Techniques of Water-Resources Investigations of the United States Geological Survey

REGRESSION MODELING OF GROUND-WATER FLOW SUPPLEMENT 1—MODIFICATIONS TO THE COMPUTER CODE FOR NONLINEAR REGRESSION SOLUTION OF STEADY-STATE GROUND-WATER FLOW PROBLEMS

BOOK 3

CHAPTER B4

SUPPLEMENT 1

Techniques of Water-Resources Investigations of the United States Geological Survey

Chapter B4
Supplement 1

REGRESSION MODELING OF GROUND-WATER FLOW SUPPLEMENT 1--MODIFICATIONS TO THE COMPUTER CODE FOR NONLINEAR REGRESSION SOLUTION OF STEADY-STATE GROUND-WATER FLOW PROBLEMS

By Richard L. Cooley

Book 3
Applications of Hydraulics

U.S. DEPARTMENT OF THE INTERIOR

MANUEL LUJAN, Jr., Secretary

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PREFACE

The series of manuals on techniques describes procedures for planning and executing specialized work in water-resources investigations. The material is grouped under major subject headings called books and is further subdivided into sections and chapters; section B of Book 3 is on ground-water techniques.

This chapter is intended to be used as a supplement to the report "Regression modeling of ground-water flow" by R.L. Cooley and R.L. Naff, which was published as Chapter B4 of Book 3. The supplement details significant improvements to a computer program that simulates ground-water flow using nonlinear regression techniques.

TECHNIQUES OF WATER-RESOURCES INVESTIGATIONS OF THE U.S. GEOLOGICAL SURVEY

The U.S. Geological Survey publishes a series of manuals describing procedures for planning and conducting specialized work in water-resources investigations. The manuals published to date are listed below and may be ordered by mail from the **U.S. Geological Survey, Books and Open-File Reports Section, Federal Center, Box 25286, Denver, Colorado 80225** (an authorized agent of the Superintendent of Documents, Government Printing Office).

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TWRI 1-D1. Water temperature--influential factors, field measurement, and data presentation, by H.H. Stevens, Jr., J.F. Ficke, and G.F. Smoot. 1975. 65 pages.

TWRI 1-D2. Guidelines for collection and field analysis of ground-water samples for selected unstable constituents, by W.W. Wood. 1976. 24 pages.

TWRI 2-D1. Application of surface geophysics to ground-water investigations, by A.A.R. Zohdy, G.P. Eaton, and D.R. Mabey. 1974. 116 pages.

TWRI 2-D2. Application of seismic-refraction techniques to hydrologic studies, by F.P. Haeni. 1988. 86 pages.

TWRI 2-E1. Application of borehole geophysics to water-resources investigations, by W.S. Keys and L.M. MacCary. 1971. 126 pages.

TWRI 2-E2. Borehole geophysics applied to ground-water investigations, by W. Scott Keys. 1990. 150 pages.

TWRI 2-F1. Application of drilling, coring, and sampling techniques to test holes and wells, by Eugene Shuter and Warren E. Teasdale. 1989. 97 pages.

TWRI 3-A1. General field and office procedures for indirect discharge measurements, by M.A. Benson and Tate Dalrymple. 1967. 30 pages.

TWRI 3-A2. Measurement of peak discharge by the slope-area method, by Tate Dalrymple and M.A. Benson. 1967. 12 pages.

TWRI 3-A3. Measurement of peak discharge at culverts by indirect methods, by G.L. Bodhaine. 1968. 60 pages.

TWRI 3-A4. Measurement of peak discharge at width contractions by indirect methods, by H.F. Matthai. 1967. 44 pages.

TWRI 3-A5. Measurement of peak discharge at dams by indirect methods, by Harry Hulsing. 1967. 29 pages.

TWRI 3-A6. General procedure for gaging streams, by R.W. Carter and Jacob Davidian. 1968. 13 pages.

TWRI 3-A7. Stage measurements at gaging stations, by T.J. Buchanan and W.P. Somers. 1968. 28 pages.

