
   12 F12            -0.195E-01
   13 F13            -0.333E-02
   14 F14            -0.101E-02
   15 F15            -0.847E-02
   16 F16            -0.111E-01
   17 F17            -0.431E-02
   18 F18             0.802E-02
   19 F19            -0.151E-01
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   20 F20           -0.335E-01
   21 F21           -0.378E-01
   22 F22           -0.272E-01
   23 F23           -0.333E-01
   24 F24           -0.236E-01
   25 F25           -0.116E-01
   26 F26           -0.522E-02
   27 F27            0.109E-02
   28 F28           -0.101E-01
   29 F29           -0.199E-02
   30 F30           -0.895E-02
   31 F31            0.520E-02
   32 F32            0.382E-01
   33 F33            0.249E-01
   34 F34            0.424E-01
   35 F35            0.147E-01
   36 F36            0.117E-02


WEIGHTED RESIDUALS AT LIMIT FOR INTERVAL     5; STARTING VALUES  1
OBSNO    OBS. NAME  WEIGHT. RES.
    1 F1             0.171E-01
    2 F2             0.175E-01
    3 F3             0.270E-01
    4 F4             0.499E-02
    5 F5            -0.197E-01
    6 F6            -0.202E-01
    7 F7             0.317E-01
    8 F8             0.250E-01
    9 F9             0.231E-01
   10 F10            0.829E-02
   11 F11           -0.174E-01
   12 F12           -0.194E-01
   13 F13           -0.333E-02
   14 F14           -0.101E-02
   15 F15           -0.846E-02
   16 F16           -0.111E-01
   17 F17           -0.431E-02
   18 F18            0.802E-02
   19 F19           -0.151E-01
   20 F20           -0.335E-01
   21 F21           -0.379E-01
   22 F22           -0.272E-01
   23 F23           -0.333E-01
   24 F24           -0.236E-01
   25 F25           -0.116E-01
   26 F26           -0.523E-02
   27 F27            0.108E-02
   28 F28           -0.101E-01
   29 F29           -0.199E-02
   30 F30           -0.895E-02
   31 F31            0.519E-02
   32 F32            0.382E-01
   33 F33            0.249E-01
   34 F34            0.424E-01
   35 F35            0.147E-01
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   36 F36             0.117E-02


WEIGHTED RESIDUALS AT LIMIT FOR INTERVAL     6; STARTING VALUES  1
OBSNO    OBS. NAME  WEIGHT. RES.
    1 F1              0.159E-01
    2 F2              0.163E-01
    3 F3              0.259E-01
    4 F4              0.387E-02
    5 F5             -0.208E-01
    6 F6             -0.213E-01
    7 F7              0.317E-01
    8 F8              0.250E-01
    9 F9              0.230E-01
   10 F10             0.774E-02
   11 F11            -0.184E-01
   12 F12            -0.204E-01
   13 F13            -0.334E-02
   14 F14            -0.103E-02
   15 F15            -0.848E-02
   16 F16            -0.111E-01
   17 F17            -0.428E-02
   18 F18             0.806E-02
   19 F19            -0.151E-01
   20 F20            -0.335E-01
   21 F21            -0.378E-01
   22 F22            -0.272E-01
   23 F23            -0.333E-01
   24 F24            -0.236E-01
   25 F25            -0.116E-01
   26 F26            -0.521E-02
   27 F27             0.110E-02
   28 F28            -0.101E-01
   29 F29            -0.198E-02
   30 F30            -0.894E-02
   31 F31             0.521E-02
   32 F32             0.382E-01
   33 F33             0.249E-01
   34 F34             0.424E-01
   35 F35             0.147E-01
   36 F36             0.118E-02


WEIGHTED RESIDUALS AT LIMIT FOR INTERVAL     7; STARTING VALUES  1
OBSNO    OBS. NAME  WEIGHT. RES.
    1 F1              0.172E-01
    2 F2              0.177E-01
    3 F3              0.273E-01
    4 F4              0.573E-02
    5 F5             -0.187E-01
    6 F6             -0.192E-01
    7 F7              0.317E-01
    8 F8              0.249E-01
    9 F9              0.227E-01
   10 F10             0.885E-02
   11 F11            -0.161E-01
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   12 F12            -0.183E-01
   13 F13            -0.332E-02
   14 F14            -0.103E-02
   15 F15            -0.847E-02
   16 F16            -0.110E-01
   17 F17            -0.418E-02
   18 F18             0.815E-02
   19 F19            -0.151E-01
   20 F20            -0.335E-01
   21 F21            -0.378E-01
   22 F22            -0.272E-01
   23 F23            -0.332E-01
   24 F24            -0.235E-01
   25 F25            -0.116E-01
   26 F26            -0.517E-02
   27 F27             0.114E-02
   28 F28            -0.100E-01
   29 F29            -0.195E-02
   30 F30            -0.892E-02
   31 F31             0.523E-02
   32 F32             0.383E-01
   33 F33             0.249E-01
   34 F34             0.424E-01
   35 F35             0.148E-01
   36 F36             0.120E-02


