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PERCOL USER'S MANUAL

R. J. Serne and R. C. Routson

Battelle
Pacific Northwest Laboratories
Richland, Washington 99352

1973

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by

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Water and Land Resources Department

1973

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SUMMARY

Research being conducted under the Radionuclides in Soils Program is attempting to predict the distribution and movement of liquid wastes in the heterogeneous subsurface environment of the Hanford Reservation. As part of this program, a transport model is being developed to predict chemical phenomena in soil-waste reactions. This document describes the use of the PERCOL model, which was developed as a simplified one-dimensional precursor to the transport model. PERCOL numerically describes the complex chemical reactions which occur during percolation of a waste solution through a porous media. This User's Manual describes the main program (PERCOL) and two subroutines (NEWTIT and DIST) and gives procedures for accessing these programs, inputting data to them and interpreting the output.

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PERCOL USER'S MANUAL

INTRODUCTION

The objective of the "Radionuclides in Soils" program being conducted by Battelle-Northwest for the Atlantic Richfield Hanford Company is development of tools for managing groundwater resources. As part of this program a transport model has been developed to predict the movement of contaminants in groundwater systems. Another model, PERCOL, was developed to describe the complex chemical reactions which occur during percolation of waste solutions through porous media such as soils. The PERCOL model can also be used as a simplified one-dimensional transport model; in this capacity, with support from experimental studies utilizing soil columns, PERCOL has been used as a precursor of the more complex transport model. This report is intended to provide the necessary direction for use of the PERCOL computer model. More detailed theory can be found in BNWL 1718.[1]

The PERCOL program is an extended and revised version of a program developed by Dutt[2] and Tanji[3] for predicting the quality of water and breakthrough of contaminants at incremental lengths throughout a soil profile. Basically the use of the computer code entails the input of the initial values for all the chemical species present in solution and in the soil as well as the values for the soil and solution volumes; in addition, the output values corresponding to the equilibrium conditions in solution and on the soil must be interpreted. The calculations thus produced are input to the transport model of the Radionuclides in Soils program.

PERCOL solves a one-dimensional version of the transport equation. Diffusion and dispersion are neglected and a Lagrangian coordinate system (following a fixed mass of fluid as it moves in space) is utilized.

This report gives detailed procedures for accessing the main program and two subroutines (NEWTIT AND DIST), inputting data, and interpreting the resulting output. The Appendices contain sample input cards, program listings, and output.

THE PERCOL PROGRAM

A soil column is divided into K separate cells, called soil subdivisions, to facilitate numerical calculations of the macro species concentrations (macro constituents are those species which are present in sufficient concentrations to appreciably affect the ionic strength of the solution and cation exchange sites available on the soil). A soil subdivision represents a homogeneous layer of soil. Thus a column consisting of several soil types is modeled with integral numbers of different soil subdivisions.

To model trace constituent sorption it was found necessary to further subdivide each K^{th} soil subdivision to prevent numerical dispersion. This partitioning is necessary only for modeling the sorption of the trace constituents and is represented by the variable JSUB.

All macro species chemical reactions take place in K soil subdivisions and all micro trace sorption reactions take place in (JSUB) X (K) partitions. In a saturated regime a pore volume of influent is introduced into the top subdivision and batch type chemical equilibria are calculated. The equilibrated effluent solution from the first subdivision becomes the influent to the second subdivision and batch type equilibria are again calculated. The pore volume of solute moves into successive subdivisions and equilibrates until it exits the last subdivision as effluent. A fresh aliquot is then initiated in the top cell and the sequence is repeated until the desired quantity of effluent is reached. Figure 1 is a conceptualization of the solute movement.

Additional assumptions which bear on the utilization of PERCOL are listed in Appendix A.

PERCOL has two subroutines, NEWTIT AND DIST. NEWTIT uses a numerical technique to solve for the real root of an equation $F(x)=0$. This equation determines the equilibrium concentrations of the chemical species which are reacting by precipitation, cation exchange, etc. Subroutine DIST calculates the empirical distribution constant Kd for sorption of each trace constituent. Details on the specific chemical reactions involved and a discussion of the empirical distribution constant can be found in BNWL 1718.[1]

PERCOL input consists of:

- soil column parameters - soil volume, number of soil subdivisions, bulk density, soluble salt content, cation exchange capacity, slightly soluble crystalline salt content

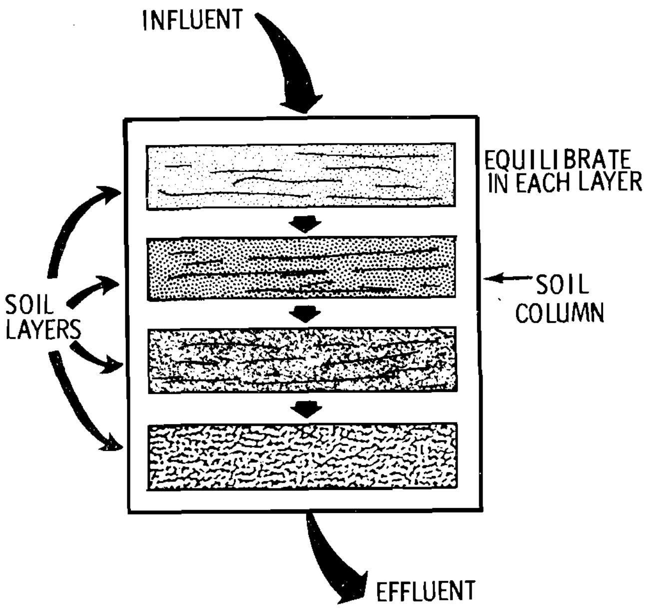

FIGURE 1. Solute Movement in PERCOL Model

- solution parameters - volume of soil to be percolated, concentration of all constituents in the solution, pH
- chemical reaction parameters - empirical ion exchange constants

Input for the subroutine NEWTIT consists of an approximation of the root x, the function F(x), the first derivative of the function and several indices containing logical information. All of this input is automatically generated in PERCOL.

Input for the subroutine DIST consists of the concentrations of chemical species in the waste solution, the soil type present, and the Kd predictor equation for the trace constituent of interest. The Kd predictor equation is added to the subroutine by the user. The other input is automatically transferred from the main program.

ACCESS

At present the PERCOL program and its subroutines are available in a FORTRAN IV punched deck consisting of about 700 cards which is set up to run on a UNIVAC 1108 computer.

INPUT REQUIREMENTS

The input requirements for the PERCOL model vary depending on the options chosen. Regardless of the options being used, all input data are transferred to the computer on data cards. The data needed if the soil column is originally dry are different from those used if the soil column is initially wet and well leached. If the soil column is nonhomogeneous each cell requires its own set of input data cards; only one set of data cards is necessary for a homogeneous soil column, however, as the computer program automatically generates the necessary input data for all the remaining soil cells.

The required input for PERCOL is arranged in four basic categories:

- descriptive or control parameters
- empirical data for ion exchange reactions
- soil column dimensions and constituents
- waste solution volumes and concentrations

Two examples of a typical input arrangement are given in Appendix B.

Descriptive Parameters

For all options, the first card in the data deck contains a number of TRUE or FALSE answers concerning the program options to be used. The TRUE or FALSE input determines conditions to be simulated. The options for TRUE or FALSE responses are presented as statements, as follows (each option statement is coded into the computer as a variable):

The first statement is, "The soil column is dry and evaporated salts are present" (the variable which controls this statement is DRY). If the statement is true, the first aliquot of waste solution containing the soil will dissolve the soluble salts present in the dry soil. If the statement is false, the column is assumed to be wet and evaporated salts have already been leached from the soil.

The second statement is, "The soil profile is homogeneous and chemical concentrations are initially the same" (the variable which controls this statement is UNI). If the statement is true, only one set of chemical data cards is needed and the computer generates identical values for the rest of the soil cells throughout the column. If the statement is false, separate sets of data cards must be input for each soil subdivision.

The third statement reads, "Print all initial and equilibrium chemical concentrations at each soil subdivision" (the variable which controls this statement is PRINT). If the statement is true, a large amount of output is generated. For the average problem this output is unnecessary, but in the debugging phase the printing may aid the user. If the statement is false, only the equilibrium concentrations of the solution effluent and of the last soil subdivision are printed. In most applications these effluent concentration data are the desired quantities.

The fourth statement is, "Print all equilibrium chemical concentrations at each subdivision" (the variable which controls this statement is PRI). This statement, when true, allows only the equilibrium values at all subdivisions to be printed. This permits a more comprehensive output of the effluent from each subdivision and the equilibrium soil conditions, but neglects the initial values entering the soil subsections. Since the effluent from subdivision K-1 is the influent to subdivision K, initial data for all but the first cell can be gleaned from this output.

Empirical Data for Ion Exchanges

Three ion exchange reactions are included in the PERCOL model.[1] Each soil type is uniquely selective for the major competing ions in the Hanford waste streams. Numerical description of the ion exchange phenomena between two cations and the soil exchange sites requires two empirical constants; the procedures for measuring the constants are described in BNWL 1721.[4] At present three sets of cation exchange reactions are included in PERCOL. The necessary input variables follow:

P1 = empirical activity correction for solid phase ratio $\frac{MgX}{CaX}$

FK1 = empirical ion exchange selectivity constant for Mg^{++} replacing Ca^{++} on the soil

P2 = empirical activity correction for solid phase ratio $\frac{NaX}{CaX}$

FK2 = empirical ion exchange selectivity constant for Na^{+} replacing Ca^{++} on the soil

P3 = empirical activity correction for solid phase ratio $\frac{KX}{NaX}$

FK3 = empirical ion exchange constant for K^+ replacing Na^+

Soil Column Parameters

The parameters which specify column sizes, numbers of subdivisions, and soil chemical characteristics are given below. Variables which must be specified whether the soil column is initially dry or wet include:

K = number of subdivisions in which soil column is divided. At present the program is dimensioned for a maximum K=20

VSOIL = total volume of soil column (units must correspond with units on solution aliquot size); i.e., cm^3-cm^3, etc.

JSUB = number of partitions into which each soil subdivision is further divided to aid the mathematical computations involved in trace constituent sorption. Macro reactions are carried out in K subdivisions and micro (trace) sorption divided in JSUB partitions for each K^{th} subdivision. A total trace partition (JSUB) X (K) equal to the physical length of the laboratory column (cm) has proven to give the best results. For example, a 50 cm column is modeled with K=10 and JSUB=5. At present, the column is dimensioned for a maximum JSUB=50

PORE = the empirically determined effective porosity of the soil column. The value is less than one and represents the drainable pore space

CAL = calcium carbonate (moles/gm) found in soil

GYP = calcium sulfate (moles/gm) found in soil

CAF = calcium fluoride (moles/gm) found in soil

SRS = initial trace constituent concentration sorbed on soil (for radioactive substances units cpm/gm, or mc/gm, etc.)

B11 = moisture percentage at which soil extract runs =

100 (gms H_2O/gm Soil)

B2 = moisture percentage at saturation

$$100 \frac{(PD-BD)}{(PD \cdot BD)}$$

where PD = particle density in gm/cm^3, usually set at 2.65, and BD = soil bulk density in gm/cm^3

B3 = percent saturation in the soil column being modeled

Additional soil parameters for initially dry soils are:

SOCA = readily soluble calcium (meq/liter) found in the B11 soil-solution extract (example: 100 gms initially dry soil is equilibrated with X mls distilled water; the solution extract is then measured for Ca)

SOMG = readily soluble magnesium (meq/liter) found in the B11 soil-solution extract

SONA = readily soluble sodium (meq/liter) found in the B11 soil-solution extract

SOK = readily soluble potassium (meq/liter) found in the B11 soil-solution extract

SOSR = readily soluble stable strontium (meq/liter) found in the B11 soil-solution extract

SOCL = readily soluble chloride (meq/liter) found in the B11 soil-solution extract

SOSO4 = readily soluble sulfate (meq/liter) found in the B11 soil-solution extract

SOHCO3 = readily soluble bicarbonate (meq/liter) found in the B11 soil-solution extract

EC = cation exchange capacity of soil (meq/gm)

Additional parameters for initially wet soil from which readily soluble salts have already been removed are:

CT = exchangeable magnesium sorbed on the soil (moles/gm)

RSR = exchangeable stable strontium sorbed on the soil (moles/gm)

ET = exchangeable calcium sorbed on the soil (moles/gm)

RP = exchangeable potassium sorbed on the soil (moles/gm)

SAT = exchangeable sodium sorbed on the soil (moles/gm)

Waste Solution Parameters

The reactions which take place as a solution percolates through porous media depend upon the chemical makeup of the solution. Thus solution constituents are necessary input to the PERCOL model. Waste solution parameters are:

WCA = calcium ion concentration in solution (meq/liter)

WMG = magnesium concentration in solution (meq/liter)

WNA = sodium concentration in solution (meq/liter)

WK = potassium concentration in solution (meq/liter)

WSR = strontium concentration in solution (meq/liter)

WCL = chloride concentration in solution (meq/liter)

WSO4 = sulfate concentration in solution (meq/liter)

WHCO3 = bicarbonate concentration in solution (meq/liter)

WNO3 = nitrate concentration in solution (meq/liter)

WFL = fluoride concentration in solution (meq/liter)

CASOI = associated calcium sulfate complex in solution (moles/liter)

APH = pH of solution

SRIN = influent concentration of trace ion being investigated; units to correspond to units on SRS (cpm/ml or mc/ml)

If more than one tracer is to be studied at once, SRIN1, SRIN2, etc., must be programmed in and appropriate variables throughout PERCOL added:

ALI = volume equivalent to one aliquot (pore volume of column/column subdivisions) times percent saturation

M = number of aliquots of this particular waste which should be percolated

LB = total number of aliquots of waste to be percolated

As many different waste solutions as are desired can be percolated through the soil. Each waste requires its own set of data cards with the input values of the above variables.