TWRI 3-A8. Discharge measurements at gaging stations, by T.J. Buchanan and W.P. Somers. 1969. 65 pages.

TWRI 3-A9.[1] Measurement of time of travel in streams by dye tracing, by F.A. Kilpatrick and J.F. Wilson, Jr. 1989. 27 pages.

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[1]This manual is a revision of "Measurement of Time of Travel and Dispersion in Streams by Dye Tracing," by E.F. Hubbard, F.A. Kilpatrick, L.A. Martens, and J.F. Wilson, Jr., Book 3, Chapter A9, published in 1982.

TWRI 3-A10. Discharge ratings at gaging stations, by E.J. Kennedy. 1984. 59 pages.
TWRI 3-A11. Measurement of discharge by moving-boat method, by G.F. Smoot and C.E. Novak. 1969. 22 pages.
TWRI 3-A12. Fluorometric procedures for dye tracing, Revised, by J.F. Wilson, Jr., E.D. Cobb, and F.A. Kilpatrick. 1986. 41 pages.
TWRI 3-A13. Computation of continuous records of streamflow, by E.J. Kennedy. 1983. 53 pages.
TWRI 3-A14. Use of flumes in measuring discharge, by F.A. Kilpatrick, and V.R. Schneider. 1983. 46 pages.
TWRI 3-A15. Computation of water-surface profiles in open channels, by Jacob Davidian. 1984. 48 pages.
TWRI 3-A16. Measurement of discharge using tracers, by F.A. Kilpatrick and E.D. Cobb. 1985. 52 pages.
TWRI 3-A17. Acoustic velocity meter systems, by Antonius Laenen. 1985. 38 pages.
TWRI 3-A18. Determination of stream reaeration coefficients by use of tracers, by F.A. Kilpatrick, R.E. Rathbun, N. Yotsukura, G.W. Parker, and L.L. DeLong. 1989. 52 pages.
TWRI 3-A19. Levels at streamflow gaging stations, by E.J. Kennedy. 1990. 31 pages.
TWRI 3-B1. Aquifer-test design, observation, and data analysis, by R.W. Stallman. 1971. 26 pages.
TWRI 3-B2.[1] Introduction to ground-water hydraulics, a programmed text for self-instruction, by G.D. Bennet. 1976. 172 pages.
TWRI 3-B3. Type curves for selected problems of flow to wells in confined aquifers, by J.E. Reed. 1980. 106 pages.
TWRI 3-B4. Regression modeling of ground-water flow, by Richard L. Cooley and Richard L. Naff. 1990. 232 pages.
TWRI 3-B4, Supplement 1. Regression modeling of ground-water flow--Modifications to the computer code for nonlinear regression solution of steady-state ground-water flow problems, by R.L. Cooley. 1993. 8 pages.
TWRI 3-B5. Definition of boundary and initial conditions in the analysis of saturated ground-water flow systems--An introduction, by O. Lehn Franke, Thomas E. Reilly, and Gordon D. Bennett. 1987. 15 pages.
TWRI 3-B6. The principle of superposition and its application in ground-water hydraulics, by Thomas E. Reilly, O. Lehn Franke, and Gordon D. Bennett. 1987. 28 pages.
TWRI 3-B7. Analytical solutions for one-, two-, and three-dimensional solute transport in ground-water systems with uniform flow, by Eliezer, J. Wexler. 1991. 193 pages.
TWRI 3-C1. Fluvial sediment concepts, by H.P. Guy. 1970. 55 pages.
TWRI 3-C2. Field methods of measurement of fluvial sediment, by H.P. Guy and V.W. Norman. 1970. 59 pages.
TWRI 3-C3. Computation of fluvial-sediment discharge, by George Porterfield. 1972. 66 pages.
TWRI 4-A1. Some statistical tools in hydrology, by H.C. Riggs. 1968. 39 pages.
TWRI 4-A2. Frequency curves, by H.C. Riggs. 1968. 15 pages.
TWRI 4-B1. Low-flow investigations, by H.C. Riggs. 1972. 18 pages.
TWRI 4-B2. Storage analyses for water supply, by H.C. Riggs and C.H. Hardison. 1973. 20 pages.
TWRI 4-B3. Regional analyses of streamflow characteristics, by H.C. Riggs. 1973. 15 pages.
TWRI 4-D1. Computation of rate and volume of stream depletion by wells, by C.T. Jenkins. 1970. 17 pages.
TWRI 5-A1. Methods for determination of inorganic substances in water and fluvial sediments, by Marvin J. Fishman and Linda C. Friedman, editors. 1989. 545 pages.
TWRI 5-A2. Determination of minor elements in water by emission spectroscopy, by P.R. Barnett and E.C. Mallory, Jr. 1971. 31 pages.
TWRI 5-A3.[2] Methods for determination of organic substances in water and fluvial sediments, edited by R.L. Wershaw, M.J. Fishman, R.R. Grabbe, and L.E. Lowe. 1987. 80 pages.
TWRI 5-A4.[3] Methods for collection and analysis of aquatic biological and microbiological samples, by L.J. Britton and P.E. Greeson, editors. 1989. 363 pages.
TWRI 5-A5. Methods for determination of radioactive substances in water and fluvial sediments, by L.L. Thatcher, V.J. Janzer, and K.W. Edwards. 1977. 95 pages.