WEIGHTED RESIDUALS AT LIMIT FOR INTERVAL     8; STARTING VALUES  1
OBSNO    OBS. NAME  WEIGHT. RES.
    1 F1             0.146E-01
    2 F2             0.156E-01
    3 F3             0.261E-01
    4 F4             0.647E-02
    5 F5            -0.173E-01
    6 F6            -0.178E-01
    7 F7             0.331E-01
    8 F8             0.253E-01
    9 F9             0.211E-01
   10 F10            0.985E-02
   11 F11           -0.136E-01
   12 F12           -0.171E-01
   13 F13           -0.276E-02
   14 F14           -0.615E-03
   15 F15           -0.803E-02
   16 F16           -0.101E-01
   17 F17           -0.259E-02
   18 F18            0.101E-01
   19 F19           -0.145E-01
   20 F20           -0.329E-01
   21 F21           -0.371E-01
   22 F22           -0.263E-01
   23 F23           -0.322E-01
   24 F24           -0.224E-01
   25 F25           -0.110E-01
   26 F26           -0.463E-02
   27 F27            0.172E-02
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   28 F28           -0.939E-02
   29 F29           -0.124E-02
   30 F30           -0.816E-02
   31 F31            0.569E-02
   32 F32            0.387E-01
   33 F33            0.254E-01
   34 F34            0.429E-01
   35 F35            0.152E-01
   36 F36            0.172E-02


WEIGHTED RESIDUALS AT LIMIT FOR INTERVAL    -1; STARTING VALUES  1
OBSNO    OBS. NAME  WEIGHT. RES.
    1 F1             0.168E-01
    2 F2             0.173E-01
    3 F3             0.269E-01
    4 F4             0.533E-02
    5 F5            -0.191E-01
    6 F6            -0.196E-01
    7 F7             0.317E-01
    8 F8             0.249E-01
    9 F9             0.227E-01
   10 F10            0.864E-02
   11 F11           -0.165E-01
   12 F12           -0.187E-01
   13 F13           -0.333E-02
   14 F14           -0.104E-02
   15 F15           -0.848E-02
   16 F16           -0.110E-01
   17 F17           -0.418E-02
   18 F18            0.814E-02
   19 F19           -0.151E-01
   20 F20           -0.335E-01
   21 F21           -0.378E-01
   22 F22           -0.272E-01
   23 F23           -0.332E-01
   24 F24           -0.235E-01
   25 F25           -0.116E-01
   26 F26           -0.517E-02
   27 F27            0.115E-02
   28 F28           -0.100E-01
   29 F29           -0.195E-02
   30 F30           -0.891E-02
   31 F31            0.522E-02
   32 F32            0.383E-01
   33 F33            0.249E-01
   34 F34            0.424E-01
   35 F35            0.148E-01
   36 F36            0.120E-02


WEIGHTED RESIDUALS AT LIMIT FOR INTERVAL    -2; STARTING VALUES  1
OBSNO    OBS. NAME  WEIGHT. RES.
    1 F1             0.131E-01
    2 F2             0.142E-01
    3 F3             0.249E-01
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    4 F4              0.575E-02
    5 F5             -0.179E-01
    6 F6             -0.184E-01
    7 F7              0.345E-01
    8 F8              0.263E-01
    9 F9              0.217E-01
   10 F10             0.100E-01
   11 F11            -0.139E-01
   12 F12            -0.177E-01
   13 F13            -0.185E-02
   14 F14             0.258E-03
   15 F15            -0.715E-02
   16 F16            -0.909E-02
   17 F17            -0.145E-02
   18 F18             0.114E-01
   19 F19            -0.137E-01
   20 F20            -0.321E-01
   21 F21            -0.363E-01
   22 F22            -0.255E-01
   23 F23            -0.314E-01
   24 F24            -0.215E-01
   25 F25            -0.105E-01
   26 F26            -0.404E-02
   27 F27             0.232E-02
   28 F28            -0.879E-02
   29 F29            -0.624E-03
   30 F30            -0.754E-02
   31 F31             0.617E-02
   32 F32             0.391E-01
   33 F33             0.258E-01
   34 F34             0.433E-01
   35 F35             0.157E-01
   36 F36             0.217E-02


