DATA INPUT GUIDE FOR SWIFT FOR WINDOWS

THE SANDIA WASTE-ISOLATION FLOW AND TRANSPORT MODEL
FOR FRACTURED MEDIA, RELEASE 2.60

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February 21, 2000

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PREFACE

The SWIFT for Windows model is the result of more than 17 years of model evolution. The predecessor codes, SWIPR, SWIFT and SWIFT II are publicly available through the National Technical Information Service and the Energy Science and Technology Center. The extension to SWIFT III was funded by HSI GeoTrans, Inc. with internal research and development funds. The PC implementation, SWIFT for Windows, was developed by HSI GeoTrans. This version is specific to the Pentium CPU processor and the Lahey LF95 Fortran compiler. The work is based on NUREG/CR-3162.

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ABSTRACT

This report is one of three which describes the three-dimensional model SWIFT for Windows. SWIFT for Windows is a fully transient, three-dimensional model which simulates the flow and transport of fluid, heat (energy), brine, and radionuclide chains in porous and fractured geologic media. It was developed for use in the analysis of deep geologic facilities for nuclear-waste disposal but can be used for a number of applications. Some of these applications include: assessment of well performance; steady-state and transient groundwater systems comprising water table, rivers, and wells; deep-well injection of hazardous waste; prediction of hazardous waste migration from land disposal sites; analysis of hydraulic barriers, liners, and containment systems; and groundwater transport of pesticides, herbicides, and agricultural products.

This document is a user's manual and should permit the analyst to use the code effectively by facilitating the preparation of input data. The second companion document, Reeves et al. [1986a], discusses the theory and implementation of the basic model and its submodels. The third document, Reeves et al. [1986b], provides illustrative problems for instructional purposes.

This report contains detailed descriptions of the data records. It also contains in an appendix a description of the input diagnostics which are coded with error numbers and record identifiers. Other useful items pertaining to the use of auxiliary files, unit conversions, and program variable descriptors also are included in this document. A utility post processing program, UNSWIFT, provides an interface to the contouring program SURFER®.

ACKNOWLEDGMENTS

The evolution of the SWIFT for Windows code is supported by HSI GeoTrans through project application and the independent efforts of the code custodian and users of the model. The code contributors include: David S. Ward, Jeff Benegar, Andrew L. Harrover, Alex H. Vincent, Barry H. Lester, Michael C. Brown and Charles R. Faust. The code custodian is Jeffrey Benegar.

1 INTRODUCTION

The input data of the SWIFT for Windows (Sandia Waste-Isolation Flow and Transport Model) model provides an important compliment to two other reports. Reeves et al. [1986a] gives the theory and formulation of the model whereas Reeves et al. [1986b] provides instruction problem sets, complete with listings of the data input and output. In addition, Finley and Reeves [1981] provides illustrative problems which, although designed for SWIFT, may be used for an initial orientation to SWIFT for Windows. Verification and validation tests of the SWIFT code are presented by Ward et al. [1984].

1.1 THE SWIFT MODELS

The SWIFT model was originally developed, maintained and applied by Sandia National Laboratories. The Nuclear Regulatory Commission has sponsored this work under its high-level nuclear-waste program. Between 1982 and 1985 the capability of SWIFT has been enlarged to include fractured media, a free-water surface and extended boundary conditions. Since 1985, HSI GeoTrans has modified the code funded through internal research and development. Revisions include a conversion to Fortran 77, extended options for matrix solutions, contour mapping and boundary conditions and postprocessing options. This code is designated as SWIFT III. In 1990, a PC version of SWIFT (SWIFT/386) was developed in which a run-time monitor was added to improve user friendliness. Since then the code has been further enhanced to include multiple values of rock compressibility. A utility program, UNSWIFT, provides an interface between the map output and the contouring program SURFER®. These models, SWIFT, SWIFT II, SWIFT III, SWIFT/386, SWIFT/486, SWIFT-98, and Swift for Windows are fully transient (with steady-state options), three-dimensional, finite-difference codes, which solve the coupled equations for flow and transport in geologic media. The models may be used for evaluation of repository site performance and repository design performance.

The processes considered are:

- fluid flow,
- heat transport,

- brine migration,
- radionuclide-chain transport.

Flow, heat and brine transport are coupled via fluid density, fluid viscosity and porosity. Together they provide the velocity field on which the radionuclide transport depends.

The media considered are:

- porous media (SWIFT, SWIFT II, SWIFT III, SWIFT/486, SWIFT-98, and SWIFT for Windows),
- fractured media (SWIFT II, SWIFT III, SWIFT/486, SWIFT-98, and SWIFT for Windows).

As discussed in Reeves et al. [1986a], the SWIFT for Windows model permits local one-dimensional subsystems to be attached, as desired, to the grid blocks comprising the global system. The local units may be used either to characterize the second porosity of a fractured media or to extend the boundaries of the system in a computationally inexpensive manner.

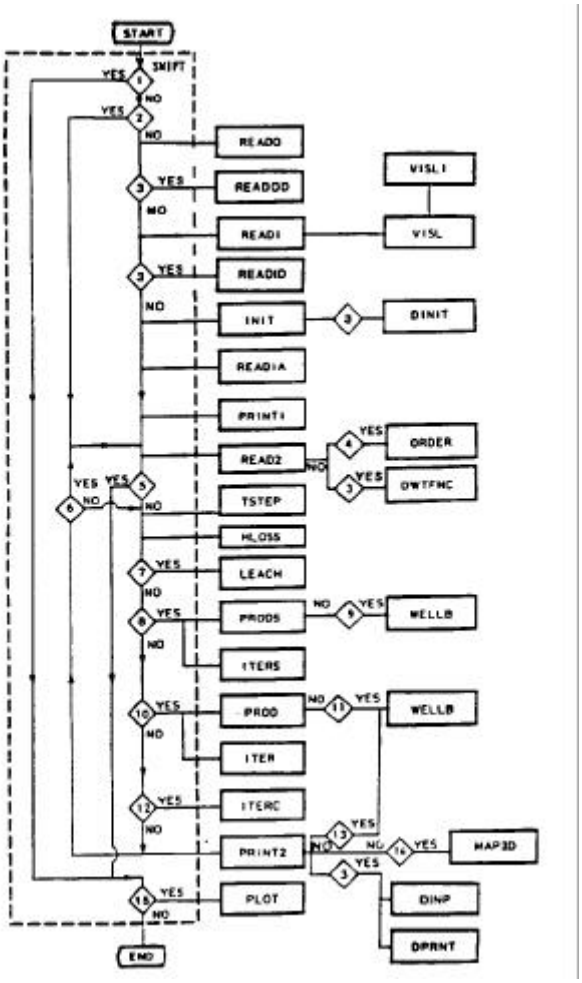
1.2 PROGRAM STRUCTURE

The SWIFT for Windows program consists of a main routine and approximately 90 supporting subroutines. Its general structure is illustrated by Figure 1-1, a flow chart of the main routine. The basic organization is focused upon the three global integration modules ITER, ITERS and ITERC. Subroutine ITER solves the coupled partial differential equations for fluid flow, heat transport and brine transport under transient conditions, ITERS integrates the flow and brine equations under steady-state conditions and ITERC solves the coupled partial differential equations for transport of a radionuclide chain. All other routines provide support functions for the integration. The support function of interest in this report is that of data input.

1.3 DATA

Data input occurs in eight of the subroutines shown in Figure 1-1, which may be viewed in several different ways. Seven of the routines are positioned outside the recurrent time-step loop extending from READ2 to PRINT2. These routines read time-independent data. The other

Figure 1-1. General Structure of SWIFT for Windows.



Conditions for Figure 1-1 (numbered diamonds) are as follows:

(1) Are plots desired for a previous run?

(2) Is this a restart run?

(3) Is dual porosity to be included?

(4) Is the reduced-bandwidth direct method of solution used? (multi-dimensional problems only)

(5) Is the run to be terminated at this time step?

(6) Are the recurrent data to be read at this time step?

(7) Is the waste-leach submodel employed?

(8) Is the steady-state pressure solution sought?

(9) Are steady-state wellbore calculations to be performed?

(10) Is the transient pressure solution sought?

(11) Are the transient wellbore calculations to be solved?

(12) Are the radionuclide transport calculations to be performed?

(13) In the transient wellbore calculations, are the well rates to be calculated semi-implicitly?

(14) Are any two-dimensional contour maps desired?

(15) Are any plots desired for this run?

routine, READ2, is positioned inside the recurrent time-step loop. Therefore, it reads time-dependent data. Regarding the storage allocation function, the three routines SWIFT, READ0 and READ0D provide data which optimally partition the common-block arrays. Here SWIFT reads such information for the global-system arrays, READ0 for the radionuclide arrays and READ0D for the local-subsystem arrays. In regard to the dual-porosity function, routines READ0D and READ1D provide input pertaining specifically to the local porosity, whereas the other routines provide input pertaining to the global porosity. Finally, the data input records divide naturally into groups depending upon the program unit in which they are read. Table 1-1 gives the "shorthand" notation used by each group and a brief description of the function of each group.

To facilitate data input, the use of record type identifiers is strongly encouraged. These identifiers, i.e., M-1, R1-1, R2-7-1 may be entered in columns 71-80 on the input data sets. Blank records are typically blank in columns 1-70 and the field identifier placed in columns 71-80, i.e., R1-26-BLK. This scheme has been used in the verification data sets and has been maintained for upward compatibility with previous versions of SWIFT. In maintaining this compatibility, an exception arises in record type R2-12 (section 8.8) where columns 1-80 are all reserved for data input.

Chapters 2 through 9 define, in detail, the data entered within each data group. Other useful items, such as auxiliary disk files, units of measurement and a variable index are treated in the remaining chapters and in the first three appendices. However, for easy reference, the final appendix is reserved for the input-error diagnostics which are printed by the code.

Table 1-1. Data Input Groups.

Routine	Notation	Data Function
SWIFT	M*	General problem setup
	P	Plotting data
READ0	R0	Radionuclide-chain information
READ0D	R0D	Dimensioning data of the local arrays
READ1	R1*	Properties of the global system
READ1D	R1D	Properties of the local subsystems
INIT	I*	Initialization data
READ1A	R1A	Specification of waste-leach submodel
NMONINP	N	Nuclide monitor block
READ2	R2*	Time-dependent data

*Indicates mandatory input. All others are optional.

2 THE M, R0 AND R0D RECORDS

2.1 THE M RECORDS, GROUP 1

The data supplied by the M records provide general program control and storage allocation for the global system. These functions include:

- primary equations to be solved in the global systems,
- primary equations to be solved in the local subsystems,
- radionuclide solution control,
- restart control,
- printing and plotting control,
- number of grid blocks in the global system,
- allocation for the coefficient matrix A.

Data input for the M Records and subsequent data groups are to be entered in the format described in the bold faced headers. Each header includes: a record title, format specifications, and a general description of the type of data to be entered. Below the header is a list of the variables in the order of entry as well as a description of each variable. Column numbers for each variable are listed for convenient location within the data set.

READ M-1 (A80/A80) Title

LIST: TITLE

TITLE Two records of alphanumeric data to serve as title for this run. Any title up to 160 characters (80/record) in length may be used.

READ M-2 (13I5) Option Parameters

LIST: NCALL, RSTRT, ISURF, IFREE, NPLP, NPLT, NPLC, IUNIT, LBIO, LMAPIT, LMBAL, LAIF, L2SORP

NCALL Control parameter for solving the primary partial differential equations within the global system. See Table 2-1 (Col. 1-5).

RSTRT Control parameter for restarting the program. (Col. 6-10)

-1 - Map from restart (Choose restart record on M-6.).
0 - A normal run starting from initial conditions.
>0 - For a calculational restart, the number (ITIME) of the time step from a previous run at which calculations are to resume.
999 - For a calculational restart in which calculations will resume from the first restart record on disk.

For a calculational restart, a restart record from a previous run, corresponding to the specified time step, ITIME, must exist on the restart unit (UNIT 4, Table 10.1). Parameter ITIME is printed each time a restart record is written. Furthermore, a restart record is written at the end of a recurrent data set providing RSTWR = 1 (READ R2-13).

ISURF Control parameter for the wellbore calculations (Col. 11-15).

0 - Rates and pressures will be specified at the reservoir formation level.
1 - Surface values will be specified. The wellbore model will calculate changes from the surface to the top of the completion zone.

IFREE Control parameter for the free-water surface (Col. 16-20).

0 - Inactive free-water surface mode (confined groundwater flow).
1 - Active free-water surface mode.

REFERENCE: The free-water surface option is described by Reeves et al. [1986a], Section 5.6.

NPLP Control parameter for plotting pressures in the wells (Col. 21-25).

1 - Bottom-hole and, if wellbore calculations are performed (ISURF), surface pressures are plotted. For an observation well, (zero well injection or production rate) the bottom-hole pressure is the grid-block pressure.
0 - No pressure plots are desired.
-1 - Pressure plots are desired for a previous run. Skip READ M-3 through R2-15 and proceed to READ P-2.

NPLT Control parameter for plotting temperatures in the well (Col. 26-30).

1 - For an observation well the grid-block temperature is plotted. For an injection well the bottom-hole temperature is plotted if wellbore calculations are performed. For a production well the bottom-hole temperature is always plotted. In addition, the surface temperature is plotted if the wellbore calculations are performed.
0 - No temperature plots are desired.
-1 - Temperature plots are desired for a previous run. Skip READ M-3 through READ R2-15 and proceed to READ P-2.

Table 2-1. Global Solution Options for the Primary Equations.*

NCALL	Pressure, P	Temperature, T	Brine, $\hat{C}$
0	T	T	T
-2	T	T	
1	T		
2	T		T
3			
4	S		
5	S		S

*"T" denotes a transient solution option.
"S" denotes a steady-state solution option.

Nuclide transport is controlled by whether nuclides are defined and present (NCP$\geq$1, Record M-3). Nuclide transport is always a transient solution. For steady-state solutions (NCALL = 4 or 5), the first recurrent data set (R2 records) controls the steady-state, after which the value of NCALL is automatically set to 3. Transient P, T or $\hat{C}$ may be simulated from a steady-state solution by setting NCALL $\neq$ 3 on R2-11.5 as flagged from ICLL=1 on R2-1.

NPLC Control parameter for plotting concentration in the well (Col. 31-35).
- 1 - The concentration in the well is plotted for both observation and production wells.
- 0 - No concentration plots are desired.
- -1 - Concentration plots are desired for a previous run. Skip READ M-3 through R2-15 and proceed to READ P-2.

IUNIT Unit specification control (Col. 36-40).
- 0 - English Engineering System (lb, ft, d).
- 1 - SI System (kg, m, s).

LBIO Nuclide monitor block control (Col. 41-45).
- 0 - No action.
- 1 - Nuclide concentrations are written on UNIT 9 (see Table 10.1) at each time step. (See Section 7.)

LMAPIT Control parameter for map matrix output as written to UNIT 13 (see Table 10.1) an controlled via R2-14 to 15 (See Section 10.5) (Col. 46-50).

LMAPIT	Pressure	File
00	No Map	
01	Pressure at Datum	ASCII
11	Environmental head	ASCII
21	Fresh water head	ASCII
02	Pressure at Datum	Binary
12	Environmental head	Binary
22	Fresh water head	Binary

LMBAL Control parameter for mass balance output to UNIT 17 (see Table 10.1) (Col. 51-55).
- 0 - No action.
- 1 - Write mass balance summary at each time step.

LAIF Control parameter for aquifer influence function output to UNIT 18 (see Table 10.1) (Col. 56-60).
- 0 - No action
- 1 - Write values of flux at each time step.

L2SORP Print frequency for L2SOR matrix inversion.
- 0 - Forced to 5 sweeps.
- >1 - Number of sweeps between printing.

Skip to READ P-1 if NPLP, NPLT or NPLC is negative.
Skip to READ R2-1 if this is a restart run, i.e., if RSTRT > 0. Skip to READ M-6 if RSTRT < 0.

READ M-3 (LIST 1: 14I5; LIST 2: 4I5) Central Memory Allocation and Program Control

LIST 1: NX, NY, NZ, HTG, NCP, NRT, KOUT, PRT, NSMAX, NABLMX, NRCHMX, METHOD, NTIME, KHEAT

NX Number of grid cells in the x direction (NX ≥ 2) (Col. 1-5). This is also the number of radial increments.