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[1]Spanish translation also available.

[2]This manual is a revision of TWRI 5-A3, "Methods of Analysis of Organic Substances in Water," by Donald F. Goerlitz and Eugene Brown, published in 1972.

[3]This manual supersedes TWRI 5-A4, "Methods for collection and analysis of aquatic biological and microbiological samples," edited by P.E. Greeson and others, published in 1977.

TWRI 5-A6. Quality assurance practices for the chemical and biological analyses of water and fluvial sediments, by L.C. Friedman and D.E. Erdmann. 1982. 181 pages.

TWRI 5-C1. Laboratory theory and methods for sediment analysis, by H.P. Guy. 1969. 58 pages.

TWRI 6-A1. A modular three-dimensional finite-difference ground-water flow model, by Michael G. McDonald and Arlen W. Harbaugh. 1988, 586 pages.

TWRI 6-A2. Documentation of a computer program to simulate aquifer-system compaction using the modular finite-difference ground-water flow model, by S.A. Leake and D.E. Prudic. 1991. 68 pages.

TWRI 6-A4. A modular finite-element model (MODFE) for areal and axisymmetric ground-water flow problems, part 2: Derivation of finite-element equations and comparisons with analytical solutions, by R.L. Cooley. 1992. 108 pages.

TWRI 7-C1. Finite difference model for aquifer simulation in two dimensions with results of numerical experiments, by P.C. Trescott, G.F. Pinder, and S.P. Larson. 1976. 116 pages.

TWRI 7-C2. Computer model of two-dimensional solute transport and dispersion in ground water, by L.F. Konikow and J.D. Bredehoeft. 1978. 90 pages.

TWRI 7-C3. A model for simulation of flow in singular and interconnected channels, by R.W. Schaffranek, R.A. Baltzer, and D.E. Goldberg. 1981. 110 pages.

TWRI 8-A1. Methods of measuring water levels in deep wells, by M.S. Garber and F.C. Koopman. 1968. 23 pages.

TWRI 8-A2. Installation and service manual for U.S. Geological Survey monometers, by J.D. Craig. 1983. 57 pages.

TWRI 8-B2. Calibration and maintenance of vertical-axis type current meters, by G.F. Smoot and C.E. Novak. 1968. 15 pages.