OUTPUT INTERPRETATION

As mentioned, the bulk of the work in using PERCOL is data manipulation. The necessary input variables were described in the previous section. The interpretation of the large amount of computer generated output follows. Besides output such as initial and equilibrium values of all the chemical species interacting in the soil-waste solution regime, diagnostic output is possible if problems with the numerical calculations are encountered.

Printed Output

The first outputs generated by PERCOL are the four option statements and replies for the particular run being submitted, followed by the printout of the chemical concentrations of the variables read as input. This provides a check on the accuracy of the data cards. The number of output lines will depend on the option taken. The values fall directly under a heading which contains a list of the input variables, so identification should be obvious.

Provided the Newton-Raphson iteration techniques (see NEWTIT) converge in fewer than 90 iterations, all output will consist of lines of heading followed by lines of numerical output for either initial or equilibrium chemical concentrations. The headings state whether the values to follow are equilibrium or initial and give the solution aliquot numbers and soil subdivisions.

The two headings are as follows:

- INITIAL CONDITIONS AFTER SOLUTION DISSOLVES SOLUBLE, COLUMN K ALIQUOT LL

• EQUILIBRIUM VALUES FOR ALL IONS, COLUMN K ALIQUOT LL

Chemical headings are explained below:

K	=	potassium concentration in solution, m/l
KX	=	potassium concentration sorbed on soil, m/gm
NA	=	sodium concentration in solution, m/l
NAX	=	sodium concentration sorbed on soil, m/gm
MG	=	magnesium concentration in solution, m/l
MGX	=	magnesium concentration sorbed on soil, m/gm
SR	=	strontium concentration in solution, m/l (stable macro portion)
SRX	=	strontium concentration sorbed in soil, m/gm (stable macro portion)
CA	=	calcium ion concentration in solution, m/l
CAX	=	calcium concentration sorbed on soil, m/gm
HCO3	=	bicarbonate concentration in solution, m/l
NO3	=	nitrate concentration in solution, m/l
SO4	=	sulfate concentration in solution, m/l
CL	=	chloride concentration in solution, m/l
FL	=	fluoride concentration in solution, m/l
CASO4UN	=	associated calcium sulfate concentration in solution, m/l
GYPSUM	=	calcium sulfate precipitated in soil, m/gm
CAL	=	calcium carbonate precipitated in soil, m/gm
CAF	=	calcium fluoride precipitated in soil, m/gm
PH	=	pH of effluent solution
KD	=	distribution constant for particular waste
B	=	soil-to-solution ratio, gm/liter

U	=	square root of ionic strength of waste solution, $\sqrt{m/l}$
SR85 SOIL	=	concentration of trace constituent sorbed on soil (cpm/gm or mc/gm)
SR85 SOL	=	concentration of trace constituent in effluent solution (cpm/ml or mc/ml)
VOLUME (MLS)	=	total volume of effluent through column, mls (but can change to any units)
COVOL	=	column volumes of effluent through column
C/CO	=	effluent trace concentration/influent trace concentration (breakthrough)

INTERNALLY GENERATED DIAGNOSTICS

One further type of numerical output is possible if NEWTIT does not converge within 90 iterations. The output will be lines consisting of the fixed point variable, ION, with values of from 1 to 5, followed by 5 to 7 floating point numbers. The fixed point number identifies the chemical reaction which is not converging.

1 = Mg-Ca Ion Exchange

2 = Na-Ca Ion Exchange

3 = Na-K Ion Exchange

4 = Calcium Carbonate Solubility

5 = Calcium Fluoride Solubility

The floating point numbers give the value of F(x), the root (x), the first derivative of F(x) which is the variable FXP, and the values of the chemical species involved. The numbers help to determine why the system is not converging.

NEWTIT SUBROUTINE

The subroutine NEWTIT is a mathematical algorithm which solves for the real root of an equation in the form of F(x)-C=0, where F(x) is any polynomial function of x and C is a constant.

The ion exchange and precipitation reactions being modeled can be put in the above form. The subroutine utilizes the Newton-Raphson iterative technique.

ACCESS

The subroutine NEWTIT is available as a FORTRAN IV punched deck of about 70 cards. It is found directly behind the main program PERCOL. NEWTIT should not have to be altered unless new chemical species which enter into reactions solved by the Newton-Raphson technique are added to the main program. This subroutine is a modification of the Program NEWTIT found in the UNIVAC 1108 Math Pack, Section 4 UP 7545.[5,6]

INPUT REQUIREMENTS

Because all input requirements for the subroutine NEWTIT are generated in the main program PERCOL, the user need not input further information. The UNIVAC 1108 Math Pack may be consulted for details of the subroutine.

Briefly, the variables automatically generated in PERCOL for subsequent input to NEWTIT include:

X	an initial estimate of the real root
FX	the polynomial function of X
FXP	the first derivative of the polynomial function of X
ERROR	the tolerance limit near zero which will satisfy convergence (the digital computer will repeatedly attempt to reach zero exactly if this tolerance limit is not specified. Defining a narrow band on the number line around zero allows the computer to accept convergence tests which are not exactly zero)
NUMB	the number of iterations the program should try before stopping (this prevents the computer from entering an infinite loop due to lack of convergence)
KAR	an integer which acts as an indicator by NEWTIT (details can be found in Reference 5)
ION	identifies the chemical equation being solved

OUTPUT INTERPRETATION

Internal Diagnostics

Built into NEWTIT are two checks to insure that computations are proceeding properly. If the chemical computations do not converge after a designated number of iterations, N (set at 100 for this program), the diagnostic occurs: "ROOT DID NOT CONVERGE WITHIN MAXIMUM NUMBER OF ITERATIONS, PROGRAM RETURNING TO NEXT SET OF DATA." Following this diagnostic are three numbers showing the soil subdivision, K; the aliquot, ISOL; and the chemical equation in which the program was stuck, ION (described in the "Internally Generated Diagnostics" section). Unless data for a new soil column follows, the run terminates.

The second diagnostic is "OVERFLOW IN COMPUTATIONS, RETURNING TO NEXT SET OF DATA." This occurs when F(x) is very large and/or FXP is very small in the Newton-Raphson scheme. If this occurs for no apparent reason, the tolerance level, E, for $F(x) \leq E$ must be increased. This is done by increasing the value of the variable ERROR in the PERCOL deck for the appropriate reaction.

Output to Main Program

NEWTIT's output to the program PERCOL is internally interpreted and unless one of the two error diagnostics is indicated the run continues.

SUBROUTINE DIST

The subroutine DIST contains the mathematical equation used to estimate the value of Kd. The equation is derived from experimental data described elsewhere.[1,4] The equation requires the input of equilibrium chemical variables of the waste solution which are automatically transferred from PERCOL.

ACCESS

The subroutine DIST is available as a FORTRAN IV punched deck of about 15 cards. It is found directly behind NEWTIT and must be altered whenever a new Kd predictor equation is to be used.

The variable AKD is the predictor equation and must be repunched whenever a new equation is used. Monitoring of more than one trace constituent requires use of several Kd equations (such as AKD1, AKD2.....); cards are added to the deck for each of these. Variables for the new wastes would also be added in appropriate spots in the main program.

INPUT REQUIREMENTS

The input requirements are the current equilibrium concentration values of all the macro constituents in the solution. These values are automatically transferred from the main program.

OUTPUT INTERPRETATION

The output is the value of Kd for the particular waste solution, soil type and trace constituent of interest. The value is automatically returned to PERCOL and computations continue.

ACKNOWLEDGMENTS

The authors acknowledge the assistance of J. F. Rheinschmidt whose comments as a potential user of this manual influenced the format followed.

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APPENDIX A

ASSUMPTIONS INTRINSIC TO PERCOL

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ASSUMPTIONS INTRINSIC TO PERCOL

- Dispersion, diffusion and evaporation are neglected.
- Seepage velocity is slow enough for equilibrium to be attained.
- Cation exchange capacity is constant for each soil type.
- Binary equations approximate the complex cation exchange in porous media.
- Equilibrium states are path independent.
- Anion exchange is negligible.
- Limestone, fluorite and gypsum are considered to be the only slightly soluble salts present and their solubility is assumed to be that of the crystalline form.
- Undissociated calcium sulfate is the only complex ion formed.
- Activity coefficients follow the Davies extension of the Debye-Huckel theory.
- Moisture content is uniform.
- Reactions of macroions present are described by factorial design regression coefficients.

APPENDIX B

SAMPLE INPUT CARDS AND PRINTED OUTPUT

APPENDIX B

SAMPLE INPUT CARDS AND PRINTED OUTPUT

1. GENERAL INPUT CARD DESCRIPTION
2. CASE ONE

   COLUMN IS WET

   COLUMN IS NONUNIFORM

   PRINT ALL VALUES

   COLUMN HAS FOUR SUBDIVISIONS

   ONE WASTE SOLUTION
3. CASE TWO

   COLUMN IS DRY

   COLUMN IS UNIFORM

   PRINT ONLY EQUILIBRIUM VALUES AT LAST SUBSECTION

   COLUMN HAS TEN SUBDIVISIONS

   ONE WASTE SOLUTION

GENERAL INPUT CARD DESCRIPTION

The data card which contains values, or answers, for the True or False Program Option Statements should be as follows: (true or false) value for each statement occupying a card column field 10 columns wide and beginning with card column 1 must be punched in the card. Each value is left justified within its card column field and statements are punched in the order they are asked. SEE FORMAT STATEMENT 1150.

The data card containing values for the variables P1, FK1, P2, FK2, P3, and FK3 must be as follows: beginning with card column 1, each value must be a real number and occupy a card column field 10 columns wide. All values are punched on the card and each is right justified within its card column field. They must be in the same order on the card as they are above. SEE FORMAT STATEMENT 1200.

The data card containing values for the variables K, JSUB, VSOIL, PORE, and B3 must have the following format: the first two values are integers, each occupying a card column field 6 columns wide beginning with card column 1. Each value must be present on the card and right justified within its field. The next three values are real numbers; each occupies a card column field 10 columns wide beginning with card column 13. Each value must be present on the card and right justified within its card column field. All values on this card must be punched in the same order as they appear above. SEE FORMAT STATEMENT 1220.

The data card containing values for the variables SOCA, SOMG, SONA, SOK, SOSR, SOCL, SOSO4, and SOHCO3 is as follows: all values are real numbers; each occupies a card column field 8 columns wide, beginning with card column 1. Each value must be right justified within its card column field. All values need not be present but card column fields for those missing must be left blank. All values punched on this card must be in the same order on the card as they are above. SEE FORMAT STATEMENT 1140.

The data card containing values for the variables SONO3, EC, CAL, B11, B2, GYP, SRS, and CAF follows the same rules and format as the data card containing values for the variables SOCA, SOMG, SONA, SOK, SOSR, SOSO4, and SOHCO3. SEE FORMAT STATEMENT 1140.

The data card containing values for the variables SAT, RP, ET, CT, and RSR must be as follows: all the values must be punched in exponential notation and each value must occupy a card column field 15 columns wide, beginning with card column 1. Each value must be right justified within its card column field. All the values need not be present but card column fields for those missing must be left blank. All the values punched must be in the same order on the card as they are above. SEE FORMAT STATEMENT 1260.

The data card containing values for the variables GYP, CAL, B2, CAF, and SRS must follow the same rules and format as the data card containing values for the variables SAT, RP, ET, CT, and RSR. SEE FORMAT STATEMENT 1260.

The data card containing values for the variables WCA, WMG, WNA, WK, WSR, WCL, WSO4, WHCO3, and M should be as follows: the first eight values are real numbers, and each must occupy a card column field 8 columns wide, beginning with card column 1. Each value must be right justified within its card column field. The last value punched on the card must be an integer number; it must occupy a card column field 5 columns wide, beginning with card column 70, and be right justified within its field. All values need not be present but card column fields for those missing must be left blank. The values must be in the same order on the card as they are above. SEE FORMAT STATEMENT 1140.

The data card containing values for the variables WNO3, SRIN, CASOI, APH, and WFL follows the same rules and format as the data card containing values for the variables WCA, WMG, WNA, WK, WSR, WCL, WSO4, WHCO3, and M. SEE FORMAT STATEMENT 1140.

The data card containing values for the variables ALI and LB must be as follows: the first value is punched in exponential notation and occupies a card column field 14 columns wide, beginning with card column 1. It must be right justified within this field. The second value punched in the card must be an integer and it must occupy a card column field 6 columns wide, beginning with card column 15. It must be right justified within its field. SEE FORMAT STATEMENT 1270.

CASE ONE (WET SOIL)

The first example of data input and computer output considers a soil column which is initially wet and has had the slightly soluble salts entirely leached from the soil. The soil column has four nonhomogeneous soil subdivisions for which input is needed. The computer generated output is in the mode which prints both the initial and final chemical concentrations for each soil cell.

The first data card contains a string of four words which answer true or false to the four questions posed by the program options. Each true or false answer is punched in a card column field 10 columns wide beginning with card column 1 and each word is left adjusted within its field. SEE FORMAT STATEMENT 1150.