NY Number of grid cells in the y direction (NY ≥ 1) (Col. 6-10). If HTG=3 for radial geometry, NY=1.

NZ Number of grid cells in the z direction (NZ ≥ 1) (Col. 11-15).

HTG Control parameter for input of reservoir description data (Col. 16-20).
- 1 - Homogeneous reservoir, Cartesian geometry.
- 2 - Heterogeneous reservoir, aquifer data entered on regional basis, Cartesian geometry.
- 3 - Cylindrical geometry. The reservoir may be heterogeneous in the vertical direction.

NCP Number of radioactive/trace components in the system (Default = 0) (Col. 21-25).

Freundlich coefficients, dispersivities, thermal conductivities and salt-dissolution coefficients are all functions of the global rock type.
Rock types of all blocks are initialized to IRT = 1. Changes of rock type to other values are entered in READ R1A-1.

NRT Number of global rock types (Default = 1) (Col. 26-30).

Enter negative values for KOUT if windowing (M-4) option is to be used.

KOUT Output control (Col. 31-35).
- 0 - All initialization output is activated. This is recommended for building data sets.
- ±1 - All initialization output except initial arrays (concentrations, pressures, etc.) is activated. This is recommended for production and sensitivity runs.
- ±3 - No initialization output is activated. A value of KOUT = 3 can be used to omit printing of most initialization data.

PRT Output array orientation control (Col. 36-40).

-1 - Print output arrays as areal layers (x-y). Block numbers in the x direction increase from left to right and in the y direction decrease down the computer page.

+1 - Print output arrays as above except that y-direction block numbers increase down the computer page.

2 - Print output arrays as vertical x-z sections.

NSMAX Maximum number of radioactive/trace component sources (Ref. R2-10) (Col. 41-45).

NABLMX Maximum number of aquifer influence-function blocks. This data is used for dimensioning the influence-function arrays (Ref. R1-27, 28) (Col. 46-50).

NRCHMX Maximum number of surface recharge blocks (Ref. R2-2.5) (Col. 51-55).

The following parameter, METHOD, is a flag which determines whether D4 ordering is to be performed in preparation for the direct-solution algorithm. Parameter METHOD may be changed in READ R2-2. Thus, for example, direct solution may be specified here, and L2S0R solution may be specified in READ R2-2. However, the converse is not true since, in that case, the coefficient matrix would not be properly ordered.

METHOD Matrix solution technique (Col. 56-60).

1 - Reduced-band-width direct solution with backward finite-difference approximation in time (BIT).

2 - Two-line successive-overrelaxation (L2SOR) solution with a backward finite-difference approximation in time (BIT).

-1 - Reduced band-width direct solution with a centered finite-difference approximation in time (CIT).

-2 - Two-line successive-overrelaxation solution (L2SOR) with a centered finite-difference approximation in time (CIT).

The following three parameters, NTIME, KHEAT and NREPB, are leach-model parameters (see R1A records).

NTIME Number of times for which concentrations of unleashed radioactive components or heat-loading densities within the repository area are to be input (Col. 61-65).

0 - Repository submodels are not used.

1 - Only the waste-leaching submodel is invoked. Initial conditions are to be specified for the unleashed concentrations and decay/production processes for such concentrations are to be calculated internally.

>1 - Both waste-leaching and repository-heating may be considered, depending on the value KHEAT below, and interpolation tables of unleashed concentrations versus time are to be used. Power-law interpolation is used in each case.

KHEAT Control parameter for heat loading in the repository blocks (Col. 66-70).
- 0 - No heat source.
- 1 - Heat source activated.

LIST 2: NREPB, KSLVD, NRTD, KOUTD

NREPB Number of repository blocks (Col. 1-5).

The following three parameters, KSLVD, NRTD and KOUTD, pertain to the local subsystems, i.e., matrix. See R0D and R1D records.

KSLVD Local control parameter for solution of both primary and radionuclide equations for the matrix. See Table 2-2 (Col 6-10).

NRTD Number of local, i.e., matrix rock types (Col. 11-15).

KOUTD Output control for the local subsystems (Col. 16-20).
- 0 - All initialization output is activated.
- 1 - No initialization output is activated.

Enter the following data if KOUT (M-3) is less than zero.

READ M-4 (6I5) Windowing of initialization output data

LIST: NI1, NI2, NJ1, NJ2, NK1, NK2

NI1,NI2 Lower and upper limits, inclusive of the window in the x-direction.

NJ1,NJ2 Lower and upper limits, inclusive of the window in the y-direction.

NK1,NK2 Lower and upper limits, inclusive of the window in the z-direction.

2.2 THE R0 RECORDS

The R0 records are read by subroutine READ0. They input information pertaining to the radioactive components. This information defines each isotope in terms of its parents, branching ratios for each parent, isotopic mass, half-life and distribution coefficient for each rock type.

Data group R0 should be entered only if RSTRT = 0 and NCP > 0. Otherwise skip READ R0-1 and READ R0-2.

Table 2-2. Local Solution Options for Both Primary and Radionuclide Equations.[1]

KSLVD	Primary Equations	Radionuclide Equations
0		
1	T	
2		T
3	T	T

[1]Only the transient solution option T is available for the local subsystems. For steady-state fracture flow and transport there is no need to simulate the local (matrix) subsystem.

READ R0-1 (LIST 1: I3,2A4,4X,3I5,E10.0; LIST 2: 4(I5,5X, E10.0)). Radioactive Component Information.

Enter NCP (READ M-3, number of components) sets of R0-1 data.

LIST 1: MASS (I), (DI(J,I),J=1,2), I, NP(I), LADJ(I), DEC(I)

MASS Mass number of the isotope (i.e., 244) (Col. 1-3). Be careful in defining the mass number as this is used in the mass decay equations. If in doubt, set to 1 for all components.

DI Identification for radioactive component I (i.e., URANIUM) (Col. 4-11).

I Component number (Col. 15-20) starting with the parent as number 1.

NP Number of parent components for I (NP $\leq$ NCP-1) (Col. 21-25).

Lambda adjustment is used for relatively short half-lived radionuclides to permit the use of time steps $\Delta t > \tau$, the half-life. See Reeves et al. [1986a], Section 7.2.2, for the meaning and limitations of this procedure.

LADJ Lambda (rate-constant) adjustment index (Col. 26-30).
- 1 - Modify rate constant of the isotope I.
- 0 - Do not modify the rate constant.

DEC Half-life of component I in years. For stable components with infinite half-life, enter zero (Col. 31-40).

Skip the following list if NP(I) = 0 (LIST 1).

LIST 2: KP(J), AP(J), J=1,NP

KP Parent component number (Col. 1-5).

AP Fraction of parent component KP that decays to the component I (LIST 1) (Col. 11-20).

READ R0-2 (LIST 1: (7E10.0); LIST 2: (7E10.0)) Rock-Dependent Freundlich Coefficients.

Read one LIST-1 set for each rock type, follow by the LIST-2 records.

LIST 1: DIS(I), I=1,NCP

DIS Adsorption coefficient κ for a Freundlich isotherm, $(ft^3/lb)^{\eta}$ or $(m^3/kg)^{\eta}$. Enter one value for each component for a total of NCP (READ M-3) values for each rock type. Start new rock-type values on a separate record.

Read one LIST-2 set for each rock type, after completing the LIST-1 records.

LIST 2: DIS(I), I = NCP+1, 2*NCP

DIS Adsorption exponent for a Freundlich isotherm, dimensionless. Enter one value for each component for a total of NCP values for each rock type. Start new rock-type values on a separate record. The default value is $\eta = 1$.

2.3 THE R0D RECORDS

The R0D records are read by subroutine READ0D. They provide both control and storage-allocation data for the local system.

If KSLVD = 0, then skip all R0D input.

READ R0D-1 (I5) Control of Convection/Dispersion

LIST: KCNVD

KCNVD Convection/dispersion control for the local subsystems, i.e., matrix.
- 0 - No convection or dispersion for either primary equations or radionuclide equations. Also, for the latter, a constant fluid density and a constant porosity are assumed. For nuclides only molecular diffusion and decay processes are solved.
- 1 - Convection and dispersion effects are included, and a variable fluid density and a variable porosity are assumed throughout.

READ R0D-2 (14I5) Number of Local Grid Blocks

LIST: NSD(IR), IR=1,NRTD

NSD Number of local, i.e., matrix grid blocks as a function of local rock type.

READ R0D-3 (8I5) Matrix Rock Types

Follow the last record of this data group with a blank record.

LIST: I1A, I1B, J1A, J1B, K1A, K1B, IR, IFD

I1A,I1B Lower and upper limits, inclusive, on the I index of the region having rock type IR.

J1A,J1B (Similar definition for J index).

K1A,K1B (Similar definition for K index).

IR Local matrix rock type.

IFD Position and orientation control for the local subsystems.
- 0 - Local subsystems positioned interior to global block (dual-porosity option).
- >0 - Local subsystems positioned exterior to the global block on both sides (discrete fracture and extended boundary-condition options).
- <0 - Local subsystems positioned exterior to the global block but on only one side (extended boundary-condition option).
- 1,-1 - Local subsystems oriented parallel to the x axis.
- 2,-2 - Parallel to the y axis.
- 3,-3 - Parallel to the z axis.

2.4 THE M RECORDS, GROUP 2

Two additional restart parameters are input in this, the second, group of M records.

If RSTRT = 0, (READ M-2), skip to READ R1-1.
The mapping data consist of sets of input records, each of which contains READ's M-6, M-7, R2-14 - R2-15. Enter as many of these sets as desired, following the last set with a blank record.

READ M-6 (I5) Time-Step Number

LIST: IMPT

IMPT The time-step number at which the maps are desired. A corresponding restart record must exist on UNIT 4, i.e., the control RSTWR = 1 (READ R2-13) must have been entered for a previous calculational run.

READ M-7 (2I5) Mapping Control

LIST: MAP, LMAPIT

MAP The four-digit mapping-variable selector as defined in READ R2-13.

LMAPIT The control parameter for output to Unit 13 as previously defined on Read M-2.
- 0 - No action.

See definition in M-3.

Skip to Read R2-14.

3 THE R1 RECORDS

The information supplied by the R1 records consists of time-independent data, all of which is read within subroutine READ1. This data specifies some of the physical properties of the global system including its geometry, boundary conditions, and initial conditions on pressure and temperature. The I data of Chapter 5 then refines the pressure initialization for the natural-flow field and provides initialization on the concentrations. The R1 records also contain a partial statement of the wellbore source/sink parameters and a definition of the discretization of the global system. The general procedure for input of the spatially dependent parameters is to specify large homogeneous regions followed by modification records to insert inhomogeneities.

3.1 PHYSICAL PROPERTIES

READ R1-1 (5E10.0) Physical Constants

LIST: CW, CR, CTW, CPW, CPR

CW Compressibility of the reservoir fluid, psi^{-1} (Pa^{-1}).

CR Compressibility of the pore structure or rock compressibility, psi^{-1} (Pa^{-1}). [For multiple entries, see R1-1.5 or R1-2.5]

CTW Coefficient of thermal expansion of the reservoir fluid, EF^{-1} (EC^{-1}).

CPW Fluid heat capacity, Btu/lb-EF (J/kg-EC).

CPR Rock heat capacity per unit volume of solid, Btu/ft^3-EF (J/m^3-EC). [For multiple entries, see R1-21 or R1-23]

If CR < 0, (READ R1-1), READ R1-1.5, otherwise, skip to R1-2.

READ R1-1.5 (List 1:(I5); List 2:(2E10.0)) Time dependent rock compressibility

LIST 1: NPTDST

NPDST Number of entries in time-compressibility table.

LIST 2: TIMTDST(I), CRTDST(I), I=1, NPTDST

TIMTDST Time, d(s).

CRTDST Rock compressibility of pore structure, psi^{-1} (Pa^{-1}).

READ R1-2 (7E10.0) Physical Constants

LIST: UKTX, UKTY, UKTZ, CONV, ALPHL, ALPHT, DMEFF

UKTX Thermal conductivity of the fluid-saturated porous medium in the x direction, Btu/ft-d-EF (J/m-s-EC) (see CONV). [For multiple entries, see R1-2.5]

UKTY Thermal conductivity of the porous medium in the y direction.

UKTZ Thermal conductivity of the porous medium in the z direction.

CONV Conversion factor for the thermal conductivities. The entered values of the thermal conductivities are multiplied by CONV to obtain units of Btu/ft-d-EF (J/m-s-EC). If entered as zero, thermal conductivities should be read in Btu/ft-d-EF (J/m-s-EC).

ALPHL Longitudinal dispersivity factor, ft (m). [For multiple entries, see R1-2.5]

ALPHT Transverse dispersivity factor, ft (m). [For multiple entries, see R1-2.5]

DMEFF Molecular diffusivity in the porous medium, includes porosity and tortuosity effects (porosity * fluid molecular diffusivity * tortuosity), ft^2/d (m^2/s). [For multiple entries, see R1-2.5]

Skip the following read if NRT = 1, and proceed to READ R1-3. Otherwise enter sequentially one group (List 1 and List 2) for each rock type. To specify block locations for different rock types, see Record R1A-1.

READ R1-2.5 (LIST 1: 4E10.0; LIST 2: 4E10.0) Rock-Dependent Properties

LIST 1: UTCX(I), UTCY(I), UTCZ(I), CONV

UTCX Thermal conductivity of the fluid-saturated media in the x direction for rock type I, Btu/ft-d-EF (J/m-s-EC).

UTCY Thermal conductivity in the y direction.

UTCZ Thermal conductivity in the z direction.

CONV Conversion factor for thermal conductivities to obtain units of Btu/ft-d-EF (J/m-s-EC).

LIST 2: ALPHAL(I), ALPHAT(I), DMEFFR(I), CRR(I)

ALPHAL Longitudinal dispersivity factor for rock-type I, ft (m).

ALPHAT Transverse dispersivity factor, ft (m).

DMEFFR Molecular diffusion coefficient for rock-type I, includes porosity and tortuosity effects, ft^2/d (m^2/s).

CRR Rock compressibility for rock-type I, psi^{-1} (Pa^{-1}).

The fluid densities are entered here for brine concentrations C = 0 (natural aquifer fluid) and concentration C = 1 (contaminated fluid). Both densities must be entered at the same reference temperature and pressure.

READ R1-3 (5E10.0) Reference Densities.

Reference: Reeves et al. [1986a], Section 3.1.

LIST: BROCK, PBWR, TBWR, BWRN, BWRI

BROCK Rock density (solid particle), lb/ft^3 (kg/m^3).

PBWR Reference pressure at which the densities are to be entered, psi (Pa).

TBWR Reference temperature at which the densities are to be entered, EF (EC).

BWRN Density of the natural reservoir fluid (C = 0) at PBWR and TBWR, (lb/ft^3).

BWRI Density of the contaminated fluid (C = 1) at PBWR and TBWR, lb/ft^3 (kg/m^3).

Note: BWRN and BWRI define the end member of fluid density. This is related to specific gravity as discussed in Section 12.4.

3.2 WELLBORE DATA

If ISURF = 0, omit READ R1-4 and READ R1-5 and proceed to READ R1-6.

Reference: Reeves et al. [1986a], Section 4.2

READ R1-4 (I5) Output Control

LIST: NOUT

NOUT Output control parameter for the wellbore calculations.
- No output is activated.

1 - An iteration summary, including the number of outer iterations, the flow rate and the bottom-hole pressure, is printed for each well.
2 - The well pressure and temperature, at the surface for an injection well and at the bottom-hole for a production well, and the flow rate are printed every time the wellbore subroutine, WELLB, is called.
3 - The pressure and temperature in the well are printed for each vertical increment (see DELPW in READ R1-5).

READ R1-5 (3E10.0) Wellbore Constants

LIST: PBASE, DELPW, TDIS

PBASE Atmospheric or reference pressure at the well-head, psi (Pa). This is used to convert absolute pressure to gauge pressure.

DELPW Incremental value of pressure over which wellbore calculations are to be performed, psi (Pa).

The pressure and temperature calculations in the wellbore proceed in increments. The length increments corresponding to DELPW are calculated, and the temperature change over each increment is simulated.

TDIS Thermal diffusivity of the rock surrounding the wellbore, ft^2/d (m^2/s).

3.3 VISCOSITY AND TEMPERATURE INITIALIZATION

The input data described in this section defines both the viscosity function and the initial-temperature definition. The latter is self evident since it consists of a simple interpolation table. The former, however, requires some explanation. Section 3.2 of Reeves et al. [1986a] provides a detailed description of the data necessary to generate the viscosity function. Thus, only a summary is given here.