CONTENTS

Regression Modeling of Ground-Water Flow Supplement 1--Modifications to the Computer Code for Nonlinear Regression Solution of Steady-State Ground-Water Flow Problems

By Richard L. Cooley

Abstract

Modifications to the computer code for nonlinear regression solution of steady-state ground-water flow problems in "Regression Modeling of Ground-Water Flow", by R.L. Cooley and R.L. Naff (U.S. Geological Survey, Techniques of Water Resources Investigations, book 3, chap. B4, 1990), improve the performance of the code. The changes 1) allow any model parameters to be transformed to natural logarithms, and 2) improve the procedure for computing the parameter that damps changes in the values of model parameters for each iteration of the solution method. In addition, the user is shown how to read prior information separately from the initial set of parameter values.

Introduction

The purpose of this supplement is to document three types of modifications to the computer code for nonlinear regression solution of steady-state ground-water flow problems given in Cooley and Naff (1990, p. 133-161). First, any parameter can be transformed to its natural logarithm. This transformation allows the use of log-normal prior information and, when applied to transmissivity, can reduce the degree of nonlinearity of the model (Carrera and Neuman, 1986, p. 214). Second, the damping parameter, ρ (Cooley and Naff, 1990, p. 63), is computed using an algorithm employed by Cooley and Vecchia (1987) and Vecchia and Cooley (1987). This algorithm often decreases the number of iterations needed for convergence and can induce convergence when the old method fails. Third, prior information can be read separately from the initial parameter values in any manner the user implements. (At present, the prior information is the set of initial parameter values.) By reading the prior information separately, the user can start the regression from a more favorable set of parameter values than those specified as prior information.

Log Transformation of Parameters

For the modified Gauss-Newton method, the nonlinear model $f(\underline{\xi},\underline{b})$ is approximated by a linear model of the form (Cooley and Naff, 1990, p. 61)

$$f(\underline{\xi},\underline{b}) \approx f(\underline{\xi},\underline{b}_0) + \underline{X}_0(\underline{b}-\underline{b}_0), \qquad (1)$$

where

$\underline{b}$ is a column p-vector of model parameter,
$\underline{b}_0$ is an initial column p-vector of model parameters,
$\underline{\xi}$ is a vector of independent variables, and
$\underline{X}_0$ is a row p-vector of sensitivities, defined by

$$\underline{X}_0 = \{X_j^0\} = \left\{ \frac{\partial f}{\partial b_j}\bigg|_{\underline{b}=\underline{b}_0} \right\}, \qquad (2)$$

where

b_j is an element of $\underline{b}$.

Let p_k be a model parameter that is to be log transformed and b_k be the log-transformed parameter, so that

$$b_k = \ln p_k, \qquad (3)$$

Then the sensitivity for this parameter is computed from

$$X_k^0 = \frac{\partial f}{\partial b_k}\bigg|_{\underline{b}=\underline{b}_0} = \left(\frac{\partial f}{\partial p_k} \frac{dp_k}{db_k} \right)_{\underline{b}=\underline{b}_0} = p_k^0 \frac{\partial f}{\partial p_k}\bigg|_{\underline{b}=\underline{b}_0}, \qquad (4)$$

where

p_k^0 is the initial value of p_k, and

$\partial f / \partial p_k$ is the sensitivity to parameter p_k calculated using the methods given in Cooley and Naff (1990, p. 83-85).

When applied to n observations, $f(\underline{\xi},\underline{b})$ becomes the n-vector $\underline{f}(\underline{\xi},\underline{b})$ and $\underline{X}_0$ becomes the $n \times p$ matrix $\underline{\underline{X}}_0$ in equations 3.3-5 and 3.3-6 in Cooley and Naff (1990, p. 61).

The model parameters to be log transformed are read in a new subroutine that is incorporated into the code (see the appendix). Input data are read as Data Set LT, which is inserted between Data Sets T and U. All initial parameter values are read as usual in Data Sets P, R and T, and values of log-transformed parameters may be read either in natural or log units, depending on the value of the user-specified indicator IEXP. Regardless of how they are read, all parameters are used in log-transformed form if identified using ILT(I) (see below). Parameters identified by ILT(I) and read for alternate solutions in Data Set V must be in log units.

Data Set LT.