The second data card contains values for the variables P1, FK1, P2, FK2, P3, and FK3, the empirical ion exchange constants for the cation exchange reactions. A real number value for each variable must occupy a 10 card column field, beginning with card column 1, and the values must be in the order specified above. SEE FORMAT STATEMENT 1200.

The third data card contains values for the variables K (the number of soil subdivisions), JSUB (the number of micro subdivisions), VSOIL (the volume of the soil column), PORE (the effective porosity), and B3 (the percent saturation) that the soil column will have. A value for each variable must be entered in the following format. The first two variable values are integers and each occupies a card column field six columns wide beginning with card column 1. The column field is right adjusted. The next three variable values are real numbers, each occupying a card column field ten columns wide beginning with card column 13. They also must be in the order specified above on the card. SEE FORMAT STATEMENT 1220.

The first three data cards are present in the described format whether the soil is wet or dry. If the soil is wet, the fourth data card contains values for the variables SAT, RP, ET, CT, and RSR; these are the exchangeable sodium, potassium, calcium, magnesium and strontium concentrations sorbed on the soil. Each of these values present must occupy a card column field 15 columns wide beginning with card column 1 and must be written in exponential notation, such as (2.221E-05). The values must appear on the card in the order specified above and the 15 card column field of each missing variable value must be left blank, or zeroed. SEE FORMAT STATEMENT 1260.

The fifth data card contains values for the variables GYP, CAL, B2, CAF, AND SRS. These are calcium sulfate, calcium carbonate found in soil, moisture percentage at saturation, calcium fluoride found in the soil, and initial trace constituent concentrations sorbed on the soil. Every one of these values need not be present, but those that are must follow the format outlined for the fourth data card. SEE FORMAT STATEMENT 1260.

The fourth and fifth data cards will be present if the soil conditions are termed WET. For DRY soil conditions different variables and card formats will be used for data cards four and five. SEE CASE TWO.

The sixth through eleventh data cards pertain to a nonuniform soil column. These cards are input in pairs containing data for the same variables found on data cards four and five and follow the same format as cards four and five. The number of pairs depends upon the number of soil cells. For this particular case there were four soil cells, hence eight data cards (data cards four through eleven).

The next three data cards are considered to be a set, and at least one set is always present. The presence of additional sets signifies that additional waste solutions will be used.

The twelfth data card contains values for the variables WCA, WMG, WNA, WK, WSR, WCl, WSO4, WHCO3, and M. These represent the calcium, magnesium, sodium, potassium, strontium, chloride, sulfate, and bicarbonate concentrations in the solution and M represents the number of aliquots of this particular waste which should be percolated. Values for all these variables need not be present; however, those that are must be in the following format: the first eight values must be real numbers and each must occupy a card column field eight columns wide beginning with card column 1. The last value to be punched on this card, "M", is an integer which occupies a card column field five columns wide beginning with card column 70; this value must be right adjusted within its card column field. All values punched must be in the order described above; the respective card column fields of those that are not to be punched must be left blank. SEE FORMAT STATEMENT 1140.

The 13th data card contains values for the variables WNO3 (the nitrate concentration in the solution), SRIN (the influent concentration of trace ion being investigated), CASOI (associated calcium sulfate complex in the solution), APH (the pH of the solution), and WFI (the fluoride concentration in the solution). All of these values need not be present, but those that are must follow the format rules of the 12th data card. Again, they must be punched on the card in the order specified, and blank card column fields must be retained. SEE FORMAT STATEMENT 1140.

The 14th data card contains values for the variables ALI (the volume equivalent to one aliquot) and LB (the total number of aliquots to be percolated). These must be present in the following format. The first variable value is punched in exponential notation and occupies a card column field 14 columns wide beginning with card column 1. The second value is an integer and occupies a card column field six columns wide beginning with card column 15. Each value must be right adjusted in its field. SEE FORMAT STATEMENT 1270.

The last card is the FIN card, signifying the end of data input. Sample CASE ONE input data cards and printed output will be found on the following pages.

The first portion of output indicates the options which are being used and the values of the data cards which were used to initialize the program. This allows a check to make sure the cards were correctly read by the computer and leaves a permanent record with the output for future reference.

Further output are the initial and equilibrium values for each soil subdivision for each aliquot of solution percolated through the soil cell.

INPUT CARDS

```
' XQT SEP
FALSE      FALSE      TRUE       FALSE
1.23       1.26       .494       2.24       1.15       8.23
    4       5  529.        .914      100.
      2.221E-05       5.636E-06       6.121E-06       2.455E-06
                      2.570E-04       2.637E+01       1.777E-06       6.261E+01
      1.447E-05       3.592E-06       9.666E-06       3.801E-06
      5.028E-07       2.570E-04       2.637E+01       1.792E-06       3.855E+00
      1.240E-05       3.411E-06       1.045E-05       4.147E-06
      2.311E-06       2.570E-04       2.637E+01       1.791E-06
      1.169E-05       3.420E-06       1.070E-05       4.244E-06
      2.232E-06       2.570E-04       2.637E+01       1.791E-06
 4.52              152.      10.30                          4.97E-03     2
 166.82 2.0   +03              7.0
   2.176   E+01        2
' FIN                                                          X
```

PRINTED OUTPUT

```
THE SOIL COLUMN IS DRY .................            F

THE SOIL PROFILE IS UNIFORM...............          F

PRINT ALL INITIAL AND FINAL VALUES .......          T

PRINT ALL EQUILIBRIUM VALUES ONLY.........          F


    P1         FK1         P2         FK2         P3         FK3
 .123+01    .126+01    .494-00    .224+01    .115+01    .823+01

     K       JSUB   VSOIL      PORE      % SAT
     4        5    .529+03   .914-00   .100+03

        SAT             RP             ET             CT            RSR
     .2221-04       .5636-05       .6121-05       .2455-05        -.0000
```

GYP	CAL	B2	CAF	SRS
-.0000	.2570-03	.2637+02	.1777-05	.6261+02

SAT	RP	ET	CT	RSR
.1447-04	.3592-05	.9666-05	.3801-05	-.0000

GYP	CAL	B2	CAF	SRS
.5028-06	.2570-03	.2637+02	.1792-05	.3855+01

SAT	RP	ET	CT	RSR
.1240-04	.3411-05	.1045-04	.4147-05	-.0000

GYP	CAL	B2	CAF	SRS
.2311-05	.2570-03	.2637+02	.1791-05	-.0000

SAT	RP	ET	CT	RSR
.1169-04	.3420-05	.1070-04	.4244-05	-.0000

GYP	CAL	B2	CAF	SRS
.2232-05	.2570-03	.2637+02	.1791-05	-.0000

WCA	WMG	WNA	WK	WSR	WCL	WSO4
.45200+01	-.00000	.15200+03	.10300+02	-.00000	-.00000	-.00000

WNO3	SRIN	CASOI	APH			WHCO3
.16682+03	.20000+04	-.00000	.70000+01			.49700-02

ALI	LB
.2176+02	2

```
INITIAL CONDITIONS AFTER SOLUTION DISSOLVES SOLUBLE. COLUMN    1 ALIQUOT     1
     K          KX         NA         NAX        MG         MGX        SR         SRX         CA
  1.030-02  5.636-06  1.520-01  2.221-05  0.000     2.455-06  0.000     -0.000     2.260-03
   HCO3        NO3       SO4        CL       CASO4UN    GYPSUM     SR85 SOL   SR85 SOIL  CAL
  4.970-06  1.668-01  0.000     0.000     -0.000     -0.000     2.000+03  6.261+01   2.570-04
   FL          CAF                                                                     CAX
  0.000     1.777-06                                                                   6.121-06
EQUILIBRIUM VALUES FOR ALL IONS  COLUMN    1 ALIQUOT     1
     K          KX         NA         NAX        MG         MGX        SR         SRX         CA
  2.993-03  7.744-06  1.215-01  3.102-05  5.076-03  9.906-07  0.000     -0.000     1.638-02
   HCO3       NO3       SO4        CL      SR85 SOL SR85 SOIL   VOLUME(ML)  COLVOL     C/CO
  4.294-04  1.668-01  0.000     0.000     2.638+01  8.219+01  2.176+01  4.113-02   1.319-02
   PH          KD      CASO4UN    GYPSUM      CAL        CAF        FL         B           U
  8.976+00  3.116+00 -0.000     -0.000     2.569-04  1.759-06  1.253-04  3.466+03   4.345-01
INITIAL CONDITIONS AFTER SOLUTION DISSOLVES SOLUBLE. COLUMN    2 ALIQUOT     1              CAX
     K          KX         NA         NAX        MG         MGX        SR         SRX         CA  2.128-06
  2.993-03  3.592-06  1.215-01  1.447-05  5.076-03  3.801-06  0.000     -0.000     1.638-02
   HCO3        NO3       SO4        CL       CASO4UN    GYPSUM     SR85 SOL   SR85 SOIL  CAL
  4.294-04  1.668-01  0.000     0.000     -0.000     5.028-07  2.638+01  3.855+00   2.570-04
   FL          CAF                                                                     CAX
  1.253-04  1.792-06                                                                   9.666-06
EQUILIBRIUM VALUES FOR ALL IONS  COLUMN    2 ALIQUOT     1
     K          KX         NA         NAX        MG         MGX        SR         SRX         CA
  1.854-03  3.921-06  1.012-01  2.032-05  7.372-03  3.138-06  0.000     -0.000     2.596-02
   HCO3       NO3       SO4        CL      SR85 SOL SR85 SOIL   VOLUME(ML)  COLVOL     C/CO
  3.474-04  1.668-01  1.227-03  0.000     1.612+00  4.224+00  2.176+01  4.113-02   8.062-04
   PH          KD      CASO4UN    GYPSUM      CAL        CAF        FL         B           U
  8.751+00  2.619+00  5.162-04  0.000     2.570-04  1.795-06  1.013-04  3.466+03   4.520-01
INITIAL CONDITIONS AFTER SOLUTION DISSOLVES SOLUBLE. COLUMN    3 ALIQUOT     1              CAX
     K          KX         NA         NAX        MG         MGX        SR         SRX         CA  7.239-06
  1.854-03  3.411-06  1.012-01  1.240-05  7.372-03  4.147-06  0.000     -0.000     2.596-02
   HCO3        NO3       SO4        CL       CASO4UN    GYPSUM     SR85 SOL   SR85 SOIL  CAL
  3.474-04  1.668-01  1.227-03  0.000     5.162-04  2.311-06  1.612+00  -0.000     2.570-04
   FL          CAF                                                                     CAX
  1.013-04  1.791-06                                                                   1.045-05
EQUILIBRIUM VALUES FOR ALL IONS  COLUMN    3 ALIQUOT     1
     K          KX         NA         NAX        MG         MGX        SR         SRX         CA     CAX
```

```
  2.202-03  3.310-06  9.549-02  1.404-05  8.264-03  3.890-06  0.000     -0.000     3.300-02 9.936-06
   HCO3      NO3      SO4        CL       SR85 SOL SR85 SOIL  VOLUME(ML)  COLVOL    C/CO
  3.160-04  1.668-01  6.501-03  0.000     1.843-02  3.844-02  2.176+01  4.113-02   9.217-06
   PH        KD       CASO4UN   GYPSUM     CAL        CAF       FL        B          U
  8.638+00  2.085+00  3.252-03  0.000     2.570-04  1.792-06  9.218-05  3.466+03   4.775-01
 INITIAL CONDITIONS AFTER SOLUTION DISSOLVES SOLUBLE. COLUMN    4 ALIQUOT    1
     K         KX        NA        NAX       MG        MGX       SR        SRX        CA        CAX
  2.202-03  3.420-06  9.549-02  1.169-05  8.264-03  4.244-06  0.000     -0.000     3.300-02  1.070-05
    HCO3      NO3       SO4       CL       CASO4UN    GYPSUM   SR85 SOL  SR85 SOIL  CAL
  3.160-04  1.668-01  6.501-03  0.000     3.252-03  2.232-06  1.843-02  -0.000     2.570-04
    FL        CAF
  9.218-05  1.791-06
 EQUILIBRIUM VALUES FOR ALL IONS  COLUMN    4 ALIQUOT    1
     K         KX        NA        NAX       MG        MGX       SR        SRX        CA        CAX
  2.569-03  3.314-06  9.396-02  1.213-05  8.766-03  4.099-06  0.000     -0.000     3.585-02  1.068-05
   HCO3      NO3      SO4        CL       SR85 SOL SR85 SOIL  VOLUME(ML)  COLVOL    C/CO
  3.065-04  1.668-01  9.282-03  0.000     2.959-04  5.485-04  2.176+01  4.113-02   1.479-07
   PH        KD       CASO4UN   GYPSUM     CAL        CAF       FL        B          U
  8.600+00  1.854+00  4.897-03  9.551-07  2.570-04  1.791-06  8.942-05  3.466+03   4.896-01
 INITIAL CONDITIONS AFTER SOLUTION DISSOLVES SOLUBLE. COLUMN    1 ALIQUOT    2
     K         KX        NA        NAX       MG        MGX       SR        SRX        CA        CAX
  1.030-02  7.744-06  1.520-01  3.102-05  0.000     9.906-07  0.000     -0.000     2.260-03  2.128-06
    HCO3      NO3       SO4       CL       CASO4UN    GYPSUM   SR85 SOL  SR85 SOIL  CAL
  4.970-06  1.668-01  0.000     0.000     -0.000    -0.000     2.000+03  8.219+01   2.569-04
    FL        CAF
  0.000     1.759-06
 EQUILIBRIUM VALUES FOR ALL IONS  COLUMN    1 ALIQUOT    2
     K         KX        NA        NAX       MG        MGX       SR        SRX        CA        CAX
  3.937-03  9.580-06  1.406-01  3.432-05  2.815-03  1.785-07  0.000     -0.000     8.721-03  3.710-07
   HCO3      NO3      SO4        CL       SR85 SOL SR85 SOIL  VOLUME(ML)  COLVOL    C/CO
  5.809-04  1.668-01  0.000     0.000     4.143+01  1.401+02  4.352+01  8.227-02   2.072-02
   PH        KD       CASO4UN   GYPSUM     CAL        CAF       FL        B          U
  9.287+00  3.382+00  -0.000    -0.000    2.569-04  1.734-06  1.695-04  3.466+03   4.232-01
 INITIAL CONDITIONS AFTER SOLUTION DISSOLVES SOLUBLE. COLUMN    2 ALIQUOT    2
     K         KX        NA        NAX       MG        MGX       SR        SRX        CA        CAX
  3.937-03  3.921-06  1.406-01  2.032-05  2.815-03  3.138-06  0.000     -0.000     8.721-03  7.239-06
    HCO3      NO3       SO4       CL       CASO4UN    GYPSUM   SR85 SOL  SR85 SOIL  CAL
  5.809-04  1.668-01  0.000     0.000     -0.000    0.000     4.143+01  4.224+00   2.570-04
    FL        CAF
  1.695-04  1.795-06
```

```
EQUILIBRIUM VALUES FOR ALL IONS  COLUMN    2 ALIQUOT    2
     K          KX         NA        NAX        MG       MGX        SR        SRX        CA        CAX
  1.665-03  4.576-06  1.122-01  2.849-05  6.781-03  1.994-06  0.000    -0.000     1.993-02  3.970-06
    HCO3       NO3       SO4        CL       SR85 SOL SR85 SOIL   VOLUME(ML)  COLVOL     C/CO
  3.917-04  1.668-01  0.000     0.000     1.789+00  5.346+00  4.352+01  8.227-02  8.944-04
    PH         KD      CASO4UN   GYPSUM       CAL       CAF        FL         B          U
  8.880+00  2.989+00 -0.000     0.000     2.570-04  1.803-06  1.143-04  3.466+03  4.405-01
INITIAL CONDITIONS AFTER SOLUTION DISSOLVES SOLUBLE. COLUMN    3 ALIQUOT    2
     K          KX         NA        NAX        MG       MGX        SR        SRX        CA        CAX

  1.665-03  3.310-06  1.122-01  1.404-05  6.781-03  3.890-06  0.000    -0.000     1.993-02  9.936-06
    HCO3       NO3       SO4        CL      CASO4UN   GYPSUM    SR85 SOL  SR85 SOIL  CAL
  3.917-04  1.668-01  0.000     0.000    -0.000     0.000     1.789+00  3.844-02  2.570-04
    FL         CAF
  1.143-04  1.792-06
EQUILIBRIUM VALUES FOR ALL IONS  COLUMN    3 ALIQUOT    2
     K          KX         NA        NAX        MG       MGX        SR        SRX        CA        CAX
  1.646-03  3.316-06  9.716-02  1.840-05  7.793-03  3.598-06  0.000    -0.000     2.644-02  8.049-06
    HCO3       NO3       SO4        CL       SR85 SOL SR85 SOIL   VOLUME(ML)  COLVOL     C/CO
  3.432-04  1.668-01  0.000     0.000     4.643-02  1.217-01  4.352+01  8.227-02  2.321-05
    PH         KD      CASO4UN   GYPSUM       CAL       CAF        FL         B          U
  8.741+00  2.622+00 -0.000     0.000     2.570-04  1.794-06  1.001-04  3.466+03  4.489-01
INITIAL CONDITIONS AFTER SOLUTION DISSOLVES SOLUBLE. COLUMN    4 ALIQUOT    2
     K          KX         NA        NAX        MG       MGX        SR        SRX        CA        CAX
  1.646-03  3.314-06  9.716-02  1.213-05  7.793-03  4.099-06  0.000    -0.000     2.644-02  1.068-05
    HCO3       NO3       SO4        CL      CASO4UN   GYPSUM    SR85 SOL  SR85 SOIL  CAL
  3.432-04  1.668-01  0.000     0.000    -0.000     9.551-07  4.643-02  5.485-04  2.570-04
    FL         CAF
  1.001-04  1.791-06
EQUILIBRIUM VALUES FOR ALL IONS  COLUMN    4 ALIQUOT    2
     K          KX         NA        NAX        MG       MGX        SR        SRX        CA        CAX
  2.096-03  3.185-06  9.191-02  1.364-05  7.992-03  4.042-06  0.000    -0.000     3.085-02  1.004-05
    HCO3       NO3       SO4        CL       SR85 SOL SR85 SOIL   VOLUME(ML)  COLVOL     C/CO
  3.217-04  1.668-01  2.225-03  0.000     9.830-04  2.250-03  4.352+01  8.227-02  4.915-07
    PH         KD      CASO4UN   GYPSUM       CAL       CAF        FL         B          U
  8.667+00  2.289+00  1.085-03  0.000     2.570-04  1.792-06  9.386-05  3.466+03  4.612-01
```