Figure 3-1 presents a useful visual aid. The minimum data necessary to specify the function shown consists of the two points VISRR = m (C =0,T=TRR) and VISIR = m (C=1,T=TIR) (READ R1-7). The remainder of the function is then generated from the generalized curve of Lewis and Squires (for the dependence on temperature) and from interpolation (for the dependence on brine concentration). As discussed in the above reference, the generalized curves may introduce as much as an 18 percent error in the temperature dependence of the viscosity function. It is therefore desirable to supply additional data whenever possible. Temperature data for C = 0 may be included by using arrays TR(I) and VISR(I) (READ

R1-9) with control parameter NTVR. Temperature data for C = 1 may be included by using arrays TI(I) and VISI(I) (READ R1-10) with control parameter NTVI. Concentration data for T = TRR may be included by using arrays SC(I) and VCC(I) (READ R1-8) with control parameter NCV. In order to define a constant value of viscosity for C = 0 (or C=1), it is necessary to specify the same value for two different temperatures. For example, a constant function m (C = 0,T) = 1 cp is determined by specifying NTVR = 1 and VISRR = VISR = 1.0 with TRR … TR.

The numbers called for immediately below (except for NDT) refer to the viscosity values to be entered in addition to the reference viscosities.

READ R1-6 (4I5) Control Parameters

LIST: NCV, NTVR, NTVI, NDT

NCV Number of entries in the concentration-viscosity table. This table is for viscosities other than the reference values entered for C = 0 and C = 1. This index refers to data points along curve c in Figure 3-1, exclusive of the end points. If only the two end-point, pure-fluid viscosities are available, enter zero and read in the viscosities of the pure fluids as reference viscosities.

NTVR Number of entries in the temperature-viscosity table for C = 0. This index refers to data points on curve r of Figure 3-1, exclusive of the end points.

NTVI Number of entries in the temperature-viscosity table for C = 1. This index refers to data points on curve i of Figure 3-1, exclusive of the end points.

NDT Number of entries in the depth-versus-temperature table.

READ R1-7 (4E10.0) Reference Viscosity Values

LIST: TRR, VISRR, TIR, VISIR

TRR Reference temperature for the resident-fluid viscosity, EF (EC).

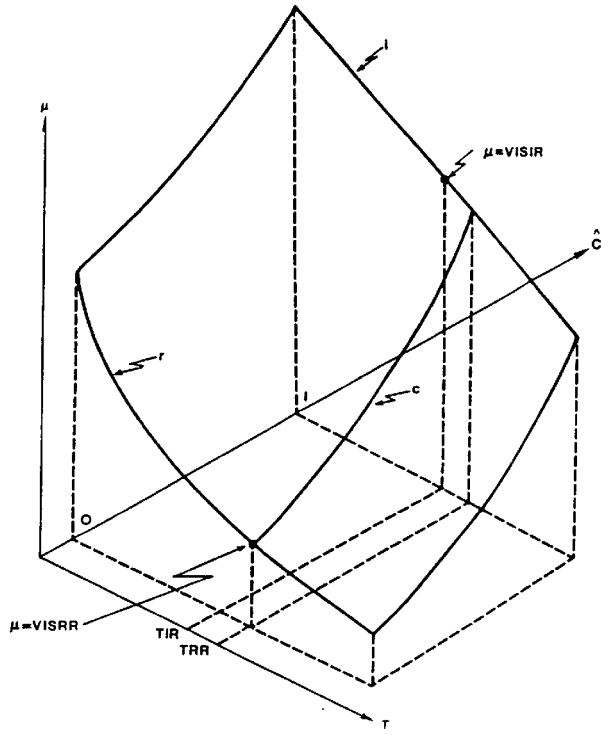
VISRR Viscosity of the resident fluid at the reference temperature, TRR, cp (Pa-s).

TIR Reference temperature for the contaminated-fluid viscosity, EF (EC).

VISIR Viscosity of the contaminated fluid at TIR, cp (Pa-s).

If NCV = 0, omit READ R1-8.

Figure 3-1. Fluid Viscosity as a Function of Temperature and Pressure.



READ R1-8 (7E10.0) Concentration-Dependent Viscosity Values

LIST: SC(I), VCC(I), I=1,NCV

SC Concentration, mass fraction.

VCC Viscosity of fluid mixture at concentration SC and temperature TRR, cp (Pa-s).

If NTVR = 0, skip READ R1-9 and proceed to READ R1-10.

READ R1-9 (7E10.0) Temperature-Dependent Viscosity Values

LIST: TR(I), VISR(I), I=1,NTVR

TR Temperature, EF (EC).

VISR Viscosity of the resident fluid at the temperature TR, cp (Pa-s). Do not re-enter the reference viscosity at TRR (READ R1-7).

If NTVI = 0, skip READ R1-10 and proceed to READ R1-11.

READ R1-10 (7E10.0) Temperature-Dependent Viscosity Values

LIST: TI(I), VISI(I), I=1,NTVI

TI Temperature, EF (EC).

VISI Viscosity of the contaminated fluid at the temperature TI, cp (Pa-s). Do not re-enter the reference viscosity at TIR (READ R1-7).

Initial temperatures in the aquifer and the over/underburden blocks are to be entered here. The initial temperature is assumed to be a function of depth only.

Reference: Reeves et al. [1986a], Section 5.1.2.

READ R1-11 (2E10.0) Initial Temperatures

LIST: ZT(I), TD(I), I=1, NDT

ZT Depth relative to reference plane, ft (m).

TD Temperature, EF (EC).

3.4 OVER/UNDERBURDEN PARAMETERS

As described in Reeves et al. [1986a], Section 5.4, heat transport between the reservoir and the overburden and/or underburden is accounted for in the SWIFT code by means of a fully coupled, completely implicit heat-transport calculation within these neighboring regions. Boundary temperatures for the top of the overburden and the bottom of the underburden are obtained from the temperature-versus-depth table (READ R1-11). Initial conditions are also obtained from this table. Except for the assumptions of no lateral transport and no fluid flow within these external zones, the calculations there are completely general. The data defined in READ R1-12 through READ R1-15 gives the information necessary to discretize the over/underburden region and to define the heat-transport parameters therein.

Reference: Reeves et al. [1986a], Section 5.4.

If NZ = 1, the underburden heat loss is assumed to be equal to the overburden heat loss, and only the parameters of the overburden are utilized.

READ R1-12 (2I5) Number of Over/Underburden Grid Blocks

LIST: NZOB, NZUB

NZOB Number of overburden blocks. If NZOB # 2, overburden heat-loss calculations are not performed.

NZUB Number of underburden blocks. If NZUB # 2, the underburden heat-loss calculations are not performed.

Skip to R1-16 if both NZOB = 0 and NZUB = 0.

READ R1-13 (4E10.0) Physical Parameters

LIST: KOB, CPOB, KUB, CPUB

KOB, KUB Vertical thermal conductivities of the overburden and the underburden blocks, respectively, Btu/ft-d-EF (J/m-s-EC).

CPOB, CPUB Heat capacities of the overburden and underburden blocks, respectively, Btu/ft^3-EF (J/m^3-EC).

Skip the following READ if NZOB = 0.

READ R1-14 (7E10.0) Discretization of the Overburden

LIST: DZOB(K), K=1,NZOB

DZOB Thickness of each overburden block, ft (m). The first overburden block is at the upper edge of the reservoir. The overburden block numbers increase moving away from the reservoir.

Skip the following READ if NZUB = 0.

READ R1-15 (7E10.0) Discretization of the Underburden

LIST: DZUB(K), K=1,NZUB

DZUB Thickness of each underburden block, ft (m). The block numbers increase moving away from the reservoir.

3.5 REFERENCE DATA AND PRESSURE INITIALIZATION

Reference: Reeves et al. [1986a], Section 5.1.1.

READ R1-16 (4E10.0) Reference Data

LIST: TO, PINIT, HINIT, HDATUM

TO Reference temperature for both hydraulic conductivities and densities, EF (EC).

PINIT Initial pressure, p_I, at the depth HINIT, psi (Pa). Also used as the reference pressure PO = PINIT. See Figure 3-2.

Permeabilities are determined assuming that the input conductivities are referenced to temperature TO. Densities are related internally to this temperature and to the pressure PINIT in that only changes from the density at TO and PO = PINIT (and C = 0) are calculated.

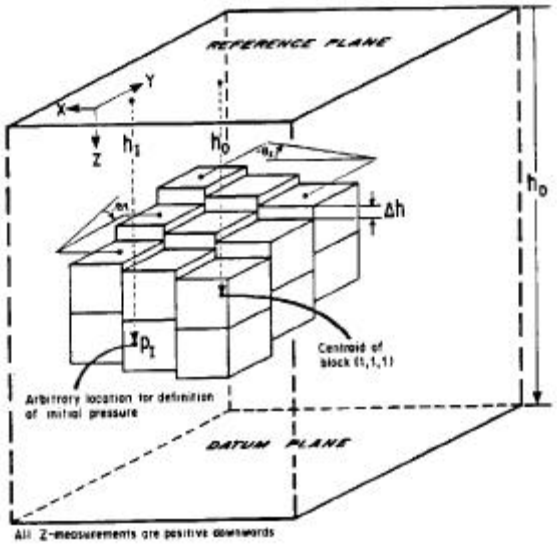
HINIT An arbitrary depth, h_I, for setting up initial conditions measured relative to the reference plane, ft (m). HINIT can be any depth within the reservoir. HINIT is used only to set up initial pressures in the reservoir. See Figure 3-2.

Quantities HINIT, HDATUM, DEPTH (READ R1-20) and UH (READ R1- 21) are all measured from the reference plane shown in Figure 3-2.

HDATUM Datum depth, h_D, measured relative to the reference plane, ft (m). See Figure 3-2.

Quantity HDATUM is used only for the printing of the dynamic pressures or pressure at datum ($p-rgh/g_c$). The pressure at block centroid depth, h, relative to the reference plane is converted to the datum plane using the reference density.

Figure 3-2. Specification of the Geometry and the Initial Pressure in a Cartesian System.



3.6 DISCRETIZATION FOR A CARTESIAN GEOMETRY

If HTG = 3 (radial geometry), skip to READ R1-22.

READ R1-17 (List Directed[1]) Grid-Block Definition

LIST: DELX(I), I=1,NX

DELX Length of each row of blocks in the x direction, ft (m).

READ R1-18 (List Directed[1]) Grid-Block Definition

LIST: DELY(J), J=1,NY

DELY Length of each row of blocks in the y direction, ft (m).

READ R1-19 (List Directed)[1] Grid-Block Definition.

LIST: DELZ(K), K=1,NZ

DELZ Thickness of each vertical layer, starting with the top-most, ft (m).

Note: To flag the stair-case grid option below, enter a negative value for DELZ(1)

READ R1-19.1 (List Directed[1]) Stair-cased Grid Definition

LIST: HTOP, (DELZ(K),K=1,NZ)

HTOP Distance below datum to top of upper-most block in column (i,j) where i refers to x-direction and j refers to y-direction, ft (m).

DELZ(K) Block thickness, starting with top-most block, ft (m).

Note: The list is read for all columns in the system. The code starts with the (1,1) columns, increments first on j (y-direction) and then i (x-direction). A total of NX * NY list are required to complete the grid definition.

---

[1]List Directed Read (also known as Free Format): Input data consists of a string of values each separated by one or more blanks or a comma and terminated by a slash. To repeat a value, an integer constant is followed by an asterisk and the constant to be repeated. Example:

2*104.8, 3*96.3 is equivalent to
104.8 104.8 96.3 96.3 96.3

Record type identifiers in the margins are illegal for records using a list directed format.

3.7 RESERVOIR DATA FOR A CARTESIAN GEOMETRY

The following data are read only if HTG = 1 or 2, and by themselves describe a homogeneous reservoir. Heterogeneity may be introduced by using READ R1-21 and/or regional modifications in READ R1-26, in addition to READ R1-20.

READ R1-20 (7E10.0) Homogeneous Reservoir Information

LIST: KX, KY, KZ, PHI, SINX, SINY, DEPTH

KX Hydraulic conductivity in x direction, ft/d (m/s).

KY Hydraulic conductivity in y direction, ft/d (m/s).

KZ Hydraulic conductivity in z direction, ft/d (m/s).

PHI Porosity (fraction).

SINX Sine of the reservoir dip angle along the x-axis (positive down). See Figure 3-2.

SINY Sine of the reservoir dip angle along the y-axis (positive down). See Figure 3-2.

DEPTH Depth, h_O, to the center of grid block (1,1,1) measured from the reference plane (positive downward). See Figure 3-2.

The following data are read only if HTG = 2. Enter as many sets of data as required. Follow the data with a blank record.

READ R1-21 (List 1: 6I5; List 2: 7E10.0) Heterogeneous Reservoir Information

LIST 1: I1, I2, J1, J2, K1, K2

I1, I2 Lower and upper limits inclusive, on the I index of the region to be described.*

J1, J2 (Similar definition for the J index).

K1, K2 (Similar definition for the K index).

LIST 2: KX, KY, KZ, PHI, UH, UTH, UCPR

KX x-direction hydraulic conductivity, ft/d (m/s).

KY y-direction hydraulic conductivity, ft/d (m/s).

KZ z-direction hydraulic conductivity, ft/d (m/s).

PHI Porosity, fraction.

UH Depth in ft (m) measured **positive downward** from reference plane to center of the cell. See Figure 3-2. If entered as zero, the depth is unaltered from the value calculated for a homogeneous aquifer.

UTH Grid-block thickness in the vertical direction, ft (m). If the layer thickness is equal to DELZ(K) (READ R1-19), UTH may be entered as zero.

UCPR Heat capacity of the rock, Btu/ft^3-EF (J/m^3-EC). If the rock heat capacity is equal to CPR (READ R1-1), UCPR may be entered as zero.

*A negative value for I1 indicates that a separate binary file will be used instead. The program will pause and request the file name. See Section 10.7 for further details.

3.8 RESERVOIR DATA FOR A CYLINDRICAL GEOMETRY

The following three records are read for a radial geometry with a well located at the center of the system. The user has the option of generating the grid block centers using an equal Dlog(r) basis, (i.e., r_i/r_{i-1} is constant) or entering the radius of each grid-block center.

Skip to READ R1-26 if HTG $\neq$ 3.

READ R1-22 (4E10.0) Geometrical Data.

Reference: Reeves et al. [1986a], Section 7.1.2.

LIST: RWW, R1, RE, DEPTH

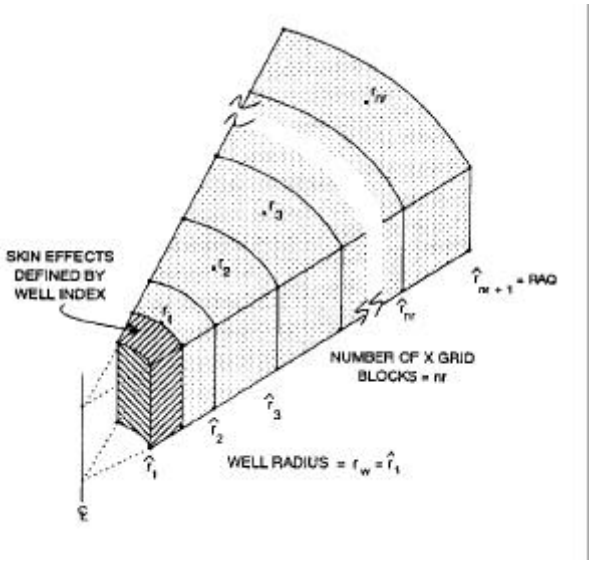
RWW Well radius, ft (m). See Figure 3-3.

R1 For mesh generation on an equal Dlog(r) basis, R1 > 0 represents the center of the first grid block. See Figure 3-3. For direct specification, R1 = 0 should be used.

RE External radius of the reservoir, ft (m). See Figure 3-3.

DEPTH Depth, h_O, from the reference plane (positive downward) to the center of the first layer of blocks, ft (m). See Figure 3-2.

Figure 3-3. Schematic of the Radial Mesh Including Grid-Block Centers, r_i, and Grid-Block Boundaries, $\hat{r}_i$.



READ R1-23 (5E10.0) Reservoir Parameters

LIST: DELZ(K), KYY(K), KZZ(K), POROS(K), CPR1(K), K=1,NZ

One record should be entered for each vertical layer.