The first line is read with format 2I5 as follows:

Line columns	Variable	Definition
1 - 5	NLTP	Number of model parameters log transformed.
6 -10	IEXP	Indicator stating whether the parameters identified by ILT(I) (see below) and read in Data Sets P, R, and T are in natural or log units. IEXP=0 if the units are natural and IEXP=1 if the units are logs.

The second and subsequent lines are only read if NLTP is greater than zero. These lines are read with format 16I5 as follows:

Line columns	Variable	Definition
1- 5	ILT(1)	Parameter numbers identifying model parameters that are log transformed.
6-10	ILT(2)	
.	.	
.	.	
.	.	
76-80	ILT(16)	
1- 5	ILT(17)	
.	.	
.	.	
.	.	
	ILT(NLTP)	

Output of data read in Data Set LT is only obtained if NLTP is greater than zero. In this case parameter numbers ILT(I) are listed. All output is transformed as appropriate to apply for the log-transformed parameters in log units.

Calculation of Damping Parameter

The damping parameter, ρ, is used to damp changes in model parameters over an iteration of the modified Gauss-Newton method (see Cooley and Naff, 1990, p. 61-72), so that

$$b_j^{r+1} = \rho_{r+1} d_j^{r+1} + b_j^r, \qquad (5)$$

where

d_j^{r+1} is the change in parameter b_j over iteration $r+1$ without damping, and

ρ_{r+1} is the damping parameter for iteration $r+1$.

The new calculation procedure for the damping parameter is as follows: Let t_{r+1} be the value of d_j^{r+1}/c_j for which $|t_{r+1}| = \max_j |d_j^{r+1}|/c_j$ (where $c_j = |b_j^r|$ if $|b_j^r| \geq 1\times10^{-10}$ and $c_j = 1$ if $|b_j^r| < 1\times10^{-10}$). Also, let t_{mx} be the maximum value of $|b_j^{r+1} - b_j^r|/c_j$ permitted for any iteration (Cooley and Naff, 1990, p. 72). Then a damping parameter ρ_{r+1} is calculated using the following three-step algorithm. In this algorithm, an intermediate damping parameter, ρ^*, is calculated to be less than unity if an oscillation in t is detected between iterations r and $r+1$. If the maximum change in a parameter value using ρ^* would be larger than permitted by t_{mx}, then ρ_{r+1} is computed by reducing ρ^* so that the maximum change equals t_{mx}; otherwise ρ_{r+1} equals ρ^*.

1. $$s = \frac{t_{r+1}}{\rho_r t_r} \quad , r > 0$$
   $$s = 1 \quad , r = 0$$

2. $$\rho^* = \frac{3+s}{3+|s|} \quad , s \geq -1$$
   $$\rho^* = \frac{1}{2|s|} \quad , s < -1$$

3. $$\rho_{r+1} = \rho^* \quad , \rho^*|t_{r+1}| \leq t_{mx}$$
   $$\rho_{r+1} = \frac{t_{mx}}{|t_{r+1}|} \quad , \rho^*|t_{r+1}| > t_{mx}$$

No new input is needed by the new method, and no new output is generated. Parameter t_{mx} is read as DMX in Data Set C and often need not be as small as required by the old method to induce convergence.

Reading Prior Information

The code may be modified to allow prior information to be different from the initial model parameter values read in Data Sets P, R, and T. Any prior value may be changed from the initial parameter value by reading a new value of P(I) (where I is the parameter number) immediately after the DO loop that ends with statement label 137 (see the appendix). Values read for log-transformed parameters must be in log units. Because no changes have been made in the code to accommodate this, the user is expected to add the appropriate read and write statements according to his or her needs.

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Carrera, Jesus, and Neuman, S.P., 1986, Estimation of aquifer parameters under transient and steady state conditions, 2--Uniqueness, stability, and solution algorithms: Water Resources Research, v. 22, no. 2, p. 211-227.

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Cooley, R.L., and Vecchia, A.V., 1987, Calculation of nonlinear confidence and prediction intervals for ground-water flow models: Water Resources Bulletin, v. 23, no. 4, p. 581-599.