CASE TWO (DRY SOIL)

For Case Two the first, second and third data cards are the same as those described in Case One; refer to Case One for their format descriptions.

The variables on the fourth data card represent the amount of calcium, magnesium, sodium, potassium, strontium, chloride, sulfate and bicarbonate in the B11 soil extracts. These values may be in real or exponential form and may or may not be present. Each value occupies a card column field eight columns wide and all exponential notations must be right justified within the card column field. Zero variables may have blank card column fields. The variables must be punched in the order listed above. SEE FORMAT STATEMENT 1140.

The fifth data card contains values for the variables SONO3, EC, CAL, B11, B2, GYP, SRF, AND CAF, representing the nitrate in the B11 extract, cation exchange capacity, calcium carbonate in soil, % moisture at which soil extract was run, % moisture of a saturated soil column, calcium sulfate in soil, initial concentration of trace ion sorbed on soil and amount of calcium fluoride present in soil. The format is identical to that of the previous card. Variables EC, B11 and B2 must be present but the other variables may or may not be present. SEE FORMAT STATEMENT 1140.

Since the soil is designated as uniform, no further dry soil data cards are needed. If the soil is nonuniform, as in Case One, a set of data cards containing the same variables as cards four and five above would be present for each soil cell. Two x K gives the number of dry soil cards needed in the general nonuniform case.

In this uniform case, one set of data cards is present and the computer automatically generates the data for the remaining uniform soil cells.

The sixth, seventh and eighth data cards represent the waste solution data. The description is the same as for Case One. SEE FORMAT STATEMENTS 1140 and 1270. Again, only one waste solution was run, thus only one set of waste solution data cards is present. The last card is a FIN card to signify the end of input data cards. Sample Case Two input data cards and printed output follow.

INPUT CARDS

```
' XQT SEP
TRUE        TRUE       FALSE      FALSE
1.23        1.26       .494       2.24       1.15       8.23
   10         5  529.           .914   100.
  11.94   5.731    27.97      1.157                    11.94
  29.13   4.5 -022.57 -04     100.    26.37   3.12 -07
 4.52               152.      10.30                                 4.97E-03   16
 166.82 2.0   +03               7.0
   2.176  E+01      16
' FIN                                                            X
```

PRINTED OUTPUT

```
THE SOIL COLUMN IS DRY ..................          T
THE SOIL PROFILE IS UNIFORM...............         T
PRINT ALL INITIAL AND FINAL VALUES .......         F
PRINT ALL EQUILIBRIUM VALUES ONLY.........         F
```