DELZ Layer thickness in the vertical direction, ft (m).

KYY Horizontal hydraulic conductivity, ft/d (m/s).

KZZ Vertical hydraulic conductivity, ft/d (m/s).

POROS Porosity, fraction.

CPR1 Rock heat capacity, Btu/ft^3-EF (J/m^3-EC). If the rock heat capacity in the layer is equal to CPR (READ R1-1), CPR1 may be entered as zero.

Skip to READ R1-26 if R1 $\neq$ 0.

READ R1-24 (7E10.0) Radial Grid-Block Centers

LIST: RR(I), I=1,NX

RR Radial grid-block centers, ft (m). See Figure 3-3.

3.9 RESERVOIR DESCRIPTION MODIFICATIONS

Read as many sets of the following data as necessary to describe all the reservoir description modifications which are desired. Follow the last set with a blank record, which the program recognizes as the end of this data set. Even if no regional modifications are desired, the blank record must be included.

READ R1-26 (LIST 1: 6I5; LIST 2: 7E10.0; LIST 3: 3E10.0)

LIST 1: I1, I2, J1, J2, K1, K2

I1, I2 Lower and upper limits, inclusive, on the I index of the region to be modified.

J1, J2 (Similar definition for J index).

K1, K2 (Similar definition for K index).

The x transmissibility indexed as (I,J,K) refers to the transmissibility at the boundary separating grid blocks (I-1,J,K) and (I,J,K). Similarly the y transmissibility indexed as (I,J,K) refers to the transmissibility at the boundary separating grid blocks (I,J-1,K) and (I,J,K).

LIST 2: FTX, FTY, FTZ, FPV, FPHI, HADD, THADD

FTX If positive or zero, this is the factor by which the x-direction transmissibilities within the defined region are to be multiplied. If negative, the absolute value of FTX will be used for the x-direction transmissibilities within the region to be modified.

FTY This has the same function of FTX, but applies to the y-direction transmissibilities.

FTZ This has the same function of FTX, but applies to the vertical transmissibilities.

FPV This has the same function of FTX, but applies to pore volumes. Set FPV to zero to make the block inactive. This will remove the block from the matrix solution and avoid printing and mapping of output with efficient storage and no loss of accuracy. Wells cannot be placed in zero pore volume blocks.

FPHI If positive, this is the factor by which the values of porosity used in the heat storage calculation within the defined region are to be multiplied. If negative, the absolute value of FPHI will be used. A zero or unit value has no effect.

HADD This is an increment that will be added to the depths within the defined region, ft (m). A positive value moves the designated cells deeper, and a negative value brings them closer to the surface. See Figure 3-2.

THADD This is an increment that will be added to the thickness values within the defined region, ft (m). A positive value makes the cell thicker, and a negative value makes it thinner. Pore volumes are implicitly modified with thickness changes.

LIST 3: FTUX, FTUY, FTUZ

FTUX If positive, this is the factor by which the x-direction Darcy velocities within the region defined are to be multiplied. The modified velocities are used in the heat and solute dispersion coefficients. A zero or unit value has no effect.

FTUY This has the same function of FTUX, but applies to the y-direction Darcy velocities.

FTUZ This has the same function of FTUX, but applies to the z-direction Darcy velocities.

In regions in which more than one modification has been made to a parameter, the order of the modifications has no effect, and the final net adjustment is simply the algebraic sum of all the additive factors or the product of all the multiplicative factors that apply to the region. The program will accept a zero modifier as a valid parameter. Therefore, if no changes are desired to data that are affected by multi-plicative factors FTX, FTY, FTZ, or FPV, read the corresponding factors as 1.0, not zero. If no changes are desired for FPHI, FTUX, FTUY or FTUZ, read the factor as 1.0 or zero. Zero additive factors (HADD AND THADD) result in no changes to the depth and thickness values.

3.10 AQUIFER-INFLUENCE FUNCTIONS AND BOUNDARY CONDITIONS

Aquifer-influence functions specify the effects of an aquifer upon the reservoir via an analytic submodel of the aquifer. Conceptually reservoir and aquifer are related as shown by Figure 3-4. For the SWIFT model three different aquifer submodels are available. These submodels are implicitly coupled to the reservoir via the influence functions. In general, both pressure and flow vary as a function of time. The application of such functions means that the aquifer itself need not be modeled as a part of the grid system. Boundary conditions, however, are more simple. They derive from specified constants for pressure, temperature and concentration. Hence, they do not implicitly vary with the internal condition of the reservoir as do the aquifer-influence functions.

Reference: Reeves et al. [1986a], Sections 5.2 and 5.3.

If no aquifer-influence functions or boundary conditions are to be specified (no flow across aquifer boundaries), insert a blank record and proceed to READ R1D-1.

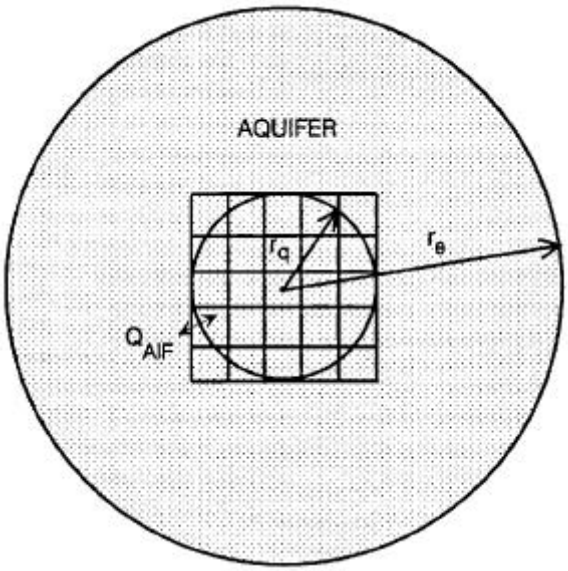
READ R1-27 (2I5) Control Parameters

LIST: IAQ, PRTAB

IAQ Control parameter for selecting the type of boundary control.

- 0 - No aquifer-influence or boundary-condition blocks are to be used. Skip to READ I-1.
- 1 - A pot-aquifer representation will be used. The aquifer is assumed to be at steady-state with a no-flow outer boundary. [Rarely used option]
- 2 - A steady-state aquifer representation will be used. The aquifer is assumed to be at steady-state with a constant pressure at the outer aquifer boundary. [Rarely used option]
- 3 - An unsteady-state aquifer representation will be implemented using the Carter-Tracy approximation.
- 4 - Constant pressure and brine-component boundary conditions will be used. Boundary conditions for heat transport may be either constant-temperature or radiative.

Figure 3-4. Geometrical Characterization of the Aquifer.



PRTAB Print control key for the aquifer-influx coefficient.
- 0 - No printing of aquifer-influence coefficients will be activated.
- 1 - The locations and values of the aquifer- influence coefficients will be printed.

3.10.1 STEADY-STATE AQUIFER-INFLUENCE FUNCTIONS AND BOUNDARY CONDITIONS

This data group consists of two records or any number of sets of two records, each set defining a rectangular region and the value of VAB to be assigned that region. Overlapping of regions is permissible. The order of the sets is immaterial except that any overlapping will result in the VAB of the last set read being assigned to the overlapping subregion.

If IAQ = 3 (READ R1-27), skip the following READ and proceed to READ R1-29.

Follow the last record of this data group by a blank record.

READ R1-28 (LIST 1: 7I5; LIST 2: 6E10.0) Region Specification

LIST 1: I1, I2, J1, J2, K1, K2, KAQ

I1, I2 Lower and upper limits, inclusive, on the I index of the aquifer-influx region.

J1, J2 (Similar definition for J index).

K1, K2 (Similar definition for K index).

KAQ Control variable for the heat-transport equation used only for IAQ = 4.
- -1 - Type 3 radiation condition only. In List 2, T1 is not used. T2 and T3 are used.
- 0 - Type 1 temperature condition only. In List 2, T1 is used. T2 and T3 are not used.
- 1 - Type 1 temperature condition and Type 3 radiation condition. In List 2, T1, T2 and T3 are all used.

LIST 2: VAB, P1, T1, C1, T2, T3

For IAQ = 1 or 2, the *Pot-Aquifer or Steady-State Options*,

VAB Aquifer influence coefficient for each block within the region defined by I1, I2, etc. The units of VAB are ft^3/psi (m^3/Pa) for a pot-aquifer representation and ft^3/psi-d (m^3/Pa-s) for a steady-state representation.

P1, T1, C1, T2, and T3 are not used.

For IAQ = 4, the *Boundary-Conditions*

VAB Face-type indicator used to assign transmissibility.
- 1.0 - Block is located on an I = 1 edge.
- 2.0 - Block is located on an I = NX edge.
- 3.0 - J = 1 edge.
- 4.0 - J = NY edge.
- 5.0 - K = 1 edge.
- 6.0 - K = NZ edge.

P1, T1, Constant values of pressure at block-centroid

C1 elevation in psi (Pa), temperature in EF (EC) and concentration (fraction) at the block boundary specified according to VAB and KAQ. See Figure 3-5.

T2 Temperature of surrounding media, EF (EC).

T3 Coefficient of surface-heat transfer, Btu/d-ft^2-EF (J/s-m^2-EC).

3.10.2 UNSTEADY-STATE AQUIFER-INFLUENCE FUNCTION

If IAQ … 3, omit the following data and proceed to READ R1-33. This section is used to enter data for the Carter-Tracy method of calculating aquifer-influence functions.

READ R1-29 (3I5) Control Parameters

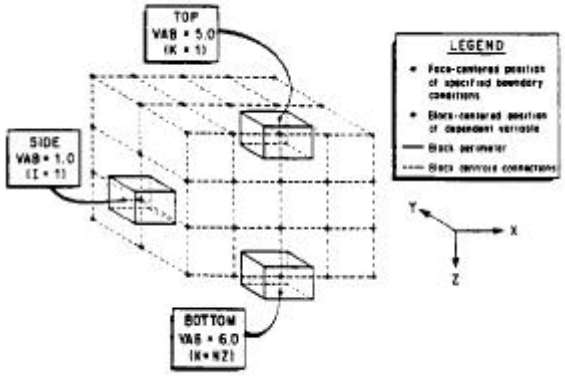
LIST: NCALC, NPT, PRTIF

NCALC Control parameter for selecting how the Carter- Tracy aquifer coefficients are to be assigned.
- 0 - The Carter-Tracy aquifer coefficients (VAB) will be read as input data.
- 1 - The VAB will be calculated by the program and assigned to each edge (perimeter) block in each areal plane, K=1,2,...,NZ (use with radial grids only).

NPT Number of points in the table of influence function versus dimensionless time ($P(t_D)$ versus t_D). If NPT = 0, then the program will select the infinite-aquifer solution for which the appropriate table is available internally.

PRTIF Print control key for the influence-function table.
- 0 - Suppress printing.
- 1 - Print the table of $P(t_D)$ versus t_D.

Figure 3-5. Positions for the Boundary Conditions.



Enter the following data only if NCALC = 0. Otherwise, skip to READ R1-31.

Follow the last VAB record of the following data group by a blank record. This READ group consists of two records, or any number of sets of two records, with each set defining a rectangular region and the value of VAB to be assigned within that region. Overlapping of regions is permissible. The order of the sets is immaterial except that any overlapping will result in the VAB of the last set being assigned to the overlapped subregion.

READ R1-30 (LIST 1: 6I5; LIST 2: E10.0) Boundary Specification

LIST 1: I1, I2, J1, J2, K1, K2

I1, I2 Lower and upper limits, inclusive, on the I index of the aquifer-influence region.

J1, J2 (Similar definition for J index).

K1, K2 (Similar definition for K index).

LIST 2: VAB

VAB Geometrical coefficient for each block within the defined region. The coefficient VAB, for the Carter-Tracy method, is actually the fraction of the total reservoir-aquifer boundary which the block surface comprises. For this reason it is possible to calculate the VAB from input data previously read, and the VAB does not have to be calculated externally.

READ R1-31 (4E10.0) Carter-Tracy Aquifer Properties.

LIST: KH, PHIH, RAQ, THETAQ

KH Conductivity-thickness for aquifer, ft^2/d (m^2/s). An average value of transmissibility along the edges should be used.

PHIH Porosity-thickness for aquifer, ft (m).

RAQ Equivalent aquifer radius, ft (m). The approximate method of Carter and Tracy is valid for circular aquifers. However, it may be used, nevertheless, to approximate the effect of an infinite aquifer upon a rectangular system.

THETAQ Angle of influence, degrees. This angle should indicate the portion of the aquifer covered by the aquifer-influence boundary. If mass flow is permitted across all the boundaries, enter 360E.

The following data are entered if NPT ≠ 0 (READ R1-29). If NPT = 0, the program will select the aquifer-influence functions for an infinite aquifer and the influence-function data need not be entered. If NPT = 0, omit this READ and proceed to READ R1-33.

READ R1-32 (2E10.0) Terminal-Rate Function

LIST: TD(I), PTD(I), I=1,NPT

TD Dimensionless time, kt/mf $(c_w c_R) r_e^2$.

PTD Terminal-rate function.

3.10.3 GEOMETRICAL-COEFFICIENT MODIFICATION

These data allow the user to modify the coefficient VAB by the relation VAB(I,J,K) = VAB(I,J,K) * FAB. This is useful when a reservoir may experience no or limited water influx across one boundary. In this case, in the region where influx is limited, the FAB may be used to reduce the VAB along that boundary.

Follow the following data with one blank record. If no modifications are desired, one blank record is still required.

READ R1-33 (LIST 1: 6I5; LIST 2: E10.0)

LIST 1: I1, I2, J1, J2, K1, K2

I1, I2 Lower and upper limits, inclusive, on the I index of the VAB to be modified.

J1, J2 (Similar definition for the J index).

K1, K2 (Similar definition for the K index).

LIST 2: FAB

FAB Factor by which the VAB will be modified in the defined region.

4 THE R1D RECORDS

The R1D input defines the physical properties and discretization of the local subsystems. These are one-dimensional units which may be attached to any global block within the system. They may be used to simulate the second porosity of a fractured media or they may be used to broaden the boundaries of the global system at minimal expense. This particular capability of the SWIFT II code is described by Reeves et al. [1986a], Sections 2.3, 5.6 and 7.1.3.

If KSLVD = 0 (READ M-3), then all R1D input should be skipped.

4.1 PHYSICAL AND DISCRETIZATION PARAMETERS

READ R1D-1 (E10.0) Rock Compressibility

LIST: CRD

CRD Compressibility of the rock within the local subsystems, psi^{-1} (Pa^{-1}).

READ R1D-2 (LIST 1: 7E10.0; LIST 2: 2I5,3E10.0; LIST 3: 7E10.0) Properties Dependent upon Local Rock Type

A set of three records is read for each local rock type assuming a natural ordering of the rock types, i.e., IR = 1,2,..., NRTD.

LIST 1: DMEFD, DMFD1, PHID, AKSD, ALPD, UKTD, CPRKD

DMEFD Diffusivity, ft^2/d (m^2/s).

DMFD1 Coefficient of thermal increase in diffusivity, $°F^{-1}$ ($°C^{-1}$).

PHID Porosity.

AKSD Permeability, ft/d (m/s).

ALPD Dispersivity, ft (m).

UKTD Thermal conductivity, Btu/ft-d-°F (J/m-s-°C).

CPRKD Heat capacity, Btu/ft^3-°F (J/m^3-°C).

LIST 2: KGDP, KGRD, SAD, DSD, DSDO

KGDP Geometry control.
- 0 - Spherical structural units.
- 1 - Prismatic structural units.

KGRD Local grid control.
- 0 - Node-to-node increment values are input.
- 1 - Single-mesh generation.
- 2 - Double-mesh generation.

SAD Length of prismatic units or radius of spherical units.

DSD Increment specification at interface of local subsystem with global system, ft(m).

DSDO Increment specification at the outer extremity of local subsystem, ft (m).

For single-mesh generation, the three parameters NSD (READ R0D-2), SAD and DSD are used to generate nodal positions for the local subsystem. See Figure 4-1a. For double-mesh generation, the four parameters, NSD, SAD, DSD and DSDO are used to generate nodal positions. See Figure 4-1b.

Reference: Reeves et al. [1986a], Section 7.1.3.

If KGRD ≠ 0 skip the following list.

