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 $\hat{M}^{a}_{\min} \le 0.01$ (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, $\hat{s}^2 = S\left(\hat{\boldsymbol{\theta}}\right)/(n-p)$.

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.