P1	FK1	P2	FK2	P3	FK3
.123+01	.126+01	.494-00	.224+01	.115+01	.823+01

K	JSUB	VSOIL	PORE	% SAT	SOSO4	SOHCO3
10	5	.529+03	.914-00	.100+03	.11940+02	-.00000

SOCA	SOMG	SONA	SOK	SOSR	SOCL
.11940+02	.57310+01	.27970+02	.11570+01	-.00000	-.00000

SONO3	EC	CAL	B11	B2	GYP
.29130+02	.45000-01	.25700-03	.10000+03	.26370+02	.31200-06

SRS	CAF
-.00000	-.00000

```
      WCA          WMG           WNA           WK          WSR           WCL           WSO4
  .45200+01    -.00000       .15200+03    .10300+02   -.00000      -.00000       -.00000

      WNO3         SR1N          CASOI         APH                                    WHCO3
  .16682+03    .20000+04    -.00000       .70000+01                               .49700-02

       ALI         LB
   .2176+02        16

                                                                                           CAX
 EQUILIBRIUM VALUES FOR ALL IONS  COLUMN   10 ALIQUOT    1                                 2.904-06
      K           KX          NA          NAX          MG          MGX          SR         SRX           CA
  9.690-03   5.725-06   5.222-01   2.934-05   1.640-01   2.061-06   0.000     -0.000       3.150-01
    HCO3         NO3         SO4          CL       SR85 SOL SR85 SOIL    VOLUME(ML)   COLVOL       C/CO
  7.920-05   1.271+00   5.191-04   0.000        5.204-13   5.264-12   2.176+01   4.113-02   2.602-16
     PH           KD       CASO4UN    GYPSUM        CAL         CAF          FL           B            U
  7.436+00   1.011+01   4.897-03   6.898-06   2.570-04  -0.000      0.000      3.466+03   1.364+00
 EQUILIBRIUM VALUES FOR ALL IONS  COLUMN   10 ALIQUOT    2
      K           KX          NA          NAX          MG          MGX          SR         SRX           CA
  2.357-03   5.725-06   1.273-01   2.940-05   1.136-02   2.022-06   0.000     -0.000       2.247-02
    HCO3         NO3         SO4          CL       SR85 SOL SR85 SOIL    VOLUME(ML)   COLVOL       C/CO
  3.895-04   1.668-01   1.504-02   0.000        1.472-07   3.872-07   4.352+01   8.227-02   7.362-11
                                                                                            CAX
                                                                                            2.916-06
     PH           KD       CASO4UN    GYPSUM        CAL         CAF          FL           B            U
  8.835+00   2.630+00   4.897-03   6.892-06   2.570-04  -0.000      0.000      3.466+03   4.962-01
 EQUILIBRIUM VALUES FOR ALL IONS  COLUMN   10 ALIQUOT    3                                      CAX
      K           KX          NA          NAX          MG          MGX          SR         SRX           CA  2.970-06
  2.357-03   5.726-06   1.277-01   2.947-05   1.064-02   1.932-06   0.000     -0.000       2.276-02
    HCO3         NO3         SO4          CL       SR85 SOL SR85 SOIL    VOLUME(ML)   COLVOL       C/CO
  3.866-04   1.668-01   1.481-02   0.000        1.640-06   4.273-06   6.528+01   1.234-01   8.201-10
     PH           KD       CASO4UN    GYPSUM        CAL         CAF          FL           B            U
  8.829+00   2.605+00   4.897-03   6.868-06   2.570-04  -0.000      0.000      3.466+03   4.950-01
 EQUILIBRIUM VALUES FOR ALL IONS  COLUMN   10 ALIQUOT    4
      K           KX          NA          NAX          MG          MGX          SR         SRX           CA
  2.357-03   5.725-06   1.282-01   2.959-05   9.561-03   1.791-06   0.000     -0.000       2.321-02
                                                                                            CAX
                                                                                            3.053-06
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  HCO3        NO3        SO4        CL       SR85 SOL SR85 SOIL    VOLUME(ML)  COLVOL     C/CO
 3.822-04  1.668-01  1.447-02  0.000      1.026-05  2.634-05  8.704+01  1.645-01  5.130-09
   PH         KD       CASO4UN    GYPSUM       CAL        CAF        FL         B          U
 8.818+00  2.568+00  4.897-03  6.832-06  2.570-04 -0.000     0.000     3.466+03  4.933-01
EQUILIBRIUM VALUES FOR ALL IONS  COLUMN   10 ALIQUOT    5                                CAX
    K          KX         NA         NAX        MG         MGX        SR         SRX      CA 3.142-06
 2.353-03  5.724-06  1.290-01  2.977-05  8.272-03  1.609-06  0.000    -0.000     2.373-02
  HCO3        NO3        SO4        CL       SR85 SOL SR85 SOIL    VOLUME(ML)  COLVOL     C/CO
 3.774-04  1.668-01  1.409-02  0.000      4.695-05  1.185-04  1.088+02  2.057-01  2.348-08
   PH         KD       CASO4UN    GYPSUM       CAL        CAF        FL         B          U
 8.807+00  2.524+00  4.897-03  6.794-06  2.570-04 -0.000     0.000     3.466+03  4.914-01
EQUILIBRIUM VALUES FOR ALL IONS  COLUMN   10 ALIQUOT    6                                CAX
    K          KX         NA         NAX        MG         MGX        SR         SRX      CA  3.206-06
 2.344-03  5.721-06  1.300-01  3.006-05  6.946-03  1.402-06  0.000    -0.000     2.420-02
  HCO3        NO3        SO4        CL       SR85 SOL SR85 SOIL    VOLUME(ML)  COLVOL     C/CO
 3.730-04  1.668-01  1.375-02  0.000      1.730-04  4.293-04  1.306+02  2.468-01  8.652-08
   PH         KD       CASO4UN    GYPSUM       CAL        CAF        FL         B          U
 8.796+00  2.481+00  4.897-03  6.765-06  2.570-04 -0.000     0.000     3.466+03  4.895-01
EQUILIBRIUM VALUES FOR ALL IONS  COLUMN   10 ALIQUOT    7                                CAX
    K          KX         NA         NAX        MG         MGX        SR         SRX      CA  3.213-06
 2.328-03  5.715-06  1.314-01  3.049-05  5.695-03  1.182-06  0.000    -0.000     2.454-02
  HCO3        NO3        SO4        CL       SR85 SOL SR85 SOIL    VOLUME(ML)  COLVOL     C/CO
 3.699-04  1.668-01  1.350-02  0.000      5.383-04  1.316-03  1.523+02  2.879-01  2.691-07
   PH         KD       CASO4UN    GYPSUM       CAL        CAF        FL         B          U
 8.789+00  2.445+00  4.897-03  6.758-06  2.570-04 -0.000     0.000     3.466+03  4.878-01
EQUILIBRIUM VALUES FOR ALL IONS  COLUMN   10 ALIQUOT    8                                CAX
    K          KX         NA         NAX        MG         MGX        SR         SRX      CA 3.144-06
 2.305-03  5.709-06  1.332-01  3.109-05  4.543-03  9.581-07  0.000    -0.000     2.469-02
  HCO3        NO3        SO4        CL       SR85 SOL SR85 SOIL    VOLUME(ML)  COLVOL     C/CO
 3.683-04  1.668-01  1.338-02  0.000      1.455-03  3.519-03  1.741+02  3.291-01  7.274-07
   PH         KD       CASO4UN    GYPSUM       CAL        CAF        FL         B          U
 8.786+00  2.419+00  4.897-03  6.777-06  2.570-04 -0.000     0.000     3.466+03  4.864-01
EQUILIBRIUM VALUES FOR ALL IONS  COLUMN   10 ALIQUOT    9                                CAX
    K          KX         NA         NAX        MG         MGX        SR         SRX      CA 3.011-06
 2.279-03  5.702-06  1.353-01  3.179-05  3.485-03  7.404-07  0.000    -0.000     2.466-02
  HCO3        NO3        SO4        CL       SR85 SOL SR85 SOIL    VOLUME(ML)  COLVOL     C/CO
 3.681-04  1.668-01  1.336-02  0.000      3.497-03  8.398-03  1.958+02  3.702-01  1.749-06
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   PH           KD        CASO4UN    GYPSUM      CAL          CAF       FL         B          U
 8.786+00   2.401+00   4.897-03   6.820-06   2.570-04 -0.000     0.000     3.466+03   4.852-01
EQUILIBRIUM VALUES FOR ALL IONS   COLUMN    10 ALIQUOT   10                                  CAX
     K          KX          NA        NAX         MG         MGX        SR        SRX       CA 2.818-06
 2.254-03   5.696-06   1.378-01   3.258-05   2.579-03   5.463-07   0.000    -0.000     2.443-02
   HCO3        NO3        SO4         CL       SR85 SOL SR85 SOIL   VOLUME(ML)  COLVOL     C/CO
 3.695-04   1.668-01   1.345-02   0.000      7.591-03   1.818-02   2.176+02   4.113-01   3.796-06
   PH           KD        CASO4UN    GYPSUM      CAL          CAF       FL         B          U
 8.790+00   2.394+00   4.897-03   6.887-06   2.570-04 -0.000     0.000     3.466+03   4.843-01
EQUILIBRIUM VALUES FOR ALL IONS   COLUMN    10 ALIQUOT   11                                  CAX
     K          KX          NA        NAX         MG         MGX        SR        SRX       CA 2.568-06
 2.231-03   5.689-06   1.406-01   3.341-05   1.839-03   3.839-07   0.000    -0.000     2.400-02
   HCO3        NO3        SO4         CL       SR85 SOL SR85 SOIL   VOLUME(ML)  COLVOL     C/CO
 3.727-04   1.668-01   1.368-02   0.000      1.506-02   3.610-02   2.394+02   4.525-01   7.528-06
   PH           KD        CASO4UN    GYPSUM      CAL          CAF       FL         B          U
 8.799+00   2.398+00   4.897-03   6.978-06   2.570-04 -0.000     0.000     3.466+03   4.838-01
EQUILIBRIUM VALUES FOR ALL IONS   COLUMN    10 ALIQUOT   12                                  CAX
     K          KX          NA        NAX         MG         MGX        SR        SRX       CA 2.279-06
 2.211-03   5.676-06   1.438-01   3.426-05   1.248-03   2.540-07   0.000    -0.000     2.337-02
   HCO3        NO3        SO4         CL       SR85 SOL SR85 SOIL   VOLUME(ML)  COLVOL     C/CO
 3.776-04   1.668-01   1.404-02   0.000      2.753-02   6.635-02   2.611+02   4.936-01   1.377-05
   PH           KD        CASO4UN    GYPSUM      CAL          CAF       FL         B          U
 8.812+00   2.410+00   4.897-03   7.033-06   2.570-04 -0.000     0.000     3.466+03   4.837-01
EQUILIBRIUM VALUES FOR ALL IONS   COLUMN    10 ALIQUOT   13                                  CAX
     K          KX          NA        NAX         MG         MGX        SR        SRX       CA 2.196-06
 2.175-03   5.614-06   1.452-01   3.465-05   7.028-04   1.700-07   0.000    -0.000     2.324-02
   HCO3        NO3        SO4         CL       SR85 SOL SR85 SOIL   VOLUME(ML)  COLVOL     C/CO
 3.786-04   1.668-01   1.410-02   0.000      4.619-02   1.111-01   2.829+02   5.347-01   2.309-05
   PH           KD        CASO4UN    GYPSUM      CAL          CAF       FL         B          U
 8.815+00   2.406+00   4.897-03   1.552-06   2.570-04 -0.000     0.000     3.466+03   4.832-01
EQUILIBRIUM VALUES FOR ALL IONS   COLUMN    10 ALIQUOT   14                                  CAX
     K          KX          NA        NAX         MG         MGX        SR        SRX       CA 7.522-07
 2.004-03   5.633-06   1.470-01   3.773-05   5.080-04   6.474-08   0.000    -0.000     1.307-02
   HCO3        NO3        SO4         CL       SR85 SOL SR85 SOIL   VOLUME(ML)  COLVOL     C/CO
 4.837-04   1.668-01   4.413-03   0.000      5.099-02   1.556-01   3.046+02   5.759-01   2.550-05
   PH           KD        CASO4UN    GYPSUM      CAL          CAF       FL         B          U
 9.090+00   3.051+00   9.654-04   0.000      2.571-04 -0.000     0.000     3.466+03   4.406-01
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                                                                                                  CAX
EQUILIBRIUM VALUES FOR ALL IONS   COLUMN    10 ALIQUOT    15                                      9.356-08
      K          KX          NA          NAX          MG         MGX         SR          SRX          CA
  2.035-03   5.651-06   1.551-01   3.914-05   2.091-04   8.529-09   0.000      -0.000      5.012-03
    HCO3         NO3        SO4          CL       SR85 SOL SR85 SOIL   VOLUME(ML)   COLVOL       C/CO
  7.597-04   1.668-01   0.000       0.000       5.853-02   2.016-01   3.264+02   6.170-01   2.926-05
     PH          KD       CASO4UN     GYPSUM        CAL         CAF         FL           B            U
  9.562+00   3.445+00  -0.000       0.000       2.571-04  -0.000      0.000      3.466+03   4.157-01
EQUILIBRIUM VALUES FOR ALL IONS   COLUMN    10 ALIQUOT    16
      K          KX          NA          NAX          MG         MGX         SR          SRX          CA
  2.089-03   5.657-06   1.597-01   3.928-05   2.818-05   7.969-10   0.000      -0.000      2.980-03
    HCO3         NO3        SO4          CL       SR85 SOL SR85 SOIL   VOLUME(ML)   COLVOL       C/CO
  9.825-04   1.668-01   0.000       0.000       4.476-02   2.349-01   3.482+02   6.581-01   2.238-05

                                                                                                   CAX
                                                                                                   2.921-08

     PH          KD       CASO4UN     GYPSUM        CAL         CAF         FL           B            U
  9.821+00   5.248+00  -0.000       0.000       2.571-04  -0.000      0.000      3.466+03   4.133-01
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APPENDIX C

FORTRAN IV LISTING
OF PERCOL, DIST, NEWTIT

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' RUN,S   8,CUB594,,RJS, 80,5000          JEFF  SERNE  SEP  PROGRAM
'M   FR5  SEP
 C       SOIL  EQUILIBRIUM  PROGRAM                                      SEP   1
         DIMENSION CHCO3(20),CNO3(20),SRSS(20,50 ),CALL(20),GYPP(20)    SEP   2
         DIMENSION CSNA(20),CSMG(20),CSCA(20),CSSR(20),CCL(20),CSO4(20) SEP   3
         DIMENSION CNA(20),CK(20),CMG(20),CCA(20),CSR(20),CSK(20)       SEP   4
         DIMENSION BB1(20),BB2(20),CAFF(20)                             SEP   5
         DIMENSION XNR(10),FXR(10)                                      SEP   6
         COMMON F,ET,B,S,AP,SAT,CT,RP,A,HCO3,FL                         SEP   7
         REAL ISOLF                                                     SEP   8
         LOGICAL DRY,UNI,PRINT,PRI                                      SEP   9
         READ (5,1150) DRY,UNI,PRINT,PRI                                SEP  10
         WRITE (6,1160) DRY                                             SEP  11
         WRITE (6,1170) UNI                                             SEP  12
         WRITE (6,1180) PRINT                                           SEP  13
         WRITE (6,1190) PRI                                             SEP  14
         READ (5,1200) P1,FK1,P2,FK2,P3,FK3                             SEP  15
         WRITE (6,1210) P1,FK1,P2,FK2,P3,FK3                            SEP  16
         READ (5,1220) K,JSUB,VSOIL,PORE,B3                             SEP  17
         WRITE (6,1230) K,JSUB,VSOIL,PORE,B3                            SEP  18
         LL=0                                                           SEP  19
         J=0                                                            SEP  20
         AKD=0.0                                                        SEP  21
         AAPH=0.0                                                       SEP  22
         ISOL=1                                                         SEP  23
         IMAX=1                                                         SEP  24
         IF (.NOT.DRY) GO TO 150                                        SEP  25
   100   READ (5,1140) SOCA,SOMG,SONA,SOK,SOSR,SOCL,SOSO4,SOHCO3        SEP  26
         WRITE (6,1090) SOCA,SOMG,SONA,SOK,SOSR,SOCL,SOSO4,SOHCO3       SEP  27
         READ (5,1140) SONO3,EC,CAL,B11,B2,GYP,SRS,CAF                  SEP  28
         WRITE (6,1100) SONO3,EC,CAL,B11,B2,GYP,SRS,CAF                 SEP  29
         IA=K                                                           SEP  30
         B1=B11
         B=B2
         SOCA=SOCA*B1/B
         SOMG=SOMG*B1/B
         SONA=SONA*B1/B
         SOK=SOK*B1/B
         SOSR=SOSR*B1/B
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      SOCL=SOCL*B1/B
      SOSO4=SOSO4*B1/B
      SOHCO3=SOHCO3*B1/B
      SONO3=SONO3*B1/B
      IF (.NOT.UNIT) GO TO 120                                SEP  31
      IA=0                                                    SEP  32