WEIGHTED RESIDUALS AT LIMIT FOR INTERVAL    -3; STARTING VALUES  1
OBSNO    OBS. NAME  WEIGHT. RES.
    1 F1              0.148E-01
    2 F2              0.152E-01
    3 F3              0.248E-01
    4 F4              0.326E-02
    5 F5             -0.212E-01
    6 F6             -0.216E-01
    7 F7              0.318E-01
    8 F8              0.249E-01
    9 F9              0.227E-01
   10 F10             0.763E-02
   11 F11            -0.184E-01
   12 F12            -0.206E-01
   13 F13            -0.331E-02
   14 F14            -0.102E-02
   15 F15            -0.846E-02
   16 F16            -0.110E-01
   17 F17            -0.416E-02
   18 F18             0.816E-02
   19 F19            -0.151E-01
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   20 F20            -0.335E-01
   21 F21            -0.378E-01
   22 F22            -0.272E-01
   23 F23            -0.332E-01
   24 F24            -0.235E-01
   25 F25            -0.115E-01
   26 F26            -0.516E-02
   27 F27             0.116E-02
   28 F28            -0.100E-01
   29 F29            -0.194E-02
   30 F30            -0.890E-02
   31 F31             0.523E-02
   32 F32             0.383E-01
   33 F33             0.249E-01
   34 F34             0.424E-01
   35 F35             0.148E-01
   36 F36             0.121E-02


WEIGHTED RESIDUALS AT LIMIT FOR INTERVAL    -4; STARTING VALUES  1
OBSNO    OBS. NAME  WEIGHT. RES.
    1 F1              0.171E-01
    2 F2              0.176E-01
    3 F3              0.273E-01
    4 F4              0.566E-02
    5 F5             -0.188E-01
    6 F6             -0.193E-01
    7 F7              0.317E-01
    8 F8              0.249E-01
    9 F9              0.227E-01
   10 F10             0.880E-02
   11 F11            -0.162E-01
   12 F12            -0.184E-01
   13 F13            -0.332E-02
   14 F14            -0.103E-02
   15 F15            -0.848E-02
   16 F16            -0.110E-01
   17 F17            -0.418E-02
   18 F18             0.814E-02
   19 F19            -0.151E-01
   20 F20            -0.335E-01
   21 F21            -0.378E-01
   22 F22            -0.272E-01
   23 F23            -0.332E-01
   24 F24            -0.235E-01
   25 F25            -0.116E-01
   26 F26            -0.517E-02
   27 F27             0.114E-02
   28 F28            -0.100E-01
   29 F29            -0.195E-02
   30 F30            -0.892E-02
   31 F31             0.522E-02
   32 F32             0.383E-01
   33 F33             0.249E-01
   34 F34             0.424E-01
   35 F35             0.148E-01
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   36 F36             0.120E-02


WEIGHTED RESIDUALS AT LIMIT FOR INTERVAL    -5; STARTING VALUES  1
OBSNO    OBS. NAME  WEIGHT. RES.
    1 F1              0.171E-01
    2 F2              0.176E-01
    3 F3              0.273E-01
    4 F4              0.567E-02
    5 F5             -0.188E-01
    6 F6             -0.193E-01
    7 F7              0.317E-01
    8 F8              0.249E-01
    9 F9              0.227E-01
   10 F10             0.881E-02
   11 F11            -0.162E-01
   12 F12            -0.184E-01
   13 F13            -0.332E-02
   14 F14            -0.103E-02
   15 F15            -0.847E-02
   16 F16            -0.110E-01
   17 F17            -0.418E-02
   18 F18             0.814E-02
   19 F19            -0.151E-01
   20 F20            -0.335E-01
   21 F21            -0.378E-01
   22 F22            -0.272E-01
   23 F23            -0.332E-01
   24 F24            -0.236E-01
   25 F25            -0.115E-01
   26 F26            -0.516E-02
   27 F27             0.115E-02
   28 F28            -0.100E-01
   29 F29            -0.195E-02
   30 F30            -0.892E-02
   31 F31             0.522E-02
   32 F32             0.383E-01
   33 F33             0.249E-01
   34 F34             0.424E-01
   35 F35             0.148E-01
   36 F36             0.120E-02