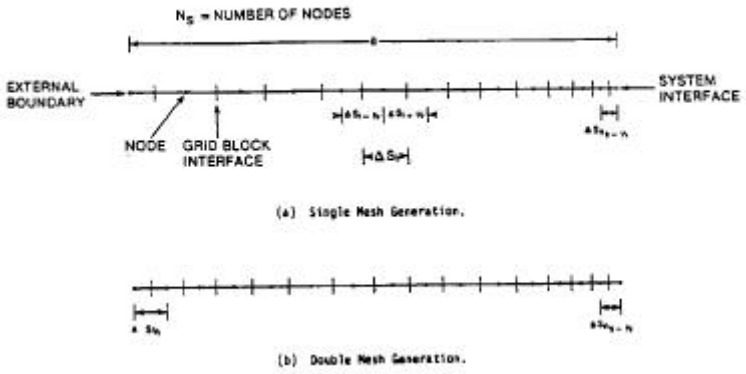
LIST 3: DS(I), I=1,NSD-1

DS Node-to-node increment values where I = 1 denotes the outermost increment and I = NSD-1 denotes the increment at the system interface, ft (m).

4.2 INITIAL AND OUTER BOUNDARY CONDITIONS FOR THE PRIMARY VARIABLES

In this section boundary conditions for the outer extremity of the local subsystem and initial conditions for the local subsystem are prescribed for the primary variables as a function of local rock type. The boundary condition at the local/global interface is not under user control since it is always matched implicitly to the value of the corresponding global variable.

Figure 4-1. Mesh generation for the local subsystems.



Enter as many records as necessary to define all initial and boundary conditions. Terminate the input here with a blank record. Even if no boundary specifications are desired, a blank record must still be used.

READ R1D-3 (LIST 1: 5I5; LIST 2: 3E10.0)

LIST 1: IR, KBC, KPB, KTPB, KSWB

IR Local rock type.

KBC Boundary-condition control
- 0 - No-flow (no-flux) conditions are invoked for all primary variables, P', T' and $\hat{C}'$.
- 1 - Dirichlet conditions are taken for all primary variables.
- 2 - Dirichlet conditions are used for the variables T' and a no-flux condition is used for P' and $\hat{C}'$.
- 3 - Dirichlet conditions are used for the variables $\hat{C}'$ and a no-flux condition is used for T'. Note: A fluid flux is calculated due to density changes.

KPB Conditional pressure control. Operative only for KBC > 0. See Figure 4-2 for a pictorial definition of the available options.
- 0 - Both boundary and initial conditions are fixed at the global-block value.
- 1 - The boundary condition is set at the value prescribed in List 2, and the initial condition is fixed at the global-block value.
- 2 - The boundary condition is set at the value prescribed in List 2, and the initial condition is fixed at the boundary-condition value.
- 3 - The boundary condition is set at the value prescribed in List 2, and the initial condition varies directly from the Dirichlet condition at the outer extremity to the global-block value at the system interface.

KTPB Temperature control. Operative for KBC = 1 and KBC = 2 only. The options here are the same as that of KPB (see Figure 4-2).

KSWB Brine control. Operative for KBC = 1 and KBC = 3 only. The options here are the same as that of KPB (see Figure 4-2).

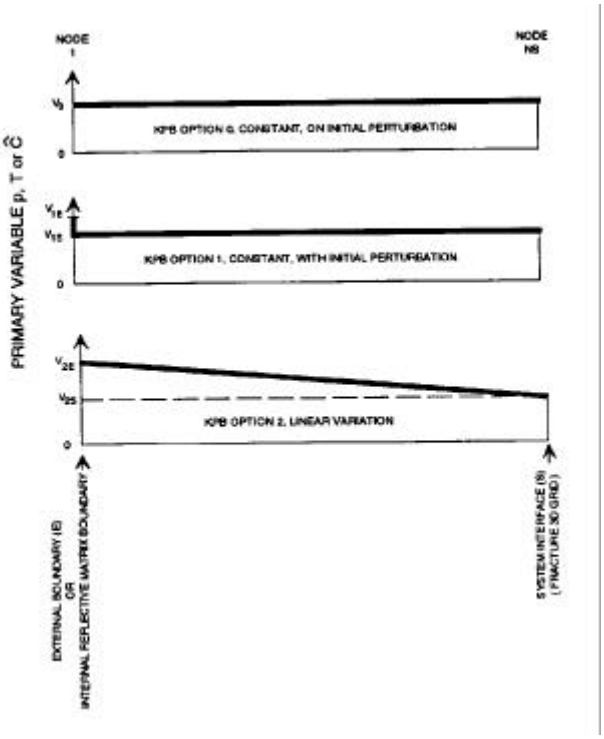
LIST 2: PBD, TPBD, SWBD

PBD Specified boundary value for pressure, psi (Pa).

TPBD Specified boundary value for temperature, °F (°C).

SWBD Specified boundary value for brine concentration, mass fraction.

Figure 4-2. Initial/boundary conditions for the primary variables within the local subsystems.



4.3 DISTRIBUTION COEFFICIENTS

If there are no radioactive components, i.e., NCP = 0 (READ M-3), skip this input set. Otherwise read one data set for each rock type.

READ R1D-4 (7E10.0)

LIST: DISD(IC), IC = 1,NCP

DISD Distribution coefficient in ft^3/lb (m^3/kg) for local rock-type IR and component IC.

4.4 RADIONUCLIDE BOUNDARY CONDITIONS

Radionuclide boundary conditions are not under the direct control of the analyst. They are set internally to be consistent with the condition used for the flow. Thus, for a constant-pressure condition, a convective flux condition is set on the radionuclide transport. For a no-flow condition, of course, a no-flux condition is used for the radionuclide equation.

4.5 DUAL POROSITY BLOCK MODIFICATIONS

Follow the data listed below with a blank record. If no modifications, a blank record is still required.

READ R1D-5 (LIST 1; 6I5; LIST 2: E10.0)

LIST 1: I1, I2, J1, J2, K1, K2

I1, I2 Lower and upper limits, inclusive on the I index of the global blocks to be modified.

J1, J2 (Similar definition for the J index.)

K1, K2 (Similar definition for the K index.)

LIST 2: FAMD

FAMD If positive, this is the factor by which the cross-sectional area within the defined region are to be multiplied. If negative, the absolute value of FAMD will be used within the region to be modified.

5 THE I RECORDS

The I data group is devoted basically to a definition of initial conditions for the global system. It supplements similar data read by subroutine READ1. Pressures are initialized within READ1 by assuming hydrostatic equilibrium with pressure PINIT at depth HINIT (READ R1-16). Temperatures are also initialized within that routine by linear interpolation from the table (ZT(I), TD(I)) (READ R1-11). The I records are read by subroutine INIT. The data obtained thereby may then be used to modify the initial pressure distribution to that appropriate for a natural flow within the reservoir. In this case, global boundary conditions prescribed in READ R1-28 for the up- and down-gradient faces of the system are respecified to their natural-flow values. In addition, both brine and radionuclide concentrations may be modified as desired from their default value of zero.

Reference: Reeves et al. [1986a], Section 5.1.

5.1 CONTROL PARAMETERS

If the initial concentrations are zero everywhere for both brine and radionuclides, and there is no natural flow, insert a blank record for READ I-1 and proceed to READ R1A-1.

READ I-1 (3I5)

LIST: ICOMP, INAT, IRD

ICOMP Control parameter for initializing brine concentrations.
- 0 - Initial concentrations in all the grid blocks are zero.
- 1 - The initial brine concentrations are not zero everywhere. Nonzero concentrations will be entered in READ I-2.

INAT Control parameter for entering initial fluid velocity.
- 0 - The reservoir fluid is static initially.
- 1 - The resident fluid velocity will be entered in READ I-3.

NOTE: While this will initialize a uniform flow field, the gradient will not necessarily be maintained during a transient flow simulation. To maintain a natural flow field, use perimeter wells (R2-4, 5, 6, 7) or prescribed pressures (R1-28).

IRD Control parameter for initializing radioactive/ trace component concentrations.
- 0 - Initial concentrations in all the grid blocks are zero.
- 1 - Nonzero concentrations for each component will be entered in READ I-4.

5.2 INITIAL BRINE CONCENTRATIONS

Skip the following READ if ICOMP = 0. If ICOMP = 1, read as many records as necessary following the last record with a blank record.

READ I-2 (6I5, E10.0)

List: I1, I2, J1, J2, K1, K2, CINIT

I1, I2 Lower and upper limits, inclusive, on the I index of the region having a nonzero initial brine concentration.

J1, J2 (Similar definition for the J index).

K1, K2 (Similar definition for the K index).

CINIT Initial brine concentration in each of the blocks of the defined region, mass fraction.

5.3 INITIAL VELOCITY CONDITION

Reference: Reeves et al. [1986a], Section 5.1.1.

If INAT = 0, skip the following record.

READ I-3 (E10.0)

LIST: VEL

VEL Initial velocity of the resident reservoir fluid in the x direction, ft/d (m/s). Initial velocities in the y and z directions are assumed to be zero.

Under this option, boundary pressures corresponding to the initial velocity are calculated and fixed at their natural-flow values. This option is not intended to replace the steady-state pressure solution, rather, initial conditions for transient simulation.

5.4 INITIAL RADIONUCLIDE CONCENTRATIONS

If IRD = 0, skip this READ. If IRD = 1, read as many records as necessary following the last record with a blank record. A total of NCP such sets of data are required, in the order of increasing component number, with a blank record terminating each set.

READ I-4 (6I5,E10.0)

LIST: I1, I2, J1, J2, K1, K2, CINIT

I1, I2 Lower and upper limits, inclusive, on the I index of the region having a nonzero initial radionuclide concentration.

J1, J2 (Similar definition for the J index).

K1, K2 (Similar definition for the K index).

CINIT Initial radionuclide concentration for the component being entered, mass fraction.

6 THE R1A RECORDS

Four different physical properties are taken to be functions of global rock type, namely thermal conductivities, dispersivities, distribution coefficients and salt-dissolution rates. Thermal conductivities and dispersivities are read by READ1 and distribution coefficients by READ0. Here, as a part of the input to READ1A, the rock-type specification and the salt dissolution rates are prescribed. In addition, all of the parameters defining the waste-leaching process within the repository are specified by the R1A input data set.

6.1 PRESCRIPTION OF ROCK TYPES AND SALT-DISSOLUTION CONSTANTS

If NRT = 1, skip to READ R1A-2 since all blocks are assumed by default to be of Type 1. Otherwise enter the desired number of changes, terminating with a blank record.

READ R1A-1 (7I5) Modification of Rock Types

LIST: I1A, I1B, J1A, J1B, K1A, K1B, IRT

I1A, I1B Lower and upper limits, inclusive, on the I index of region of modified rock type.

J1A, J1B (Similar definition for the J index).

K1A, K1B (Similar definition for the K index).

IRT Rock type.

Reference: Reeves et al. [1986a], Section 3.3.

READ R1A-2 (7E10.0) Salt-Dissolution Coefficients

LIST: (ACS(I), I=1,NRT)

ACS Product of the rate dissolution constant and the mass fraction of solubles to total dry mass, d^{-1} (s^{-1}).

6.2 DEFINITION OF THE REPOSITORY PARAMETERS

Reference: Reeves et al. [1986a], Section 3.4.

The user should skip to READ R2-1 if NREPB = 0. If NCP = 0 and NREPB ≠ 0, skip to READ R1A-5.

READ R1A-3 (I5) Waste Type

LIST: ILEVEL

ILEVEL Waste-type identifier.
- 0 - The waste-volume density is to be input directly.
- 1 - Canistered-storage data is to be input and used internally to calculate the waste-volume density.

READ R1A-4 (4E10.0) Storage Specifications

LIST: SDRIFT, SCNSTR, DCNSTR, HCNSTR

See Figure 6-1 for a pictorial definition of the following parameters for canistered waste (ILEVEL = 1).

SDRIFT Separation of rows of canisters, ft (m). Used only for storage of canistered wastes.

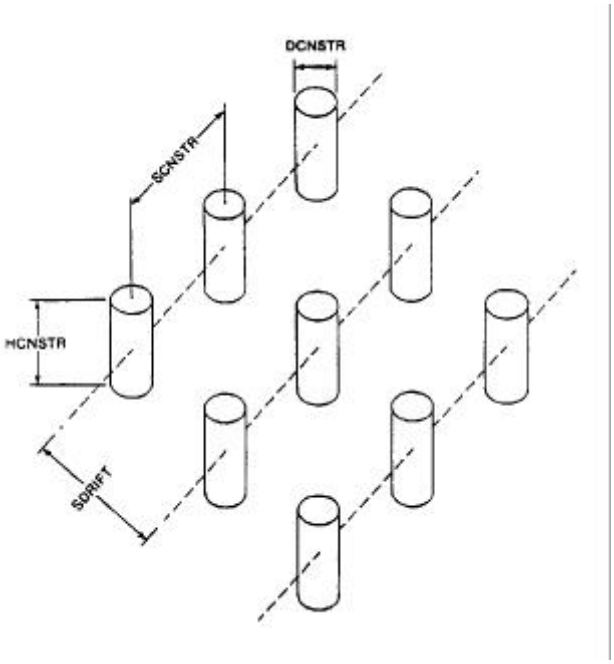
SCNSTR Center-to-center canister separation within each row, ft (m). Used only for storage of canistered wastes.

DCNSTR For canistered wastes (ILEVEL = 1) DCNSTR is the diameter of each canister, ft (m). For uncanistered wastes (ILEVEL = 0) DCNSTR is the volumetric waste density (volume of wastes per bulk volume of repository blocks).

HCNSTR Canister height, ft (m). Used only for storage of canistered wastes.

Arbitrary units may be used above and then converted to the English Engineering System (SI System) via R1A-5.

Figure 6-1. Specification of the Canistered Waste.



READ R1A-5 (4E10.0) UNIT Conversions

LIST: CONVL, CONVC, CONVT, CONVH

CONVL For canistered wastes (ILEVEL = 1) CONVL multiplies SDRIFT, SCNSTR, DCNSTR, and HCNSTR to convert to ft (m). For uncanistered wastes (ILEVEL = 0) CNVL multiplies only DCNSTR to convert to ft^3 (m^3) of wastes per bulk ft^3 (m^3).

CONVC This parameter multiplies the waste concentrations (R1A-8) to convert to lb/ft^3 (kg/m^3).

CONVT This parameter multiplies the given interpolation times (R1A-7) to convert to days (seconds).

CONVH This parameter multiplies the repository heat loadings (R1A-8.5) to convert to Btu/ft^2-d (J/m^2-s).

The default value for CONVL, CONVC, CONVT and CONVH is one. Thus, a blank or zero input value is reset to unity.

READ R1A-6 (6I5) Repository Location.

LIST: I1A, I1B, J1A, J1B, K1A, K1B

I1A, I1B Upper and lower limits, inclusive, on the I index of the repository region.

J1A, J1B (Similar definition for the J index).

K1A, K1B (Similar definition for the K index).

The repository blocks are assumed to be contiguous. Thus, only one input record R1A-6 is permitted, and no terminating blank record is necessary.

An error condition exists if the specified repository region contains more than NREPB blocks.

READ R1A-7 (7E10.0) Interpolation Times.

Waste concentrations may be obtained either by interpolation from a table of values or by integration of the radionuclide-transformation equations. If the integration option has been specified (NTIME = 1), then insert a blank record here and proceed to READ R1A-8.

LIST: CTIME(I), I=1,NTIME

CTIME Interpolation times, d (s).

Arbitrary units may be used here and then converted via CONVT (READ R1A-5) if desired.

If NCP = 0, skip to READ R1A-8.5.

The user must enter NCP groups of records below. However, the information will be used only for those components being tracked within the entire global system, i.e., the information will be used only if CNAME below matches one of the DI identifiers (READ R0-1).

READ R1A-8 (2A4,2X,6E10.0/(7E10.0)) Interpolation of Unleached Concentrations

LIST: (CNAME(I), I=1,2), (CNDUM(I), I=1,NTIME)

CNAME Identification of radioactive component.

CNDUM If interpolation is to be used, then CNDUM represents the concentrations at the interpolation times expressed as mass per unit volume of waste. If interpolation is not used, then CNDUM(1) is the initial condition for the chain decay.

If KHEAT = 0, skip to READ R1A-9.

READ R1A-8.5 (7E10.0) Repository Heat Loadings.

LIST: (ARHLD(I), I=1,NTIME)

ARHLD Repository heat loading expressed as energy input per unit time per unit area in the x-y plane.