110   IA=IA+1                                                 SEP  33
120   J=J+1                                                   SEP  34

      SAR=SONA/SQRT((SOCA+SOMG)/2.)                           SEP  35
      ESP=0.01475*SAR/(1.+.01475*SAR)                         SEP  36
      CNA(J)=ESP*EC                                           SEP  37
      PAR=SOK/SQRT((SOCA+SOMG)/2.)                            SEP  38
      EPP=(0.0360+0.1051*PAR)/(1.+(0.0360+0.1051*PAR))        SEP  39
      CK(J)=EPP*EC                                            SEP  40
      ZE=EC-CK(J)-CNA(J)                                      SEP  41
      IF (SOMG.EQ.0.0) CMG(J)=0.0                             SEP  42
      IF (SOMG.EQ.0.0) GO TO 130                              SEP  43
      RA=SOCA/(SOMG*(0.625))                                  SEP  44
      CMG(J)=ZE/(RA+1.)                                       SEP  45
130   CCA(J)=-CMG(J)+ZE                                       SEP  46
      CSR(J)=CCA(J)*SOSR/(1.3*SOCA)                           SEP  47
      CNA(J)=CNA(J)/1000.                                     SEP  48
      CK(J)=CK(J)/1000.                                       SEP  49
      CMG(J)=CMG(J)/2000.                                     SEP  50
      CCA(J)=CCA(J)/2000.                                     SEP  51
      CSR(J)=CSR(J)/1000.                                     SEP  52
      CSNA(J)=SONA/1000.                                      SEP  53
      CSK(J)=SOK/1000.                                        SEP  54
      CSMG(J)=SOMG/2000.                                      SEP  55
      CSCA(J)=SOCA/2000.                                      SEP  56
      CSSR(J)=SOSR/2000.                                      SEP  57
      J1=0                                                    SEP  58
      DO 140 LBJ=1,JSUB                                       SEP  59
      J1=J1+1                                                 SEP  60
      SRSS(J,J1)=SRS                                          SEP  61
140   CONTINUE                                                SEP  62
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      CCL(J)=SOCL/1000.                                             SEP  63
      CSO4(J)=SOSO4/2000.                                           SEP  64
      CHCO3(J)=SOHCO3/1000.                                         SEP  65
      CNO3(J)=SONO3/1000.                                           SEP  66
      CALL(J)=CAL
      GYPP(J)=GYP                                                   SEP  68
      CAFF(J)=CAF                                                   SEP  69
      BBI(J)=BI1                                                    SEP  70
      BB2(J)=B2                                                     SEP  71
      IF (IA.NE.K) GO TO 110                                        SEP  72
      IF (J.LT.K) GO TO 100                                         SEP  73
      J=0                                                           SEP  74
      L=1                                                           SEP  75
      GO TO 200                                                     SEP  76
  150 READ (5,1260) SAT,RP,FT,CT,RSR                                SEP  77
      WRITE (6,1240) SAT,RP,FT,CT,RSR                               SEP  78
      READ (5,1260) GYP,CAL,B2,CAF,SRS                              SEP  79
      WRITE (6,1250) GYP,CAL,B2,CAF,SRS                             SEP  80
      IA=K                                                          SEP  81
      IF (.NOT.UNI) GO TO 170                                       SEP  82
      IA=0                                                          SEP  83
  160 IA=IA+1                                                       SEP  84
  170 J=J+1                                                         SEP  85
      GYPP(J)=GYP                                                   SEP  86
      BBI(J)=B2                                                     SEP  87
      BB2(J)=B2                                                     SEP  88
      CSR(J)=RSR                                                    SEP  89
      CMG(J)=CT                                                     SEP  90
      CCA(J)=ET                                                     SEP  91
      CALL(J)=CAL
      CK(J)=RP                                                      SEP  93
      J1=0                                                          SEP  94
      DO 180 LBJ=1,JSUB                                             SEP  95
      J1=J1+1                                                       SEP  96
      SRSS(J,J1)=SRS                                                SEP  97
  180 CONTINUE                                                      SEP  98
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      CNA(J)=SAT                                              SEP  99
      CAFF(J)=CAF                                             SEP 100
      B=BB2(J)
      IF (IA.NE.K) GO TO 160                                  SEP 101
      IF (J.LT.K) GO TO 150                                   SEP 102
      J=0                                                     SEP 103
      L=2                                                     SEP 104
      GO TO 200                                               SEP 105
  190 IF (M.NE.LL) GO TO 220                                  SEP 106
  200 READ (5,1140) WCA,WMG,WNA,WK,WSR,WCL,WSO4,WHCO3,M       SEP 107
      WRITE (6,1110) WCA,WMG,WNA,WK,WSR,WCL,WSO4,WHCO3,M      SEP 108
      READ (5,1140) WNO3,SRIN,CASOI,APH,WFL                   SEP 109
      WRITE (6,1120) WNO3,SRIN,CASOI,APH                      SEP 110
      READ (5,1270) ALI,LB                                    SEP 111
      WRITE (6,1280) ALI,LB                                   SEP 112
      J=J+1                                                   SEP 113
      IF (L-I) 230,230,210                                    SEP 114
  210 WCA=WCA/2000.                                           SEP 115
      WMG=WMG/2000.                                           SEP 116
      WSR=WSR/2000.                                           SEP 117
      WSO4=WSO4/2000.                                         SEP 118
      WNA=WNA/1000.                                           SEP 119
      WK=WK/1000.                                             SEP 120
      WHCO3=WHCO3/1000.                                       SEP 121
      WCL=WCL/1000.                                           SEP 122
      WNO3=WNO3/1000.                                         SEP 123
      WFL=WFL/1000.                                           SEP 124
      A=WCA                                                   SEP 125
      F=WMG                                                   SEP 126
      S=WNA                                                   SEP 127
      ASR=WSR                                                 SEP 128
      AP=WK                                                   SEP 129
      HCO3=WHCO3                                              SEP 130
      H=WCL                                                   SEP 131
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      G=WSO4                                                            SEP 132
      AN=WNO3                                                           SEP 133
      FL=WFL                                                            SEP 134
      B1=BB1(J)                                                         SEP 135
      B=BB2(J)                                                          SEP 136
      CASO=CASOI                                                        SEP 137
      SR=SRIN                                                           SEP 138
      GO TO 240                                                         SEP 139
  220 A=WCA                                                             SEP 140
      F=WMG                                                             SEP 141
      S=WNA                                                             SEP 142
      ASR=WSR                                                           SEP 143
      AP=WK                                                             SEP 144
      HCO3=WHCO3                                                        SEP 145
      H=WCL                                                             SEP 146
      G=WSO4                                                            SEP 147
      AN=WNO3                                                           SEP 148
      FL=WFL                                                            SEP 149
      J=J+1                                                             SEP 150
      B1=BB1(J)                                                         SEP 151
      B=BB2(J)                                                          SEP 152
      CASO=CASOI                                                        SEP 153
      SR=SRIN                                                           SEP 154
      GO TO 240                                                         SEP 155
  230 WCA=WCA/2000.                                                     SEP 156
      WMG=WMG/2000.                                                     SEP 157
      WNA=WNA/1000.                                                     SEP 158
      WK=WK/1000.                                                       SEP 159
      WSR=WSR/2000.                                                     SEP 160
      WNO3=WNO3/1000.                                                   SEP 161
      WHCO3=WHCO3/1000.                                                 SEP 162
      WSO4=WSO4/2000.                                                   SEP 163
      WCL=WCL/1000.                                                     SEP 164
      WFL=WFL/1000.                                                     SEP 165
      B1=BB1(J)                                                         SEP 166
      B=BB2(J)                                                          SEP 167
      H=WCL+CCL(J)*100./B3                                              SEP 168
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      G=WSO4+CSO4(J)*100./B3                                            SEP 169
      AN=WNO3+CNO3(J)*100./B3                                           SEP 170
      HCO3=WHCO3+CHCO3(J)*100./B3                                       SEP 171
      AP=WK +CSK(J)*100./B3                                             SEP 172
      ASR=WSR+CSSR(J)*100./B3                                           SEP 173
      S =WNA+CSNA(J)*100./B3                                            SEP 174
      F=WMG+CSMG(J)*100./B3                                             SEP 175
      A =WCA+CSCA(J)*100./B3                                            SEP 176
      FL=WFL                                                            SEP 177
      CASO=CASOI                                                        SEP 178
      SR=SRIN                                                           SEP 179
  240 XXT=GYPP(J)                                                       SEP 180

      B=1.0E+05*PORE/(B*B3/100.)                                        SEP 181
      RSR=CSR(J)                                                        SEP 182
      CT=CMG(J)                                                         SEP 183
      FT=CCA(J)                                                         SEP 184
      CAL=CALL(J)                                                       SEP 185
      RP=CK(J)                                                          SEP 186
      SRS=SRSS(J,JSUB)                                                  SEP 187
      SAT=CNA(J)                                                        SEP 188
      CAF=CAFF(J)                                                       SEP 189
      IF (PRINT.OR.PRI.AND.J.EQ.K) WRITE (6,1360) J,ISOL                SEP 190
      IF (PRINT.OR.PRI.AND.J.EQ.K) WRITE (6,1380)                       SEP 191
      IF (PRINT.OR.PRI.AND.J.EQ.K) WRITE (6,1370) AP,RP,S,SAT,F,CT,ASR,RSEP 192
     1SR,A,ET                                                           SEP 193
      IF (PRINT.OR.PRI.AND.J.EQ.K) WRITE (6,1290)                       SEP 194
      IF (PRINT.OR.PRI.AND.J.EQ.K) WRITE (6,1370) HCO3,AN,G,H,CASO,XXT,SSEP 195
     1R,SRS,CAL                                                         SEP 196
      IF (PRINT.OR.PRI.AND.J.EQ.K) WRITE (6,1300)                       SEP 197
      IF (PRINT.OR.PRI.AND.J.EQ.K) WRITE (6,1370) FL,CAF                SEP 198
  250 A11=A                                                             SEP 199
      IF (XXT) 260,260,270                                              SEP 200
  260 U=SQRT(2.0*(A+F+G+ASR)+0.5*(S+H+HCO3+AP+AN+FL))                   SEP 201
      AA=EXP(-9.366*(U/(U+1.)-.2*U*U))                                  SEP 202
      IF (2.4E-5-A*G*AA) 270,330,330                                    SEP 203
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```
270   X=0.0                                                        SEP 204
      U=SQRT(2.0*(A+F+G+ASR)+0.5*(S+H+HCO3+AP+AN+FL))              SEP 205
      BB=A+G                                                       SEP 206
      FX=(9.366*(U/(1.+U)-.2*U*U))                                 SEP 207
      CC=A*G-(2.4E-5)*EXP(EX)                                      SEP 208
      R=SQRT(BB*BB-4.0*CC)                                         SEP 209
      X=(-BB+R)/2.0                                                SEP 210
      CAS1=4.897E-3-CASO                                           SEP 211
      DEL=B*XXT-CAS1                                               SEP 212
      IF (DEL-X) 280,360,360                                       SEP 213
280   X=XXT*B                                                      SEP 214
      XXT=0.0                                                      SEP 215
      CAS1=0.0                                                     SEP 216
      A=A+X                                                        SEP 217
      G=G+X                                                        SEP 218
      U=SQRT(2.0*(A+F+G+ASR)+0.5*(S+H+HCO3+AP+AN+FL))              SEP 219
      AA=EXP(-9.366*(U/(U+1.)-.2*U*U))                             SEP 220
290   BB=-(4.9E-03+AA*A+AA*G)                                      SEP 221
      CC=AA*A*G-4.9E-3*CASO                                        SEP 222
      XXXX=BB*BB-4.0*AA*CC                                         SEP 223
      IF (XXXX) 300,300,310                                        SEP 224
300   X1=0.0                                                       SEP 225
      GO TO 320                                                    SEP 226
310   X1=(-BB-SQRT(XXXX))/(2.0*AA)                                 SEP 227
320   CASO=CASO+X1                                                 SEP 228
      A=A-X1                                                       SEP 229
      G=G-X1                                                       SEP 230
      GO TO 370                                                    SEP 231
330   IF (G) 350,350,340                                           SEP 232
340   IF (A) 350,350,290                                           SEP 233
350   IF (CASO) 370,370,290                                        SEP 234
360   A=A+X                                                        SEP 235
      G=G+X                                                        SEP 236
      XXT=XXT-X/B                                                  SEP 237