Vecchia, A.V., and Cooley, R.L., 1987, Simultaneous confidence and prediction intervals for nonlinear regression models with application to a groundwater flow model: Water Resources Research, v. 23, no. 7, p. 1237-1250.

Appendix: Coding Changes

In the following listings taken from files INVFD.FOR and INVSUB.FOR, lines changed or added are shaded, and adjacent unchanged lines are included so that the user can locate the changes to be made. Array B, which originally had a minimum dimension of N_R+N_n (where N_R is the total number of regression parameters and N_n is the number of zonal aquifer properties that are not regression parameters), now must have a minimum dimension of N_R. Array BD must have a minimum dimension of N_R+N_n, and array ILT must have a minimum dimension equal to the number of log-transformed parameters.

Changes to INVFD.FOR.

```
      DIMENSION TITLE(20),DX(30),DY(30),CX(500),CY(500),VL(500)
     1,QR(500),WELL(500),HR(500),HC(500),HCI(70),BK(70),BL(70)
     2,BM(70),BN(70),HO(70),W(70),PAR(4),QBF(50),PLA(50),PLB(50)
     3,CXHR(50),CXHL(50),CYHT(50),CYHB(50),AU(5,250),AL(20,250)
     4,V(500),X(20,70),S(20,90),XV(500),XS(4),P(20),WP(20)
     5,A(20,20),B(20)
      DIMENSION BD(50),ILT(20)
      DIMENSION JPOS(30),IZN(500),IBZN(50),IPRM(4,20),IBNA(50)
     1,IBNB(50),IBPA(10),IBPB(10),IBHN(50),IHSN(100),KOBS(70)
     2,LN(4),NCBA(20),NCEA(20),NCBF(20),NCEF(20),NCBH(20)
     3,NCEH(20),ILOC(500),JLOC(500),IN(500),IC(5,250)
      COMMON/INT/NIJ,NEQ,ICR,ICR1,IB1,LH1,ID,JD,IM,JM,NOBS,NQSD,NBH
     1,NVAR,NVX2,KOUNT,INDT,IPO
      COMMON/LOC/ILOC,JLOC
      COMMON/TNME/IIN,IOUT
      COMMON/FLT/CX,CY,VL,QR,WELL,HR,HC,BK,BL,BM,BN,HO,W
      COMMON/SOLV/AU,AL
      COMMON/REG/DMX,DMAX,ADMX,AP,CSA,AMP,RP,BP,YSQ
      EQUIVALENCE (TITLE(1),A(1,1),S(1,1),AU(1,1)),(HC(1),XV(1))
     1,(CX(1),HCI(1)),(ILOC(1),IC(1,1))


      DO 40 K=1,4
      L=IPRM(K,I)
      IF(L.GT.0) GO TO 40
      M=M+1
      L=M
      IPRM(K,I)=L
   40 BD(L)=PAR(K)
   45 CONTINUE


      K=K+1
      TEMP=DX(K)
      IF(M.EQ.ID) TEMP=DY(K)
      QBF(N)=QBM*TEMP
   66 IBZN(N)=IP
   68 BD(IP)=QB
      WP(IP)=SDQB
      GO TO 80
   70 TMP=QB*QBM
```

```
      IBPA(IZ)=M
      IBPB(IZ)=N
      IF(M.LT.1) GO TO 97
      BD(M)=V(1)