If NCP = 0, skip to READ R2-1.

READ R1A-9 (7E10.0) Solubility Limits.

LIST: CS(I), I=1,NCP

CS Solubility limits expressed as mass fractions.

The code applies the solubility constraint $C(I) \leq CS(I)$ for component I only within the repository region specified in READ R1A-6.

7 THE N RECORDS

The nuclide monitor blocks are identified to facilitate postprocessing of radionuclide simulations. Nuclide concentrations are written to UNIT 9 (Section 10.8) at each time step for each block as identified. The file is formatted beginning with the value of time, followed by a set of concentration values. In each record the nuclide component is identified, followed by a sequential list of concentrations; one for each monitor block. Subsequent components follow sequentially.

Postprocessing may consist of time series plots or tables. Because of device dependence of graphics software, a postprocessing must be provided by the user. The output file may be imported to a spreadsheet or processed by other user programs (see Section 10.8).

Nuclide monitor blocks can be used to obtain nuclide mass faction breakthrough; time series concentration data, and with the water mass flux rate, calculate in nuclide mass discharge rate. This would be useful in risk assessment or evaluating the performance of a remedial strategy.

7.1 NUCLIDE MONITOR BLOCK

Skip to R2-1 if LBI0 = 0 (M-2).

READ N-1 (3I5) Monitor block location

LIST: IDSC, JDSC, KDSC

IDSC I index for block location.

JDSC J index for block location.

KDSC K index for block location.

Read as many records as necessary, terminating with a blank record.

8 THE R2 CARDS

In contrast to that of previous sections, the R2 data are time-dependent. Two different time regimes are used by the code. The first regime is a set of relatively coarse recurrent time steps. The time-dependent parameters are changed at the beginning of each such step by input from subroutine READ2. The second regime is a relatively finer time grid within each recurrent time step used for numerical integration of the transport equations. The recurrent data consists of control integers, source information, numerical-solution control and output control.

The minimum number of records for one recurrent data set is 3, R2-1 (options), R2-12 (time stepping), and R2-13 (print control). There is no limit to the number of recurrent data sets. A data set is terminated by an additional R2-1 record in which ITHRU=1.

For steady-state analysis, one set of recurrent data is required. The user can terminate the run or continue execution in one of two ways. For example, steady-state flow (NCALL = 4, M-3) completes and sets the solution option to NCALL = 3 (no primary equations). The run can be terminated and a restart file written (RSTWR = 1, R2-13) or continued. In either case, the solution control NCALL must be set to 1 or 2 etc. This is accomplished in the recurrent data using ICLL(R2-1) and NCALL (R2-11.1). Thus the first time change TCHG (R2-12) is zero and "real" time stepping appears in the second recurrent data set.

8.1 CONTROL INTEGERS

READ R2-1 (11I5)

LIST: INDQ, IWELL, IMETH, ITHRU, IRSS, IPROD, IOPT, INDT, ICLL, IRCH, ICHCR

INDQ Control parameter for reading well rates (Col. 1-5).
- 0 - Do not read well rates. No change in well rates
- 1 - Read seven well rates per card in READ R2-5.
- 2 - Read one card per well rate in READ R2-6.

IWELL Control parameter for reading well definition data (R2-7) (Col. 6-10).
- 0 - Do not read well data. No change in well data.
- 1 - Read new or altered well data.

IMETH Control parameter for reading method of solution (R2-2) (Col. 11-15).
0 - Do not read method of solution. No change in method.
1 - Read new or altered method of solution.

ITHRU Run termination (Col. 16-20).
0 - Run is to continue.
1 - Run is to terminate at this point. No more recurrent data will be read after this card. If no plots are desired, i.e., if NPLP, NPLT and NPLC are all zero, this should be the last card in your data deck.

IRSS Control parameter for reading radionuclide source data (R2-9, R2-10, R2-10.5) (Col. 21-25).
0 - Do not read source data for the trace components. No change in source data.
1 - Read new or altered source-rate data (R2-10).
2 - read new or altered waste-leach data (R2-10.5).

IPROD Control parameter for reading wellbore data (R2-8) (Col. 26-30).
0 - Do not read well-head data. No change in well-head data.
1 - Read new or altered well-head data.

IOPT Control parameter for reading iteration data for the wellbore solution (R2-3) (Col. 31-35).
0 - Do not read wellbore iteration data. If it is a new run and if wellbore calculations are desired, then default values of the iteration parameters will be used for the wellbore calculations.
1 - Read new or altered wellbore iteration data.

INDT Control parameter for reading iteration data for the reservoir solution (R2-11, R2-11.1) (Col. 36-40).
0 - Do not read iteration data. If no such data has been read for previous recurrent data sets, then default values are used.
1 - Read new or altered iteration data (R2-11).
2 - Read new or altered iteration data and L2SOR data (R2-11, R2-11.1).

ICLL Equation-solution control (R2-11.5) (Col 41-45).
0 - Do not read change in equation solution control, NCALL.
1 - Read new equation solution control, NCALL.

IRCH Control parameter for reading recharge data (R2-2.5) (Col. 46-50).
0 - Do not read recharge data. No change in recharge data.
1 - Read new or altered recharge data.

ICHCR Control parameter for reading rock compressibility and local rock parameters (R2-2.6) (Col. 51-56).

0 - Do not read compressibility data. No change in compressibility data
1 - Read new or altered compressibility data.

8.2 DIFFERENCING AND MATRIX SOLUTION CONTROL

The following data are entered if IMETH ≠ 0. If it is a new run and IMETH = 0, the program selects METHOD = 1 and WTFAC = 1.0 (direct solution with backward space and time approximations).

Reference: For a description of time and space differencing, see Reeves et al. [1986a], Sections 6.1.4 and 6.1.5. For a description of the matrix-solution options see Section 8.2.

READ R2-2 (I5,E10.0)

LIST: METHOD, WTFAC

METHOD Method of solution. Direct solution may be entered only if direct solution is specified in READ M-3.
- 1 - Reduced-band-width direct solution with backward finite-difference approximation in time (BIT).
- 2 - Two-line successive-overrelaxation (L2SOR) solution with a backward finite-difference approximation in time (BIT).
- -1 - Reduced band-width direct solution with a centered finite-difference approximation in time (CIT).
- -2 - Two-line successive-overrelaxation solution (L2S0R) with a centered finite-difference approximation in time (CIT).

WTFAC Weight factor for the finite-difference approximation in space.
- 1.0 - Backward differencing (BIS).
- 0.5 - Central differencing (CIS).

If WTFAC ≤ 0 is entered, the program selects WTFAC = 1.0.

8.3 SURFACE RECHARGE SPECIFICATION

The following data are entered if IRCH ≠ 0. Read as many records as necessary and follow the last record with a blank record.

READ R2-2.5 (4I5,E10.0)

LIST: I1, I2, J1, J2, RCHG

I1, I2 Lower and upper limits, inclusive, for the I index of the region having recharge rate, RCHG.

J1, J2 (Similar definition for the J index).

RCHG Recharge rate, ft/d (m/s).

The following data are entered if ICHCR ≠ 0.

READ R2-2.6 (LIST 1: 2E10.0; LIST 2: I5, E10.0; LIST 3: I5,4E10.0)

LIST 1: CR, CRD

CR Global rock compressibility (see R1-1).

CRD Local rock compressibility (see R1D-1).

LIST 2: IRT, CRR

IRT Global rock type (see R1A-1).

CRR Global rock compressibility (see R1-2.5).

Enter as many LIST 2 records as desired, terminating with a blank record.

LIST 3: IR, AKSD, PBD, TPBD, SWBD

IR Local rock type (see ROD-3).

AKSD Local rock hydraulic conductivity (see R1D-2).

PBD Specified boundary pressure (see R1D-3).

TPBD Specified boundary temperature.

SWBD Specified brine concentration.

Enter as many LIST 3 records as desired, terminating with a blank record.

8.4 WELL DATA

The following data are entered if IOPT > 0 (READ R2-1). If default values are desired, insert a blank record and proceed to READ R2-4. The default values of the parameters are discussed below.

****THIS FEATURE DOES NOT CONFORM TO QUALITY ASSURANCE STANDARDS. USE OF THIS IS NOT RECOMMENDED.****

READ R2-3 (I5,4E10.0) Wellbore Data.

Reference: Reeves et al. [1986a], Section 4.2.

LIST: NITQ, TOLX, TOLDP, DAMPX, EPS

NITQ Maximum number of outer iterations in the wellbore calculations. For example, if the injection rate for a well is specified, the well-head pressure is calculated iteratively to obtain the bottom-hole pressure necessary to inject the specified rate. If NITQ $\leq$ 0, the program selects the default value of 20.

TOLX The tolerance on the fractional change in pressure over an iteration. If TOLX $\leq$ 0, the default value of 0.001 is selected.

TOLDP The tolerance on pressure, psi (Pa). The default value is 7000 psi (4.8×10^7 Pa).

DAMPX Damping factor in estimating the next value of the pressure (at the surface for an injection well and at the bottom-hole for a production well). If the frictional pressure drop in the well is high, a linear extrapolation may lead to oscillations around the right value. The default value is 2.0.

EPS The tolerance on calculating temperature from given values of enthalpy and pressure. The fluid temperatures in the wellbore are calculated over each pressure increment as specified in READ R1-3. The default value is 0.001.

If INDQ = 0 (READ R2-1), skip READ R2-4 through READ R2-6 and proceed to READ R2-7.

READ R2-4 (I5) Rate Specifications

LIST: NWT

NWT Total number of wells.

Enter the following data only if INDQ = 1.

READ R2-5 (7E10.0) Rate Specifications.

LIST: Q(I), I=1,NWT

Q Production rate, ft^3/d (m^3/s). For an injection well, enter the value as a negative production rate. All the well rates must be entered even if all of them have not changed from the previous recurrent time step.

Enter the following data only if INDQ = 2. Read as many records as necessary to describe all the modified injection and production well rates. Follow the last record with a blank record.

READ R2-6 (I5, E10.0) Rate Specifications

LIST: I, QWELL

I Well number.

QWELL Production rate, ft^3/d (m^3/s). Enter negative values for injection rates. Enter only the well rates which are to be changed from an earlier recurrent data set.

The following data are entered for IWELL = 1. Read one set of data for each well, and follow the last record with a blank record.

READ R2-7 (LIST 1: (6I5); LIST 2: (4E10.0); LIST 3: (8E10.0); LIST 4: (7E10.0)) Definition of Well Options.

LIST 1: I, IIW, IJW, IIC1, IIC2, IINDW1 Well number.

IIW I index of the grid cell containing the well.

IJW J index of the grid cell containing the well.

IIC1 Uppermost layer in which the well is completed.

IIC2 Lowermost layer in which the well is completed.

IINDW1 Well specification option.

- 1 - Layer allocation via mobilities alone. Rate control only.
- ±2 - Layer allocation via mobility and pressure drop between wellbore and grid block. Rate control only.
- ±3 - Layer allocation via mobility and pressure drop between wellbore and grid block. Variable rate-pressure control.
- 2,3 - Explicit implementation.
- -2,-3 - Semi-implicit implementation.
- -4 - Steady-state pressure-limited.

Reeves et al. [1986a], Section 4.1, discusses the four topics, pressure/rate control, explicit/implicit rate terms, layer allocation and transient/steady-state implementation, all of which are crucial to a proper implementation of the well submodels. There is another point, however, which should be reiterated here related to pressure control.

Specifically, the point of application of the bottom-hole pressure. Figure 8-1 shows a well completed into three layers. As indicated there, the enforcement position for the specified bottom-hole pressure is the block center of the top layer of the completion zone. Usually this is also the position of the physical pressure measurement.

LIST 2: WI, BHP, TINJ, CINJ

WI Well index, ft^2/d (m^2/s).

BHP Bottom-hole pressure, psi (Pa). This must be specified only if IINDW1 = 3 or 4.

TINJ Temperature of the injected fluid, °F (°C). If surface conditions are being specified, TINJ is the temperature at the surface.

CINJ Brine concentration of the injection fluid, dimensionless.

Reeves et al. [1986a], Section 4.1, discusses how the well index is calculated and its function of relating the pressure of source or sink at a sub-grid scale to the average grid block pressure.

Skip LIST 3 if ISURF = 0 (READ M-2).

Reference: Reeves et al. [1986a], Section 4.2.

LIST 3: X, DW, ED, OD, TTOPW, TBOTW, UCOEF, THETA

X Wellbore length from surface to top of perforations, ft (m).

DW Inside diameter of the tubing, ft (m).

ED Roughness of the inner surface of the tubing for a smooth pipe, ft (m).

OD Outside diameter of the casing, ft (m).

TTOPW Initial rock temperature at the top-hole, °F (°C).

TBOTW Initial rock temperature at the bottom-hole, °F (°C).

UCOEF Overall heat transfer coefficient between the inner surface of the tubing and the outer surface of the casing, Btu/ft^2-°F-d (J/m^2-°C-s).

THETA Angle of deviation of the well bore from the vertical direction, degrees.

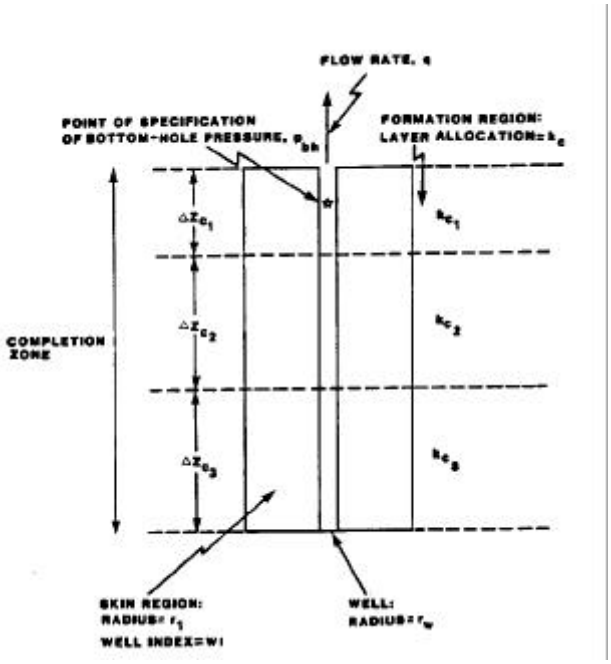
Skip LIST 4 if the well is completed in only one layer, i.e., if IIC1 = IIC2.

LIST 4: KHL(K), K=IIC1,IIC2

KHL(K) Layer allocation factors for well I, layer K, dimensionless.

Layer-allocation factors should be proportional to the total productivity of the individual layers, taking into account layer values of kΔz (permeability x thickness). Only relative values are important since these factors are renormalized to a unit sum. The productivity (injectivity) of layer K is computed as WI x KHL(K).

Figure 8-1. Characterization of a Well.



Skip the following READ if IPR0D = 0 (READ R2-1). However, it is used only for those wells having specification option IINDW1 = ±3.

READ R2-8 (7E10.0) Wellbore Data

LIST: THP(I), I=1,NWT

THP Surface pressure for each well, psi (Pa).

8.5 SINK/SOURCE INFORMATION

If IRSS = 0, skip this section of input and proceed to READ R2-11.

If NREPB > 0, skip to READ R2-10.5.

READ R2-9 (I5) Specified-Rate Data

LIST: NSS

NSS Number of sink/source blocks.

Enter one set of data for each source and follow the last set with a blank record.

Reference: Reeves et al. [1986a], Section 4.3.

If IRSS = 1, READ R2-10 and skip R2-10.5.

Enter NSS sets of data.

READ R2-10 (LIST 1: 4I5; LIST 2: 7E10.0) Specified-Rate Data

LIST 1: I, IIS, IJS, IKS

I Source Number.

IIS I index of the source block.

IJS J index of the source block.

IKS K index of the source block.

LIST 2: QWW(I), QHH(I), (QCC(I,J)J=1,NCP)

QWW Fluid discharge rate, lb/d (kg/s). A negative rate denotes a source, and a positive rate denotes a sink.

QHH Heat discharge rate, Btu/d (J/s).

QCC Discharge rates of radioactive components, lb/d (kg/s). Omit this parameter if NCP = 0.

Note: be careful not to doubly specify the water flow rate using QWW in this record and also as a well R2-5,6,7. For clarity it is recommended that fluid sources associated with heat or radionuclide input be entered on R2-10 records.

If IRSS = 2, READ R2-10.5.