      CASO=CASO+CAS1                                               SEP 238
      XXT=XXT-CAS1/B                                               SEP 239
```

```
370   A2=A                                                            SEP 240
      SFI=S                                                           SEP 241
      IF ((RP.EQ.0.0.OR.S.EQ.0.0).AND.(AP.EQ.0.0.OR.SAT.EQ.0.0)) GO TO 4SEP 242
     160                                                              SEP 243
      ERROR=1.200E-06                                                 SEP 244
      KAR=0                                                           SEP 245
      NUMB=100                                                        SEP 246
      X=.5*AP/B-5.0E-09                                               SEP 247
      IF (X.GE.SAT) X=.6*SAT-5.0E-10                                  SEP 248
      IF (-X.GT.RP) X=-RP+1.0E-11                                     SEP 249
      IF (-X.GT.S/B) X=-S/B+1.0E-11                                   SEP 250
      ION=3                                                           SEP 251
      GO TO 390                                                       SEP 252
380   X=X+.1*X                                                        SEP 253
390   X70=X                                                           SEP 254
400   SI=S+B*X                                                        SEP 255
      AP1=AP-B*X                                                      SEP 256
      SATI=SAT-X                                                      SEP 257
      RP1=RP+X                                                        SEP 258
      IF (S1.LT.0.0.OR.SAT1.LT.0.0.OR.RP1.LT.0.0.OR.AP1.LT.0.0) GO TO 41SEP 259
     10                                                               SEP 260
      GO TO 420                                                       SEP 261
410   X=.5*X70                                                        SEP 262
      X70=X                                                           SEP 263
      GO TO 400                                                       SEP 264
420   FX=(S1/AP1)*(RP1/SAT1)**P3-FK3                                  SEP 265
      FXP=(FX+FK3)*(P3/RP1+P3/SAT1+B/S1+B/AP1)                        SEP 266
      CALL NEWTIT (X,FX,FXP,ERROR,NUMB,KAR,ION)                       SEP 267
      IF (NUMB.GE.50) WRITE (6,1130) ION,FX,X,FXP,S1,AP1,SAT1,RP1     SEP 268
      GO TO (400,450,430,450,380,440), KAR                            SEP 269
430   WRITE (6,1310)                                                  SEP 270
      WRITE (6,1320) J,ISOL,ION                                       SEP 271
      GO TO 1080                                                      SEP 272
440   WRITE (6,1330)                                                  SEP 273
      WRITE (6,1320) J,ISOL,ION                                       SEP 274
      GO TO 1080                                                      SEP 275
450   Y=X                                                             SEP 276
      S=S+B*Y                                                         SEP 277
      AP=AP-B*Y                                                       SEP 278
```

```
      SAT=SAT-Y                                                         SEP 279
      RP=RP+Y                                                           SEP 280
  460 INDEX=8                                                           SEP 281
      SE2=S                                                             SEP 282
      IF ((ET.EQ.0.0.OR.S.EQ.0.0).AND.(A.EQ.0.0.OR.SAT.EQ.0.0)) GO TO 53SEP 283
     10                                                                 SEP 284
      ERROR=1.000E-06                                                   SEP 285
      NUMB=100                                                          SEP 286
      KAR=0                                                             SEP 287
      ION=2                                                             SEP 288
      X=.1*S/B-5.0E-09                                                  SEP 289
      IF (X.GE.ET) X=.8*ET-5.0E-10                                      SEP 290
      IF (-X.GT.SAT/2.) X=-SAT/2.+1.0E-11                               SEP 291
      IF (-X.GT.A/B) X=-A/B+1.0E-11                                     SEP 292
      GO TO 480                                                         SEP 293
  470 X=X+.1*X                                                          SEP 294
  480 X70=X                                                             SEP 295
  490 A1=A+B*X                                                          SEP 296
      S1=S-2.*B*X                                                       SEP 297
      ET1=ET-X                                                          SEP 298
      SAT1=SAT+2.*X                                                     SEP 299
      IF (A1.LT.0.0.OR.S1.LT.0.0.OR.ET1.LT.0.0.OR.SAT1.LT.0.0) GO TO 500SEP 300
      GO TO 510                                                         SEP 301
  500 X=.5*X70                                                          SEP 302
      X70=X                                                             SEP 303
      GO TO 490                                                         SEP 304
  510 U=SQRT(2.0*(A+F+G+ASR)+0.5*(S+H+HCO3+AP+AN+FL))                   SEP 305
      AA=EXP(-2.344*(U/(U+1.)-.2*U*U))                                  SEP 306
      FX=AA*(A1/(S1*S1))*(SAT1/ET1)**P2-FK2                             SEP 307
      FXP=(FX+FK2)*((2.*P2)/SAT1+P2/ET1+B/A1+(4.*B)/S1)                 SEP 308
      CALL NEWTIT (X,FX,FXP,ERROR,NUMB,KAR,ION)                         SEP 309
      IF (NUMB.GE.90) WRITE (6,1130) ION,FX,X,FXP,S1,A1,SAT1,ET1        SEP 310
      GO TO (490,520,430,520,470,440), KAR                              SEP 311
  520 Y=X                                                               SEP 312
      A=A+B*Y                                                           SEP 313
      S=S-2.*B*Y                                                        SEP 314
      ET=ET-Y                                                           SEP 315
      SAT=SAT+2.*Y                                                      SEP 316
```

```
530   A3=A                                                                SEP 317
      IF (CT.LT.1.01E-11) CT=0.0                                          SEP 318
      IF ((ET.EQ.0.0.OR.F.EQ.0.0).AND.(A.EQ.0.0.OR.CT.EQ.0.0)) GO TO 600SEP 319
      ERROR=1.000E-06                                                     SEP 320
      NUMB=100                                                            SEP 321
      KAR=0                                                               SEP 322
      ION=1                                                               SEP 323
      X=.1*F7B-5.0E-09                                                    SEP 324
      IF (X.GE.ET) X=.8*ET-5.0E-10                                        SEP 325
      IF (-X.GT.CT) X=-CT+1.0E-11                                         SEP 326
      IF (-X.GT.A/B) X=-A/B+1.0E-11                                       SEP 327

      GO TO 550                                                           SEP 328
540   X=X+.1*X                                                            SEP 329
550   X70=X                                                               SEP 330
560   AI=A+B*X                                                            SEP 331
      F1=F-B*X                                                            SEP 332
      ET1=ET-X                                                            SEP 333
      CT1=CT+X                                                            SEP 334
      IF (AI.LT.0.0.OR.F1.LT.0.0.OR.ET1.LT.0.0.OR.CT1.LT.0.0) GO TO 570 SEP 335
      GO TO 580                                                           SEP 336
570   X=.5*X70                                                            SEP 337
      X70=X                                                               SEP 338
      GO TO 560                                                           SEP 339
580   FX=(A1/F1)*(CT1/ET1)**P1-FK1                                        SEP 340
      FXP=(FX+FK1)*(P1/ET1+P1/CT1+B/A1+B/F1)                              SEP 341
      CALL NEWTIT (X,FX,FXP,ERROR,NUMB,KAR,ION)                           SEP 342
      IF (NUMB.GE.90) WRITE (6,1130) ION,FX,X,FXP,F1,A1,CT1,FT1           SEP 343
      GO TO (560,590,430,590,540,440), KAR                                SEP 344
590   Y=X                                                                 SEP 345
      A=A+B*Y                                                             SEP 346
      F=F-B*Y                                                             SEP 347
      ET=ET-Y                                                             SEP 348
      CT=CT+Y                                                             SEP 349
600   A4=A                                                                SEP 350
      IF (RSR) 620,620,610                                                SEP 351
610   BB=A+B*(RSR+1.23*ET)+1.23*ASR                                       SEP 352
```

```
      AA=B*(1.0-1.23*ASR*ET)
      CC=(A*RSR-1.23*ASR*ET)
      R=SQRT(BB*BB-4.0*AA*CC)
      Y=(-BB+R)/(2.0*AA)
      A=A+B*Y
      ASR=ASR-B*Y
      ET=ET-Y
      RSR=RSR+Y
      A5=A
  620 U=SQRT(2.0*(A+F+G+ASR)+0.5*(S+H+HCO3+AP+AN+FL))
      AA=EXP(-7.034*(U/(U+1.)-.2*U*U))
      Z3=4.676E-10-A*HCO3**2*AA
      IF (Z3) 630,700,700
  630 ERROR=1.0E-11
      KAR=0
      NUMB=100
      ION=4
      XJ=SQRT(4.676E-10/(AA*A))
      X=(XJ-HCO3)/2.
      IF (-X.GT.A) X=-(.93*A-5.0E-07)
      GO TO 650
  640 X=X+.1*X
  650 X70=X
  660 CA1=A+X

      HC1=HCO3+2.*X
      IF (CA1.LT.0.0.OR.HC1.LT.0.0) GO TO 670
      GO TO 680
  670 X=.5*X70
      X70=X
      GO TO 660
  680 FX=CA1*HC1**2-4.676E-10/AA
      FXP=HC1**2+4.*CA1*HC1
      CALL NEWTIT (X,FX,FXP,ERROR,NUMB,KAR,ION)
      IF (NUMB.GE.90) WRITE (6,1130) ION,FX,X,FXP,CA1,HC1,A,HCO3
      GO TO (660,690,430,690,640,440), KAR
```

```
690   A=A+X                                                 SEP 388
      HCO3=HCO3+2.*X                                        SEP 389
      CAL=CAL-X/B                                           SEP 390
      IF (A.LT.0.0.OR.HCO3.LT.0.0) GO TO 1080               SEP 391
      GO TO 730                                             SEP 392
700   IF (CAL.GT.0.0) GO TO 710                             SEP 393
      GO TO 730                                             SEP 394
710   XM=CAL*B                                              SEP 395
      AOLD=A                                                SEP 396
      HCOLD=HCO3                                            SEP 397
      COLD=CAL                                              SEP 398
      A=A+XM                                                SEP 399
      HCO3=HCO3+2.*XM                                       SEP 400
      QU=SQRT(2.0*(A+F+G+ASR)+.5*(S+H+HCO3+AP+AN+FL))       SEP 401
      CAL=0.0                                               SEP 402
      QA=EXP(-7.034*(QU/(QU+1.)-.2*QU*QU))                  SEP 403
      Z3=4.676E-10-A*HCO3**2*QA                             SEP 404
      IF (Z3) 720,730,730                                   SEP 405
720   A=AOLD                                                SEP 406
      HCO3=HCOLD                                            SEP 407
      CAL=COLD                                              SEP 408
      GO TO 630                                             SEP 409
730   A6=A                                                  SEP 410
      U=SQRT(2.0*(A+F+G+ASR)+0.5*(S+H+HCO3+AP+AN+FL))       SEP 411
      AA=EXP(-7.034*(U/(U+1.)-.2*U*U))                      SEP 412
      Z4=3.98E-11-A*FL**2*AA                                SEP 413
      IF (Z4) 740,840,840                                   SEP 414
740   ERROR=3.0E-12                                         SEP 415
      KAR=0                                                 SEP 416
      NUMB=100                                              SEP 417
      ION=5                                                 SEP 418
      XJ=SQRT(3.98E-11/(AA*A))                              SEP 419
      X=(XJ-FL)/2.                                          SEP 420
      IF (-X.GT.A) X=-(.93*A-5.0E-07)                       SEP 421
      XS=X                                                  SEP 422
      INR=0                                                 SEP 423
      GO TO 760                                             SEP 424
750   X=X+.1*X                                              SEP 425
```

```
      WRITE (6,1340)
 760  X70=X
 770  CA2=A+X
      FL2=FL+2.*X
      IF (CA2.LT.0..OR.FL2.LT.0.) GO TO 800
      GO TO 810
 780  IF (ABS(FXR(4)).GT.ABS(FXR(3)).AND.ABS(FXR(3)).GT.ABS(FXR(2)).AND.
     1ABS(FXR(2)).GT.ABS(FXR(1))) GO TO 790
      GO TO 770
 790  X=(XS+XNR(1))/2.
      GO TO 830
 800  X=.5*X70
      X70=X
      GO TO 770
 810  FX=CA2*FL2**2-3.98E-11/AA
      FXP=FL2**2+4.*A2*FL2
      CALL NEWTIT (X,FX,FXP,ERROR,NUMB,KAR,ION)
      IF (NUMB.GE.90) WRITE (6,1130) ION,FX,X,FXP,CA2,FL2,A,FL
      GO TO (820,830,430,830,750,440), KAR
 820  INR=INR+1
      XNR(INR)=X
      FXR(INR)=FX
      IF (INR.EQ.4) GO TO 780
      GO TO 770
 830  A=A+X
      FL=FL+2.*X
      CAF=CAF-X/B
      IF (A.LT.0..OR.FL.LT.0.) GO TO 1080
      GO TO 870
 840  IF (CAF.GT.0.) GO TO 850
      GO TO 870
 850  XM=CAF*B
      AOLD=A
      FOLD=FL
      COLD=CAF
```

```
      FL=FL+2.*XM                                                       SEP 461
      CAF=0.                                                            SEP 462
      QU=SQRT(2.*(A+F+G+ASR)+.5*(S+H+HCO3+AP+AN+FL))                    SEP 463
      QA=EXP(-7.034*(QU/(QU+1.)-.2*QU*QU))                              SEP 464
      Z4=3.98E-11-A*FL**2*QA                                            SEP 465
      IF (Z4) 860,870,870                                               SEP 466
  860 A=AOLD                                                            SEP 467
      FL=FOLD                                                           SEP 468
      CAF=COLD                                                          SEP 469
      GO TO 740                                                         SEP 470
  870 DEL=A-A11                                                         SEP 471
      IF (DEL+1.0E-5) 250,880,880                                       SEP 472
  880 IF (DEL-1.0E-5) 890,890,250                                       SEP 473
  890 DEL=A-A2                                                          SEP 474
      IF (DEL+1.0E-5) 250,900,900                                       SEP 475
  900 IF (DEL-1.0E-5) 910,910,250                                       SEP 476
  910 DEL=A-A3                                                          SEP 477
      IF (DEL+1.0E-5) 250,920,920                                       SEP 478
  920 IF (DEL-1.0E-5) 930,930,250                                       SEP 479
  930 DEL=A-A4                                                          SEP 480
      IF (DEL+1.0E-5) 250,940,940                                       SEP 481
  940 IF (DEL-1.0E-5) 950,950,250                                       SEP 482
  950 DEL=S-SF1                                                         SEP 483
      IF (ABS(DEL)-1.0E-5) 960,960,250                                  SEP 484
  960 DEL=S-SF2                                                         SEP 485
      IF (ABS(DEL)-1.0E-5) 970,970,250                                  SEP 486