      WP(M)=SDHA
   97 IF(N.LT.1) GO TO 98
      BD(N)=V(NN)
      WP(N)=SDHB
   98 J=JLOC(1)


  122 CONTINUE
C**SET UP D4 ORDERING
      CALL ORDER(JPOS,IN,IC)
C**COMPUTE INITIAL SOLUTION
      DO 130 I=1,NVAR
  130 B(I)=BD(I)
      CALL SETLT(B,BD,ILT,NLTP)
      CALL COEF(WELL,HR,HC,CX,CY,VL,QR,CXHR,CXHL,CYHT,CYHB,QBF,BD,AU,AL
     1,V,IZN,IBZN,IPRM,IBNA,IBNB,IN,IC,NAD)
      CALL D4SOLV(HC,AU,AL,V,IN,IC,NAD)
      WRITE(IOUT,846)


      DO 137 I=1,NVAR
      P(I)=B(I)
      IF(WP(I).LE.0.) GO TO 137
      WP(I)=EV/(WP(I)*WP(I))
      NPRIR=NPRIR+1
  137 CONTINUE
      WRITE(IOUT,848) NPRIR
C**INSERT READ AND WRITE STATEMENTS HERE FOR NEW VALUES OF P(I)
C**INITIALIZE BEGINNING AND END POINT ARRAYS
      DO 148 I=1,NVAR


  174 INDT=0
      ER=.01
      ERP=.001
      DMAX=DMX
      AP=1.
      AMP=0.
      NVX2=NVAR+NVAR
      KOUNT=0
  176 KOUNT=KOUNT+1
      REWIND ITA
C**SOLVE FOR SENSITIVITIES:
      KLT=1
      DO 260 N=1,NVAR
      DO 178 I=1,NEQ
  178 V(I)=0.
```

```
      DO 240 I=2,II
      L=IC(I,KK)
      V(KK)=V(KK)-AU(I,KK)*V(L)
  240 CONTINUE
  250 CONTINUE
      CALL SENLT(BD,V,ILT,N,KLT,NEQ)
      WRITE(ITA) (V(I),I=1,NEQ)
C**COMPUTE SENSITIVITIES AT OBSERVATION POINTS


  265 CONTINUE
C**CALL LEAST SQUARES
  270 CALL LSTSQ(HC,BK,BL,BM,BN,HO,W,P,WP,X,A,B,V,KOBS,IN,NVD)
      DO 280 I=1,NVAR
  280 BD(I)=B(I)
      IF(NLTP.GT.0) CALL LOGT(BD,ILT,NLTP)
      IF(INDT.GT.0) GO TO 515
C**COMPUTE NEW SPECIFIED HEADS
      IF(NBH.LT.1) GO TO 310


  300 CONTINUE
C**CHECK FOR CONVERGENCE
  310 IF(ADMX.LT.ER) GO TO 350
C**COMPUTE NEW HEADS AT GRID POINTS
      CALL COEF(WELL,HR,HC,CX,CY,VL,QR,CXHR,CXHL,CYHT,CYHB,QBF,BD,AU,AL
     1,V,IZN,IBZN,IPRM,IBNA,IBNB,IN,IC,NAD)
      CALL D4SOLV(HC,AU,AL,V,IN,IC,NAD)
C**CHECK FOR PARAMETERS GOING TO ZERO
      IND=0


  670 B(I)=PR
      WRITE(IOUT,892)
      CALL PRTOT(B,NVAR,0,1)
      DO 675 I=1,NVAR
  675 BD(I)=B(I)
      IF(NLTP.GT.0) CALL LOGT(BD,ILT,NLTP)
      IF(NBH.LT.1) GO TO 685
      DO 680 N=1,NBH
      M=IBZN(N+NQSD)
      K=IBPA(M)
      TMPA=0.


      J=IBHN(N)
  680 HC(J)=HC(J)+TMPA+TMPB
  685 CALL COEF(WELL,HR,HC,CX,CY,VL,QR,CXHR,CXHL,CYHT,CYHB,QBF,BD,AU,AL
     1,V,IZN,IBZN,IPRM,IBNA,IBNB,IN,IC,NAD)
      CALL D4SOLV(HC,AU,AL,V,IN,IC,NAD)
```