If NREPB = 0, skip the following READ.
Reference: Reeves et al. [1986a], Section 3.4.

READ R2-10.5 (2E10.0) Waste-Leach Data

LIST: ALCH, BLCH

ALCH Leach time for radioactive waste within the repository boundaries, d (s).

BLCH Lag time from start of simulation to initiation of waste leaching or heat loading of the repository.

8.6 ITERATION AND L2SOR DIRECTIONAL CONTROL

The following data are entered if INDT ≠ 0 (READ R2-1). If default values are desired, enter INDT = 0 and skip to READ R2-11.5.

READ R2-11 (3I5)

LIST: MINITN, MAXITN, IMPG

MINITN Minimum number of outer (nonlinear-property due to density variation or water table) iterations in the subroutine ITER and ITERS. The default value is one.

MAXITN Maximum number of outer (nonlinear-property due to density variation or water table) interactions in subroutine ITER and ITERS. The default value is 2. For constant density use 1.

Note: For many variable-density or transient water table simulations, a value of 3 is adequate for MAXITN. Under steady-state water table conditions 5 to 15 iterations are recommended.

Reference: Reeves et al. [1986a], Section 8.2.

IMPG Number of time steps (transient) or iterations (steady state) after which the optimum parameters for the inner iterations are recalculated for the two-line successive over relaxation method. These data need be entered only if METHOD = 2. The default value for IMPG is 5.

If INDT = 1, skip to R2-11.5. Enter only if INDT = 2.

READ R2-11.1 (2I5, 2E10.0) L2SOR solution data

LIST: IXYZ, IBUD, TBUD, TPARM

IXYZ

- 0 - Code automatically chooses optimal direction for solution sweep based on minimum over-relaxation parameter.
- ±1 - Override to force sweep in x-direction.
- ±2 - Override to force sweep in y-direction.
- ±3 - Override to force sweep in z-direction.

IBUD Maximum number of L2SOR sweeps. The default value is 100. Usually 50-200 iterations will suffice.

TBUD Convergence (not normalized) criteria for iterations. The default value is 1 x 10^{-5} units. Be careful not to simply use the default. For example, 10^{-5} psi may be too small causing an excessive number of iterations. A default of 10^{-5} mass fraction is too large when simulating concentrations at 10^{-3} or less.

TPARAM Over or under-relaxation parameter (if IXYZ < 0). A value greater than 1.0 accelerates the solution and less than 1.0 dampens or under-relaxes the iterations. Generally 1.8 - 1.95 is used. Occasionally a coupled pressure-brine simulation will require an under relaxation of 0.85 - 0.99.

One record is required for each equation solution being solved. The order of equations is pressure, temperature, brine, radionuclides. Only one set of parameters is used for all radionuclide components.

8.7 EQUATION CONTROL

This section of input is frequently used for computational efficiency in the transient coupled solution of the primary and radionuclide equations. In such solution, the primary transport processes frequently reach steady-state. The radionuclide processes, however, due to the usual time dependence of the decay/production processes and of the source strength, frequently never reach steady-state. The ICLL option allows one to "turn-off" the primary solution after steady-state has been reached so that the major computational effort may then be devoted to the radionuclide solution.

Skip this READ if ICLL = 0 (READ R2-1).

READ R2-11.5 (I5) Equation solution control

LIST: NCALL

NCALL Same definition as for READ M-2 (see Table 2-1).

In the case of a steady-state run with NCALL = 4 or 5, the code automatically sets NCALL to 3 at the end of the solution. If one initiates a restart record from a previous steady-state simulation, the value of NCALL must be specified, otherwise the code will pick up a value of 3 contained in the restart file.

8.8 RECURRENT TIME AND TIME-STEP SPECIFICATION

READ R2-12 (8E10.0) Time values

LIST: TCHG, DT, DCMX, DSMX, DPMX, DTPMX, DTMAX, DTMIN

TCHG Time at which next set of recurrent data will be read, d (s). For steady-state, enter a zero (Col. 1-10).

The restart records can be written at TCHG only. Also, the mapping subroutine can be activated at TCHG only.

DT Time step specification, d (s). If DT is positive it will be the time step used from the current time to TCHG. If DT is zero, the program will select the time step automatically (Col. 11-20).
>0 - Time step to be used from the current time to TCHG.
0 - Automatic time stepping to be used for transient analysis or zero for steady-state analysis.

DT must not be zero for the first time step of the simulation time, unless the steady-state option (NCALL = 4 or 5) is used. If transient radionuclide solutions are to simulated after a steady-state flow analysis, enter a zero TCHG and DT for the first recurrent data set. In the second recurrent data set introduce the nuclide source and enter non-zero DT.

The following six parameters are used only if the automatic time-step feature is selected, i.e., if DT = 0. If this feature is selected, the program will automatically vary the time-step as it seeks a value such that the maximum changes in the concentration, pressure and temperature are less than or equal to the specified values.

DCMX Maximum change desired per time step for the radioactive/trace-component concentration. The default value is 0.95 (Col. 21-30).

DSMX Maximum change desired per time step for the brine concentration. The default value is 0.25 (Col. 31-40).

DPMX Maximum change desired per time step for the pressure, psi (Pa). The default value is 50 psi (350,000 Pa) (Col. 41-50).

DTPMX Maximum change desired per time step for the temperature, °F (°C). The default value is 9°F (5°C) (Col. 51-60).

DTMAX Maximum time step allowed, d (s). The default value is 30 d (2.6×10^6 s) (Col. 61-70).

DTMIN Minimum time step required, d (s). The default value is 1.0 d (8.64×10^4 s) (Col. 71-80).

Note: Column identified in cols. 71-80 cannot be used on this record. use beyond col. 81 to label this record if desired.

8.9 OUTPUT CONTROL

READ R2-13 (14I5) Output Control

LIST: I01, I02, I03, I04, I05, I06, I08, RSTWR, MAP, MDAT, IIPRT, IO5D, I08D, IIPRTD

I01 Control parameter for the frequency of time-step summary. The time-step summary gives mass-balance information for both the global system and the local subsystems. It also characterizes the state of the global system via the average reservoir pressure, and the maximum pressure, concentration and temperature changes in any block during the time step (Col. 1-5).

I02 Control parameter for the frequency of the well summary. For each well this summary gives production and injection rates of fluid, heat and brine, cumulative production and injection, well-head and bottom-hole pressures, well-head and bottom-hole temperatures and the grid-block pressure in which the bottom-hole of the well is located. This summary also gives the total production and injection rates and the total cumulative production and injection (Col. 6-10).

I03 Frequency control for listing the grid-block values of concentration, temperature and pressure for the global system and the local subsystems (Col. 11-15).

I04 Control parameter for printing the injection/ production rates in each layer for each well (Col. 16-20).

I05 Control parameter for listing the grid-block values of radionuclide concentrations for the global system (Col. 21-25).

I06 Control parameter for listing of aquifer-influence and boundary rates (Col. 26-30).

The following values apply to all six of the above parameters:

-1 - Omit printing for all time steps from the current time through TCHG, inclusive.

0 - Print at the end of each time step.
1 - Print only at time TCHG.
n(>1) - Print at the end of every n-th time step and at the time TCHG.

I08 Control parameter for selectively listing the grid-block values of the primary variables for the global system. The listings are printed according to the frequency specified by I03. This parameter gives one the option for not printing selected tables, as desired. This parameter requires a three-digit specification. The first (left-most) digit refers to pressure, the second to temperature and the third to brine concentration. A negative number allows for windowing via R2-16 (Col. 31-35).
0 - The grid-block values will be printed.
1 - The grid-block values (pressure at datum or temperature or brine concentration) will not be printed.
2 - Refers to the first digit only. Neither the pressure nor the pressure at datum will be printed.

For example, if only grid block values of temperature are desired, then enter I08 = 201.

RSTWR Restart-record control parameter (Col. 36-40).
0 - No restart record will be written.
1 - Restart record will be written on UNIT 8 at time TCHG.

MAP Parameter for printing contour maps at time TCHG. Only two-dimensional maps are printed. The maps are printed for r-z coordinates in a cylindrical system and for x-y coordinates (areal maps) in a Cartesian system. If NY = 1 then maps may also be obtained for x-z coordinates (vertical cross sections) in a Cartesian system. Areal maps cannot be printed for a cylindrical system. This parameter requires a four digit specification, the first digit referring to all of the radionuclide concentrations, the second to pressures, the third to temperatures and the fourth to brine concentrations (Col. 41-45).
0 - The variable will not be mapped.
1 - Areal map (x-y) at TCHG.
2 - Vertical cross-sectional map (x-z or r-z).
3 - Vertical cross-sectional map (y-z).

For example, if contour maps are desired for areal pressure at datum and vertical temperature only, enter MAP = 0120.

For radionuclides, all components are mapped.

For pressure, either pressure at datum, environmental head or freshwater head in printing depending on the value of LMAPIT (M-2).

The type of map output is controlled on Record R2-14. This includes listable output, matrix and x, y, z formats.

MDAT Control parameter for entering the mapping specifications (R2-14, R2-14.5, R2-15) (Col. 46-50).
0 - The mapping specifications are not to be changed.

1 - Read new mapping specifications. If activating the printing of contour maps for the first time during the current run, MDAT must be entered as one and MAP must be greater than zero.

IIPRT Intermediate print control for the global system. This parameter requires two or more digits for its specification of the form 10n + i. Here n is the frequency control with the same options as those used for IO1 through IO6 (see note following IO6). Parameter i is the function control with the following options (Col. 51-55).

0 - None of the output listed below will be activated.
1 - Darcy velocities will be printed.
2 - Transmissibilities, Peclet and Courant number will be printed in addition to the velocities.
3 - Fluid densities, viscosities, enthalpies and dispersions will be printed, in addition to the quantities listed above.

For example, to print velocity at the end of the time change TCHG (R2-12), enter a value of 11. It may be desirable to use the value of 13 during debugging, but this will create significantly large output files. Also, as the parameters don't change significantly with time, it is not recommended to print values every time step. If output is not desired, enter 00.

IO5D Control parameter for listing the grid-block values of the radionuclide concentrations for the local subsystems, i.e., matrix (Col. 56-60).

IO8D Control parameter for selectively listing the grid-block values of the primary variables for the local subsystems. The listings are printed according to the frequency specified by IO3 (Col. 61-65).

IIPRTD Intermediate print control for the local sub-systems. This parameter is analogous to the global control IIPRT. It also has the form 10n + i where n carries the frequency options used for IO1 through IO6 (see note following IO6) and where i carries the function control given under IIPRT (Col. 66-70).

8.10 MAPPING CONTROL

Enter the following data in Reads R2-14, R2-14.5, R2-15 only if contour maps are desired, i.e., if MAP ≠ 0000 (READ R2-13) and if MDAT = 1 (READ R2-13).

It is not necessary to enter these records each time a map is to be printed. One only needs to enter R2-14, R2-14.5 and R2-15 once, unless mapping specifications are to be changed with time.

READ R2-14 (6I5) Map Orientation Control

LIST: NORNXY, NORNXZ, NORNYZ, KMP6, KMP10, KMP13

NORNXY, Map orientation factors for areal and vertical maps, respectively.
NORNXZ,
NORNYZ

0 - The map is printed with the first-coordinate (r for radial geometry) increasing from left to right and the second ordinate increasing up the computer page, i.e., the x=0, y=0 point is the bottom left hand corner for areal map.

1 - First ordinate increases from left to right and second ordinate increases down the computer page. The origin is the upper left hand corner. Use this for cross-sections where depth is positive downward.

-1 - Use this for cross sections where elevation is positive upwards.

KMP6, Control parameters for listing and writing of map output files on Unit 6
KMP10, (line printer), Unit 10 (x,y,z format as specified in Section 10.5) and Unit 13
KMP13 (matrix grids). See Table 10.1 for file naming.

0 - Write to file.

-1 - No file writing.

READ R2-14.5 (6E10.0) Physical Dimensions of Map

LIST: XYXL, XYYL, XZXL, XZZL, YZYL, YZZL

XYXL,XYYL The x and y map lengths in inches, respectfully, for all the areal maps.

XZXL,XZZL The x/r and z map lengths in inches, respectively, for all the vertical (x-z) maps.

YZYL,YZZL The y and z map lengths in inches, respectively, for all the vertical (y-z) maps.

Assume output device is 10 characters per inch, 6 lines per inch.

READ R2-15 (6I5, 2E10.0)

Enter one record for each map requested on R2-13 record. For example, if MAP = 0103, areal pressures and vertical brine concentration maps will be generated. Therefore, 2 data records should be entered here for this example. Note that all nuclide components of concentration are mapped. These data are used for all components present in the simulation.

LIST: I1(I), I2(I), J1(I), J2(I), K1(I), K2(I), AMIN (I), AMAX(I), I=1, Number of MAPS requested.

I1, I2 Lower and upper limits, inclusive, on the I-coordinate of the region to be mapped.

J1, J2 Lower and upper limits, inclusive, on the J-coordinate of the region to be mapped.

K1, K2 Lower and upper limits, inclusive, on the K-coordinate of the region to be mapped.

AMIN, AMAX The minimum and maximum values of the variable used to derive the 20 contour intervals. If the variable in any grid block is higher than AMAX, it will be indicated as AMAX. If AMAX is entered as zero, the program will search for the maximum among all the grid block values and use as AMAX. Similarly, a large negative number for AMIN ($\leq$-99) will cause the program to search for the minimum and use as AMIN.

The data entered up to this point are sufficient for simulation of the system through time TCHG. To continue, another recurrent data set is attached. However, to terminate the simulation phase of the run, one should enter ITHRU = 1 in a single READ R2-1 termination card. If any plots are desired, i.e., if NPLP or NPLT or NPLC equals one, then the plotting data (READ P-2 through P-4) should follow. If no plots are desired, then ITHRU = 1 will terminate the execution.

8.11 WINDOW CONTROL

Enter the following data if I08 (R2-13) is less than zero.

READ R2-16 (6I5) Windowing Output Control

LIST: NI1, NI2, NJ1, NJ2, NK1, NK2

NI1, NI2 Lower and upper limits, inclusive of the window in the x-direction.

NJ1, NJ2 Lower and upper limits, inclusive of the window in the y-direction.

NK1, NK2 Lower and upper limits, inclusive of the window in the z-direction.

9 THE P RECORDS

The P records, like the M records, are read by the main routine. Here, however, the input is identified by its function (plotting) rather than by the routine from which it is read. Plotting, within the SWIFT model, is identified with well data in that pressure, temperature and brine concentrations, both at the surface and at the bottom-hole, may be plotted as functions of time. Table 9-1 exhibits the various dependent variables which may be plotted as functions of the well characteristics. Plots for an observation well are particularly useful since they simply indicate the behavior of the grid-block variables as functions of time.

In order to facilitate model calibrations, printer plots are used. The time axis is always directed down the page with range and resolution determined by the input parameters. The dependent-variable axes, on the other hand, are always directed across the page. Here the range is determined externally by the input parameters, but the resolution is fixed internally in that the specified range is divided into 100 columns in each case. The plotting symbols which are used are given in Table 9-2. If there are several values of the dependent variables within the prescribed resolution on the time scale, then the average value is plotted. If there are no such values, then, of course, no values are plotted.

Calculated plot data is stored by the code on UNIT 12. If plots are desired for a previous run, then UNIT 12 should be attached.

If NPLP = 0, NPLT = 0, and NPLC = 0, (i.e., no plots are desired), skip all P records.

The plotting data for one well consist of the data from READ P-2 through READ P-4. Enter as many sets of these data as there are wells for which plots are desired. If plots are desired for all the wells enter NWT sets of these data. If less than NWT sets are entered, then follow the last set with a blank record to end the input of plotting data.

READ P-2 (I5, 5X, 10A4) Well Identity

LIST: KW, ID

KW The well number.

ID A title to the plots for well number KW.

Table 9-1. Dependent plotting variables versus well characteristics.

Well Type	Point of Specification[1]	Plotting Variables[2,3]	
		Bottom-Hole	Surface
Observation[4]	--	P, T, $\hat{C}$	
Injection	Bottom-Hole	P	
Injection	Surface	P, T	P
Production	Bottom-Hole	P, T, $\hat{C}$	
Production	Surface	P, T, $\hat{C}$	P, T

[1]The point of specification is controlled by integer ISURF (READ M-2), i.e., ISURF = 0 for bottom-hole conditions and ISURF = 1 for surface conditions.
[2]Notation here is consistent with that of Reeves et al. [1986a], i.e.,
P - pressure,
T - temperature,
$\hat{C}$ - brine concentrations.