WEIGHTED RESIDUALS AT LIMIT FOR INTERVAL    -6; STARTING VALUES  1
OBSNO    OBS. NAME  WEIGHT. RES.
    1 F1              0.165E-01
    2 F2              0.170E-01
    3 F3              0.267E-01
    4 F4              0.504E-02
    5 F5             -0.194E-01
    6 F6             -0.199E-01
    7 F7              0.317E-01
    8 F8              0.249E-01
    9 F9              0.227E-01
   10 F10             0.849E-02
   11 F11            -0.167E-01
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   12 F12           -0.189E-01
   13 F13           -0.334E-02
   14 F14           -0.104E-02
   15 F15           -0.848E-02
   16 F16           -0.110E-01
   17 F17           -0.418E-02
   18 F18            0.814E-02
   19 F19           -0.151E-01
   20 F20           -0.335E-01
   21 F21           -0.378E-01
   22 F22           -0.272E-01
   23 F23           -0.332E-01
   24 F24           -0.235E-01
   25 F25           -0.115E-01
   26 F26           -0.516E-02
   27 F27            0.115E-02
   28 F28           -0.100E-01
   29 F29           -0.195E-02
   30 F30           -0.892E-02
   31 F31            0.523E-02
   32 F32            0.383E-01
   33 F33            0.249E-01
   34 F34            0.424E-01
   35 F35            0.148E-01
   36 F36            0.120E-02


WEIGHTED RESIDUALS AT LIMIT FOR INTERVAL    -7; STARTING VALUES  1
OBSNO    OBS. NAME  WEIGHT. RES.
    1 F1             0.171E-01
    2 F2             0.175E-01
    3 F3             0.271E-01
    4 F4             0.499E-02
    5 F5            -0.197E-01
    6 F6            -0.202E-01
    7 F7             0.317E-01
    8 F8             0.250E-01
    9 F9             0.231E-01
   10 F10            0.829E-02
   11 F11           -0.174E-01
   12 F12           -0.194E-01
   13 F13           -0.333E-02
   14 F14           -0.101E-02
   15 F15           -0.846E-02
   16 F16           -0.111E-01
   17 F17           -0.431E-02
   18 F18            0.802E-02
   19 F19           -0.151E-01
   20 F20           -0.335E-01
   21 F21           -0.379E-01
   22 F22           -0.272E-01
   23 F23           -0.333E-01
   24 F24           -0.236E-01
   25 F25           -0.116E-01
   26 F26           -0.524E-02
   27 F27            0.108E-02
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   28 F28           -0.101E-01
   29 F29           -0.199E-02
   30 F30           -0.895E-02
   31 F31            0.519E-02
   32 F32            0.382E-01
   33 F33            0.249E-01
   34 F34            0.424E-01
   35 F35            0.147E-01
   36 F36            0.118E-02


WEIGHTED RESIDUALS AT LIMIT FOR INTERVAL    -8; STARTING VALUES  1
OBSNO    OBS. NAME  WEIGHT. RES.
    1 F1             0.140E-01
    2 F2             0.150E-01
    3 F3             0.255E-01
    4 F4             0.603E-02
    5 F5            -0.177E-01
    6 F6            -0.182E-01
    7 F7             0.328E-01
    8 F8             0.249E-01
    9 F9             0.206E-01
   10 F10            0.954E-02
   11 F11           -0.138E-01
   12 F12           -0.173E-01
   13 F13           -0.303E-02
   14 F14           -0.895E-03
   15 F15           -0.832E-02
   16 F16           -0.104E-01
   17 F17           -0.283E-02
   18 F18            0.990E-02
   19 F19           -0.147E-01
   20 F20           -0.331E-01
   21 F21           -0.373E-01
   22 F22           -0.265E-01
   23 F23           -0.324E-01
   24 F24           -0.226E-01
   25 F25           -0.112E-01
   26 F26           -0.477E-02
   27 F27            0.158E-02
   28 F28           -0.954E-02
   29 F29           -0.139E-02
   30 F30           -0.832E-02
   31 F31            0.556E-02
   32 F32            0.386E-01
   33 F33            0.253E-01
   34 F34            0.428E-01
   35 F35            0.152E-01
   36 F36            0.161E-02
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