Changes to INVSUB.FOR.

```
      SUBROUTINE LSTSQ(HC,BK,BL,BM,BN,HO,W,P,WP,X,C,B,V,KOBS,IN,NVD)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION HC(1),BK(1),BL(1),BM(1),BN(1),HO(1),W(1),P(1),WP(1)
     1,X(NVD,1),C(NVD,1),B(1),V(3)
      DIMENSION KOBS(1),IN(1)
      COMMON/INT/NIJ,NEQ,ICR,ICR1,IB1,LH1,ID,JD,IM,JM,NOBS,NQSD,NBH
     1,NVAR,NVX2,KOUNT,INDT,IPO
      COMMON/TNME/IIN,IOUT
      COMMON/REG/DMX,DMAX,ADMX,AP,CSA,AMP,RP,BP,YSQ
C**CHECK FOR NONZERO MARQUARDT PARAMETER
      NM1=NVAR-1
      IF(AMP.LT.-.5) GO TO 105


C**COMPUTE AND PRINT PARAMETERS
  200 ADMX=0.
      DMXO=DMAX
      DO 202 J=1,NVAR
      V(J)=V(J)/V(J+NVX2)
      TMPA=DABS(B(J))
      IF(TMPA.LT.1.D-10) TMPA=1.
      TMPA=V(J)/TMPA
      TMPB=DABS(TMPA)
      IF(TMPB.LT.ADMX) GO TO 202
      DMAX=TMPA
      ADMX=TMPB
  202 CONTINUE
      IF(KOUNT.LT.2) GO TO 205
      SPR=DMAX/(AP*DMXO)
      IF(SPR.LT.-1.) GO TO 204
      AP=(3.+SPR)/(3.+DABS(SPR))
      GO TO 205
  204 AP=.5/DABS(SPR)
  205 IF(AP*ADMX.GT.DMX) AP=DMX/ADMX
      DO 206 J=1,NVAR
      V(J)=AP*V(J)
  206 B(J)=V(J)+B(J)
      WRITE(IOUT,220) KOUNT,YSQ,DET,AMP,AP
      WRITE(IOUT,230) (B(J),J=1,NVAR)
      RETURN
```

Added subroutines.

```
      SUBROUTINE SETLT(B,BD,ILT,NLTP)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION B(1),BD(1),ILT(1)
      COMMON/TNME/IIN,IOUT
      ILT(1)=0
C**READ PARAMETER NUMBERS FOR LOG-TRANSFORMED PARAMETERS
      READ(IIN,40) NLTP,IEXP
      IF(NLTP.LT.1) RETURN
      WRITE(IOUT,50) IEXP
      READ(IIN,40) (ILT(I),I=1,NLTP)
      WRITE(IOUT,60) (ILT(I),I=1,NLTP)
C**EXPONENTIATE PARAMETERS
      IF(IEXP.LT.1) GO TO 20
      DO 10 I=1,NLTP
      J=ILT(I)
   10 BD(J)=DEXP(BD(J))
      RETURN
C**TAKE LOGS OF PARAMETERS
   20 DO 30 I=1,NLTP
      J=ILT(I)
   30 B(J)=DLOG(B(J))
      RETURN
C
   40 FORMAT (16I5)
   50 FORMAT (43H0ARE INITIAL PARAMETERS LOGS? (1=YES, 0=NO),I5)
   60 FORMAT (49H0PARAMETER NUMBERS FOR LOG-TRANSFORMED PARAMETERS
     1/(1H ,16I5))
      END
      SUBROUTINE LOGT(BD,ILT,NLTP)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION BD(1),ILT(1)
C**EXPONENTIATE LOG-TRANSFORMED PARAMETERS
      DO 20 I=1,NLTP
      J=ILT(I)
   20 BD(J)=DEXP(BD(J))
      RETURN
      END
      SUBROUTINE SENLT(BD,X,ILT,J,K,NEQ)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION BD(1),X(1),ILT(1)
C**TRANSFORM SENSITIVITIES CORRESPONDING TO LOG-TRANSFORMED PARAMETERS
      IF(J.NE.ILT(K)) RETURN
      K=K+1
      TMP=BD(J)
      DO 10 I=1,NEQ
   10 X(I)=X(I)*TMP
      RETURN
      END
```

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