  970 IF (RSR) 990,990,980                                              SEP 487
  980 DEL=A-A5                                                          SEP 488
      IF (ABS(DEL)-1.0E-5) 990,990,250                                  SEP 489
  990 DEL=A-A6                                                          SEP 490
      IF (ABS(DEL)-1.0E-5) 1000,1000,250                                SEP 491
 1000 CALL DIST (B,A,AP,S,F,ASR,APH,AKD,HCO3,AN,H,G,AAPH,U,FL)          SEP 492
      IF (AKD.LT.0.0) AKD=0.0                                           SEP 493
      J1=0                                                              SEP 494
      B=B/FLOAT(JSUB)                                                   SEP 495
```

```
      DO 1040 LBJ=1,JSUB                                              SEP 496
      J1=J1+1                                                         SEP 497
      Y=(AKD*SR-SRSS(J,J1))/(1.+AKD*B)                                SEP 498
      IF (Y) 1010,1020,1020                                           SEP 499
 1010 IF (-Y.GT.SRSS(J,J1)) Y=-SRSS(J,J1)                             SEP 500
      GO TO 1030                                                      SEP 501
 1020 IF (Y*B.GT.SR) Y=SR/B                                           SEP 502
 1030 SR=SR-Y*B                                                       SEP 503
      SRSS(J,J1)=SRSS(J,J1)+Y                                         SEP 504
 1040 CONTINUE                                                        SEP 505
      B=B*1000.*FLOAT(JSUB)                                           SEP 506
      SRS=SRSS(J,JSUB)                                                SEP 507
      ISOLF=ISOL                                                      SEP 508
      VOL=ALI*ISOLF                                                   SEP 509
      COVOL=VOL/VSOIL                                                 SEP 510
      BREAK=SR/SRIN                                                   SEP 511
      IF(PRINT.OR.PRI.OR.J.EQ.K)WRITE(6,1350)J,ISOL
      IF(PRINT.OR.PRI.OR.J.EQ.K)WRITE(6,1380)
      IF(PRINT.OR.PRI.OR.J.EQ.K)WRITE(6,1370)AP,RP,S,SAT,F,CT,ASR,RSR,A,
     CET
      IF(PRINT.OR.PRI.OR.J.EQ.K)WRITE(6,1390)
      IF(PRINT.OR.PRI.OR.J.EQ.K)WRITE(6,1410)HCO3,AN,G,H,SR,SRS,VOL,COVOL,
     CL,BREAK
      IF(PRINT.OR.PRI.OR.J.EQ.K)WRITE(6,1400)
      IF(PRINT.OR.PRI.OR.J.EQ.K)WRITE(6,1420)APH,AKD,CASO,XXT,CAL,CAF,FL,B
     C,B,U
      CSR(J)=RSR                                                      SEP 521
      CMG(J)=CT                                                       SEP 522

      CCA(J)=ET                                                       SEP 523
      CK(J)=RP                                                        SEP 524
      CNA(J)=SAT                                                      SEP 525
      GYPP(J)=XXT                                                     SEP 526
      CALL(J)=CAL
      CAFF(J)=CAF                                                     SEP 528
      IFX=0                                                           SEP 529
```

```
      J=J+1                                                             SEP 530
      B1=BB1(J)                                                         SEP 531
      B=BB2(J)                                                          SEP 532
      IF (J-K) 1050,1050,1070                                           SEP 533
 1050 IF (L-I) 1060,1060,240                                            SEP 534
 1060 H =H+CCL(J)*100./B3                                               SEP535
      G =G+CSO4(J)*100./B3                                              SEP 536
      AN=AN+CNO3(J)*100./B3                                             SEP 537
      HCO3=HCO3+CHCO3(J)*100./B3                                        SEP 538
      AP=AP+CSK(J)*100./B3                                              SEP 539
      ASR=ASR+CSSR(J)*100./B3                                           SEP 540
      S =S+CSNA(J)*100./B3                                              SEP 541
      F =F+CSMG(J)*100./B3                                              SEP 542
      A =A+CSCA(J)*100./B3                                              SEP 543
      GO TO 240                                                         SEP 544
 1070 CONTINUE                                                          SEP 545
      ISOL=ISOL+1                                                       SEP 546
      J=0                                                               SEP 547
      L=2                                                               SEP 548
      LL=LL+1                                                           SEP 549
      IF (LL-LB) 190,1080,1080                                          SEP 550
 1080 CALL EXIT                                                         SEP 551
C                                                                       SEP 552
 1090 FORMAT (T9,4HSOCA,T21,4HSOMG,T34,4HSONA,T48,3HSOK,T60,4HSOSR,T73,4SEP 553
     1HSOCL,T86,5HSOSO4,T97,6HSOHCO3/8(3X,E10.5)//)                     SEP 554
 1100 FORMAT (T9,5HSONO3,T21,2HEC,T34,3HCAL,T48,3HB11,T60,2HB2,T73,3HGYPSEP 555
     1,T86,3HSRS,T99,3HCAF/8(3X,E10.5)//)                               SEP 556
 1110 FORMAT (T9,3HWCA,T21,3HWMG,T34,3HWNA,T48,2HWK,T60,3HWSR,T73,3HWCL,SEP 557
     1T86,4HWSO4,T100,5HWHCO3,T112,1HM/8(3X,E10.5)3X,I5//)              SEP 558
 1120 FORMAT (T9,4HWNO3,T21,4HSRIN,T34,5HCASOI,T48,3HAPH/4(3X,E10.5)//) SEP 559
 1130 FORMAT (1I6,7E15.5)                                               SEP 560
 1140 FORMAT (8F8.0,5X,I5)                                              SEP 561
 1150 FORMAT (4L10)                                                     SEP 562
 1160 FORMAT (1H1,'THE SOIL COLUMN IS DRY ..................'L10)       SEP 563
 1170 FORMAT (1H0'THE SOIL PROFILE IS UNIFORM................'L10)      SEP 564
 1180 FORMAT (1H0,'PRINT ALL INITIAL AND FINAL VALUES ........'L10)     SEP 565
 1190 FORMAT (1H0,'PRINT ALL EQUILIBRIUM VALUES ONLY..........'L10,//)  SEP 566
```

```
 1200  FORMAT (6F10.4)                                                    SEP 567
 1210  FORMAT (T6,3H P1,T16,4H FK1,T26,3H P2,T36,4H FK2,T46,3H P3,T56,4H SEP 568
      1FK3/6E10.3//)                                                      SEP 569
 1220  FORMAT (2I6,3F10.3)                                                SEP 570
 1230  FORMAT (T6,2H K,T13,5H JSUB,T19,6H VSOIL,T31,5H PORE,T40,6H ( SAT/

      C2I8,3E10.3//)                                                      SEP 571
 1240  FORMAT (T10,4H SAT,T25,3H RP,T40,3H ET,T55,3H CT,T70,4H RSR,/5E15.SEP 572
      14//)                                                               SEP 573
 1250  FORMAT (T10,4H GYP,T25,4H CAL,T40,3H B2,T55,4H CAF,T70,4H SRS/5E15SEP 574
      1.4//)                                                              SEP 575
 1260  FORMAT (5E15.4)                                                    SEP 576
 1270  FORMAT (E14.4,I6)                                                  SEP 577
 1280  FORMAT (T9,4H ALI,T19,2HLB/E14.4,I6//)                             SEP 578
 1290  FORMAT (89H      HCO3        NO3       SO4          CL       CASO4UN    GSEP 579
      1YPSUM    SR85 SOL  SR85 SOIL  CAL  )                               SEP 580
 1300  FORMAT (21H       FL          CAF   )                              SEP 581
 1310  FORMAT (96HOROOT DID NOT CONVERGE WITHIN MAXIMUM NUMBER OF ITERATISEP 582
      1ONS,PROGRAM RETURNING TO NEXT SET OF DATA)                         SEP 583
 1320  FORMAT (3I6)                                                       SEP 584
 1330  FORMAT (54HOOVERFLOW IN COMPUTATION,RETURNING TO NEXT SET OF DATA)SEP 585
 1340  FORMAT (18H WENT THRU NUMB 21)                                     SEP 586
 1350  FORMAT (40H EQUILIBRIUM VALUES FOR ALL IONS  COLUMN,I5,8H ALIQUOTISEP 587
      15)                                                                 SEP 588
 1360  FORMAT (60H INITIAL CONDITIONS AFTER SOLUTION DISSOLVES SOLUBLE. CSEP 589
      1OLUMN,I5,8H ALIQUOT,I5)                                            SEP 590
 1370  FORMAT (1X,10(1PE10.3),10X,2(1PE10.3))                             SEP 591
 1380  FORMAT (102H       K          KX          NA         NAX         MG      SEP 592
      1 MGX        SR        SRX         CA         CAX        )          SEP 593
 1390  FORMAT (107H      HCO3        NO3       SO4          CL       SR85 SOL SR85SEP 594
      1 SOIL    VOLUME(ML)  COLVOL      C/CO                    )         SEP 595
 1400  FORMAT (97H      PH          KD       CASO4UN    GYPSUM       CAL      SEP 596
      1 CAF         FL          B           U          )                  SEP 597
 1410  FORMAT (1X,10(1PE10.3))                                            SEP 598
 1420  FORMAT (1X,10(1PE10.3))                                            SEP 599
       END                                                                SEP 600
```

```
'M   FR5 DIST
      SUBROUTINE DIST (B,A,AP,S,F,ASR,APH,AKD,HCO3,AN,H,G,AAPH,U,FL)      DIS   1
      IF (HCO3.LE.0.0) GO TO 100                                          DIS   2
      U=SQRT(2.0*(A+F+G+ASR)+0.5*(S+H+HCO3+AP+AN+FL))                     DIS   3
      APH=6.65-.5*ALOG(A)+1.018*(U/(1.+U)-.2*U*U)                         DIS   4
      AAPH=6.6-.5*ALOG10(A)                                               DIS   5
100   B=B/1000.                                                           DIS   6
      IF (A.LT..005) GO TO 110                                            DIS   7
      AKD=1.9337-60.72*(A-.0275)-.5287*(40.*AP-1.)+17.831*(40.*AP-1.)*(ADIS   8
     1-.0275)-3.263*(S-.11)+126.52*(S-.11)*(A-.0275)+5.43*(S-.11)*(40.*ADIS   9
     2P-1.)-222.864*(S-.11)*(40.*AP-1.)*(A-.0275)                         DIS  10
      RETURN                                                              DIS  11
110   AKD=4.325-683.3*(A-.0035)-1.67*(40.*AP-1.)+493.3*(A-.0035)*(40.*APDIS  12
     1-1.)-11.*(S-.11)+3259.26*(S-.11)*(A-.0035)+11.94*(S-.11)*(40.*AP-1DIS  13
     2.)-1000.*(S-.11)*(A-.0035)*(40.*AP-1.)                              DIS  14
      RETURN                                                              DIS  15
      END                                                                 DIS  16-
'M   FR5 NEWTIT,NEWTIT
      SUBROUTINE NEWTIT (X,FX,FXP,E,N,K,ION)                              NEW   1
      COMMON F,ET,B,S,AP,SAT,CT,RP,A,HCO3,FL                              NEW   2
      IF (K.GT.0) GO TO 100                                               NEW   3
      J=K                                                                 NEW   4
      K=1                                                                 NEW   5
      NMAX=N                                                              NEW   6
      N=0                                                                 NEW   7
100   T=FX                                                                NEW   8
      IF (J.EQ.0) GO TO 110                                               NEW   9
      IF (ABS(X).LT.1.E-34) GO TO 120                                     NEW  10
      T=T/X                                                               NEW  11
110   IF (.NOT.ABS(T).GT.E) GO TO 260                                     NEW  12
120   IF (N.EQ.NMAX) GO TO 270                                            NEW  13
      IF (.NOT.ABS(FXP).GT.0.) GO TO 290                                  NEW  14
      T=X                                                                 NEW  15
      X=X-FX/FXP                                                          NEW  16
      GO TO (130,160,190,220,230), ION                                    NEW  17
130   IF (F.EQ.0.) GO TO 140                                              NEW  18
      IF (B*X.GE.F) X=.95*F/B                                             NEW  19
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      IF (FT.EQ.0.) GO TO 150                                           NEW   20
140   IF (X.GE.FT) X=.95*FT                                             NEW   21
150   IF (-X.GT.CT) X=-CT+1.0E-11                                       NEW   22
      IF (-X.GT.A/B) X=-A/B+1.0E-11                                     NEW   23
      GO TO 240                                                         NEW   24
160   IF (S.EQ.0.) GO TO 170                                            NEW   25
      IF (2.*B*X.GE.S) X=.95*S/(2.*B)                                   NEW   26
      IF (ET.EQ.0.) GO TO 180                                           NEW   27
170   IF (X.GE.ET) X=.95*ET                                             NEW   28
180   IF (-X.GT.SAT/2.) X=-SAT/2.+1.0E-11                               NEW   29
      IF (-X.GT.A/B) X=-A/B+1.0E-11                                     NEW   30
      GO TO 240                                                         NEW   31
190   IF (AP.EQ.0.) GO TO 200                                           NEW   32
      IF (B*X.GE.AP) X=.95*AP/B                                         NEW   33
      IF (SAT.EQ.0.) GO TO 210                                          NEW   34
200   IF (X.GE.SAT) X=.95*SAT                                           NEW   35
210   IF (-X.GT.RP) X=-RP+1.0E-11                                       NEW   36
      IF (-X.GT.S/B) X=-S/B+1.0E-11                                     NEW   37
      GO TO 240                                                         NEW   38
220   XY=X                                                              NEW   39
      IF (-X.GT.A) X=-.95*A                                             NEW   40
      IF (-X/2..GT.HCO3) X=-.45*HCO3                                    NEW   41
      IF (XY.NE.X) WRITE (6,310) XY,X                                   NEW   42
      GO TO 240                                                         NEW   43
230   XY=X                                                              NEW   44
      IF (-X.GT.A) X=-.95*A                                             NEW   45
      IF (-X/2..GT.FL) GO TO 250                                        NEW   46
240   N=N+1                                                             NEW   47
      CALL OVERFL (I)                                                   NEW   48
      IF (I.EQ.1) GO TO 300                                             NEW   49
      IF (.NOT.ABS(T-X).GT.0.) GO TO 280                                NEW   50
      RETURN                                                            NEW   51
250   X=9.4E-05                                                         NEW   52
      WRITE (6,320) XY,X,A,F                                            NEW   53
      GO TO 230                                                         NEW   54
```

```
260    K=2                                              NEW  55
       RETURN                                           NEW  56
270    K=3                                              NEW  57
       RETURN                                           NEW  58
280    K=4                                              NEW  59
       RETURN                                           NEW  60
290    K=5                                              NEW  61
       RETURN                                           NEW  62
300    K=6                                              NEW  63
       RETURN                                           NEW  64
C                                                       NEW  65
310    FORMAT (22H NEWTON RAPHSON CHANGE,2E10.4)        NEW  66
320    FORMAT (17H WENT THRU NEWTIT,4E10.4)             NEW  67
       END                                              NEW  68
' XQT SEP
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