[3]The list of plotting variables given here assumes that NCALL = 0 (READ M-2).
[4]An observation well is defined by the flow rate, Q = 0.

Table 9-2. Plotting symbols.

Symbol	Data Type
X	Calculated
O	Observed
*	Coincident Calculated and Observed

READ P-3 (7E10.0) Variable Ranges and Resolutions

LIST: TMN, TMX, D1, PWMN, PWMX, PSMN, PSMX, TWMN, TWMX, TSMN, TSMX, CMN, CMX

TMN Lower limit on time, d (s).

TMX Upper limit on time, d (s).

D1 Time step for each row, d (s).

The three parameters immediately above determine the number of rows, NROWS, to be used, i.e., NROWS = (TMX - TMN)/D1. Current fixed dimensions restrict this quantity to NROWS $\leq$ 400.

If D1 is set to zero, a default value is calculated assuming 50 rows, i.e., D1 = (TMX - TMN)/50.

PWMN, PSMN, TWMN, TSMN CMN — Lower limits on bottom-hole pressure, psi (Pa); face pressure, psi (Pa); bottom-hole temperature, °F (°C); surface temperature, °F (°C); and brine concentration, dimensionless, respectively.

PWMX, PSMX, TWMX, TSMX, CMX — Upper limits on bottom-hole pressure, psi (Pa); surface pressure, psi (Pa); bottom-hole temperature, F° (°C); surface temperature, °F (°C);cand brine concentration, dimensionless, respectively.

If there are no observed data, then enter any negative number in the first field of the following record. Fixed dimensions limit the number of values for any one variable to 300 or less. If there are such data, then enter up to 300 (inclusive) of these records in the read set below, and terminate the read with any negative number in the first field.

READ P-4 (6E10.0) Observed Data.

Read as many records (up to 300) as there are observed data points (one record for each value of time at which the observed values are available). Follow the last record with a negative number in the first field specification (E10.0).

LIST: TOX, POW, POS, TOW, TOS, COC

TOX Observation time, d (s).

POW Bottom-hole pressure, psi (Pa).

POS Surface pressure, psi (Pa).

TOW Bottom-hole temperature, °F (°C).

TOS Surface temperature, °F (°C).

COC Brine concentration, dimensionless.

10 USE OF AUXILIARY DISK FILES

Auxiliary disk files are used by the SWIFT model to perform the six different functions given in Table 10-1. Two of these functions are standard input and standard output, which require no discussion. The others consist of calculational restarts, mapping restarts, plots of well data mapping, mass balance, heterogeneous reservoir, nuclide monitor block, aquifer influence function, and streamline postprocessing. These functions do require further discussion which is provided herein. These files are written as controlled by various input data specifications. Note that creation of these files requires CPU time and disk space. For example, a restart file contains virtually all input and calculated values. Multiple restarts in one file for a large three-dimensional run can require tens of megabytes of storage. On the other hand, the use of a binary heterogeneous reservoir specification can be used to replace voluminous R1-21 ASCII records. This could reduce a 10 MB section of the standard input file with a substantially smaller binary. This binary file needs to be stored only once for a set of runs.

10.1 CALCULATIONAL RESTARTS

Figure 10-1 shows the basic sequence of events for restarting a calculation. As illustrated there, UNIT 8 is written during the execution of the direct run. This information is then read from UNIT 4 and the first restart run commences. Although it is not illustrated by the figure, another restart record may be written (on UNIT 8) during the second execution and the restarting process may be continued indefinitely.

Aside from the temporary-store variables, which are defined locally within each subroutine, all scalars and arrays are partitioned within the four common-block arrays. A restart procedure is initiated by simply setting the control

RSTWR = 1 (READ R2-13) (10-1)

If this is done, say, by the direct run of Figure 10-1, then the common-block arrays are written on auxiliary storage using the following unformatted write commands:

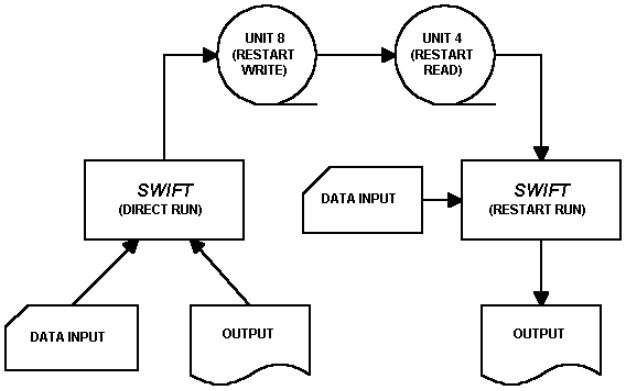
Table 10-1. Definition of auxiliary files.

UNIT	Function	Default File Suffix
4	Input for restart calculation	.RST
7	Output for streamline postprocessing	.VL
8	Output for subsequent restart calculation	.WR
9	Output for nuclide monitor post-processing	.NM
10	Output for contouring based on mapping options	.XYZ
11	Input for heterogeneous reservoir R1-21	.BIN
12	Input and output for plotting via SWIFT	.WL
13	Output for contour mapping using MODFLOW format	.MAP
15	Standard 80 column input	.DAT
16	Standard 132 column output for printer	.OUT
17	Output for mass balance summary	.MBL
18	Output for aquifer influence function flux values	.AIF

Unformatted files:

- Restart: UNIT 4 and 8.
- Heterogeneous reservoir (optional, see R1-21): UNIT 11.
- Contour mapping (optional) UNIT 10: Format is formatted if LMAPIT = x1 (M-3) and unformatted if LMAPIT = x2 (M-3). Also the creation is further controlled via KMP10 (R2-14).

Figure 10-1. Schematic of a Restart Calculation.



```
WRITE(8)  (TWRITE(I),I=1,LTWRT)
WRITE(8)  (G3(I),I=1,IG3LST)                                    (10-2)
WRITE(8)  (G2(I),I=1,IG2LST)
WRITE(8)  (G(I),I=1,IGLSTR)
WRITE(8)  (IG(I),I=1,IGLSTI)
```

For protection against an abnormal termination, it is a good practice to write restart records at several different times during a relatively long run.

The calculation may be restarted by so indicating with the control

```
RSTRT = ITIME          (READ M-2)                               (10-3)
```

where ITIME indicates the time step of the particular restart record which is to be used to initialize the follow-up calculation. The code then simply reads the list of restart records written during the previous run(s) until the appropriate one is found, loads the common-block arrays and continues the calculation. A list of the appropriate data input is given in Table 10-2.

10.2 MAPPING RESTARTS

Assume that an auxiliary disk file has been loaded with several restart records, as described in the preceding section, and that it is desired to map the results present in some of those records. There are options in SWIFT which permit such to be done. The configuration is similar to that shown on the right-hand side of Figure 10-1. Thus, UNIT 4 contains the restart data which is read by the code, along with data from records, and maps are obtained in the output. The necessary record input is presented in Table 10-3. Basically, the function of this entire set of input data is to search the auxiliary unit for the appropriate restart record(s), as indicated by the time-step number(s) and then to map the primary variables as contour plots over the specified spatial domain. Mapping specifications may be changed from that originally given (at the time the restart record was made) as desired.

Table 10-2. Data input for a calculational restart.

Card Identifier	Function
M-1	Title
M-2	Option Parameters (RSTRT > 0)
R2 Group(s)	Recurrent-Data Input
P Group[1]	Plotting of Well Data

[1]Optional depending upon values of NPLP, NPLT and NPLC.

Table 10-3. Data input for a map from a restart file.

Card Identifier	Function
M-1	Title
M-2	Option Parameters (RSTRT = -1)
	---First Map from Restart Record---
M-6	Time-Step Number (IMPT > 0)
M-7	Mapping Control
R2-14 - R2-15[1]	Map Specifications
	--Additional Maps From Restart Records[2]--
M-6 - R2-15	
•	
•	
M-6	Blank

[1]Optional depending on MDAT and MAP (READ M-7)
[2]Enter as many sets of these data as desired.

10.3 PLOTS OF WELL DATA

As in the case of mapping, plots may be obtained either at the time of a calculational run or from a separate plotting run. The purpose of this section is to elaborate on the latter. Figure 10-2 configures the case to be considered. As illustrated there, all plotting variables are written UNIT 12 by SWIFT. Providing, then, that this auxiliary file has been properly preserved, it may be attached for a plotting run.

To write UNIT 12, a formatted output statement is used, specifically in Subroutine PRINT2,

> WRITE(IOU12,1630) KW, I2, TCX(IPT), PCW(IPT), PCS(IPT), TCW(IPT), TCS(IPT), CCC(IPT), QW(IPT) 1630 FORMAT (2I5,7E12.5)

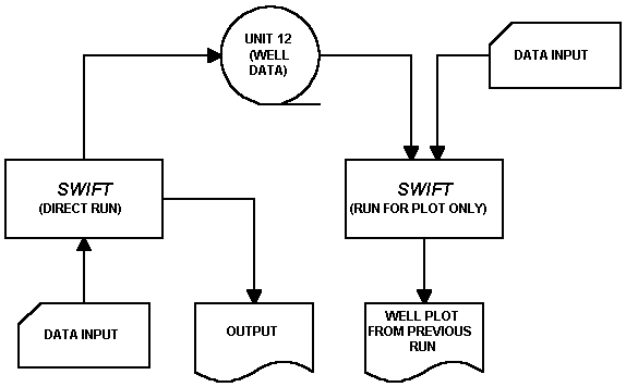
Here the parameters and variables are defined as follows:

Parameter	Alias	Definition
KW	I1	Well number
I2	I2	Control parameter
TCX	U1	Time
PCW	U2	Pressure at bottom-hole
PCS	U3	Pressure at surface
TCW	U4	Temperature at bottom-hole
TCS	U5	Temperature at surface
CCC	U6	Brine concentration
QW	U7	Well flow rate

A record of the above form is written for each time step during the calculation.

In contrast to the writing of a restart record, the writing of UNIT 12 is not controlled by an integer such as RSTWR (READ R2-13). It is controlled only by the requirement that there must be wells in the system, i.e., NWT > 0. The control parameter I2 specifies the plots which are to be made. As discussed in Chapter 9 (see especially Table 9-1) the specification of plotting variables depends upon the well characteristics. Thus, only a selected number of the dependent variables of the above output list will be plotted depending upon whether the well is an injection, production or observation well and on whether surface or bottom-hole conditions are specified. Parameter I2 takes into account these factors.

Figure 10-2. Schematic of Plotting from a Previous Run.



The additional information necessary for plotting is that deriving from the standard input unit, i.e., the data on records. Table 10-4 characterizes this data. As illustrated, negative values of the plot controls NPLP, NPLT and NPLC are necessary to trigger the plotting from a previous run in that control is transferred immediately to the plotting routines. As many wells as desired may be used for the plotting.

The plot file ___.WL can easily be imported to a spreadsheet. The file format groups all wells for a time step, thus the data may require some rearrangement in order to develop a time series. For radionuclide discharge, it may be necessary to merge the ___.WL file with the nuclide monitor output (Section 10.8).

10.4 STREAMLINE POSTPROCESSING

It is frequently helpful to present flow results in terms of streamlines. For this reason the appropriate information is written to the auxiliary file so that it may be processed by a streamline postprocessor. Figure 10-3 gives the configuration of such an operation. As shown there, UNIT 7 is prepared during the SWIFT run and is subsequently read by a streamline utility. The latter is denoted there by the acronym "STLINE."

The first record contains the current version number.

(1) WRITE(7) 'VERSION 2.54'

The second record contains the depth to datum for converting between block depth and elevation.

(2) WRITE(7) HDATUM /See R1-16

The third record of information of UNIT 7 comes from the unformatted output statement:

(3) WRITE(7) NX, NY, (DELX(I),I=1,NX), (DELY(I),J=1,NY)

It contains the incrementation integers, NX, NY and the increments, DELX, DELY. The next nine records on UNIT 7 are derived from the following unformatted writes:

(4) WRITE(7) (H(M),M=1,NB) /Block centroid elevation

(5) WRITE(7) (FR(M),M=1,NB) /Saturated block thickness

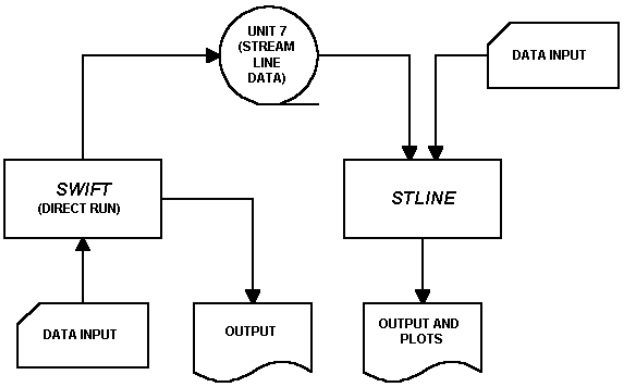
(6) WRITE(7) (PV(M),M=1,NB) /Saturated pore volume

Table 10-4. Data input for plots from a previous run.

Card Identifier	Function
M-1	Title
M-2	Option Parameters (NPLP < 0, NPLT < 0 or NPLC < 0
P-2 - P-4	Data for One Well
P-2 - P-4	Data for Another Well[1]
P-1	Blank

[1]Enter date for each well for which plots are desired.

Figure 10-3. Schematic of Streamline Postprocessing.



```
(7)   *WRITE(7)  (UXX(M),M=1,NB)  /x-direction Darcy velocity
(8)   *WRITE(7)  (UYY(M),M=1,NB)  /y-direction Darcy velocity
(9)   *WRITE(7)  (UZZ(M),M=1,NB)  /z-direction Darcy velocity
(10)  *WRITE(7)  (P(M),M=1,NB)    /Fluid pressure at elevation
(11)  *WRITE(7)  (BW(M),M=1,NB)   /Fluid density
(12)  *WRITE(7)  TIME             /Elapsed simulation time
```

*For transient flow analysis, only these arrays are written at time steps 2 and thereafter.

They contain saturated block thickness, FR; pore volumes, PV; Darcy velocities, UXX, UYY and UZZ; and fluid pressure at elevation. At present, simulation times are not written, instead the writing of UNIT 7 is controlled by the integer IIPRT (see READ R2-13).

Note: All real variables are double precision (REAL*8) and integer variables are long integers (Integer*4).

10.5 MAPPING POSTPROCESSING

While the contour maps from the output file are invaluable in trial simulations, ultimately report quality figures will be needed. This may be accomplished by an auxiliary file and postprocess the dependent variable with other software such as SURFER, PLOT88, DISSPLA, or DI-3000. The "map" file is written to UNITs 10 and 13. The file is controlled by the options for the printer (UNIT 6) contour map (see R2-13 to R2-15).

The map data are written to two files as well as optionally being listed with the other output on UNIT 6. The ASCII file on unit 10 may be processed by entering the data as randomly-spaced input to contouring packages. Alternatively, the grid or matrix format file on unit 13 allows for post processing consistent with the U.S. Geological Survey Modular Groundwater Flow code MODFLOW (McDonald and Harbarugh, 1988). In either case, the control for writing these files is the same.

The ASCII file on UNIT 10 is a header record and a continuous string of records containing the x-coordinate, y-coordinates and dependent variable for the window of the map as specified in the R2-13 to R2-15 records. The format is:

Header Record

TIME, ITIME, (TEXT(I),I=1,3) using format (E10.3, I10, 3A4)

Triad List

Col. 1-15	16-30	31-45
))))	))))	))))))
X(I)	Y(J)	A(I,J) (3G15.7)

X() and Y() are the grid block centroid coordinates and A(I,J) is the dependent variable mapped (see MAP on R2-13). In the case of zero pore volume blocks, the value of the dependent variable will be -9999. In addition, to avoid the possibility of underflows the minimum absolute value of the dependent variable is set to 1.0 E-30.

The grid or matrix file, written to UNIT 13, is styled after MODFLOW (McDonald and Harbaugh, 1988). The MODFLOW file structure is adopted as a standard convention to facilitate the postprocessing of contour maps. The UNSWIFT utility in Section 11 describes the translation procedure to interface with SURFER®. In contrast, SWIFT does not use stress periods, nor are the data files designed on a horizontal layering concept. It is nevertheless worthwhile to adopt the MODFLOW format to allow for interchangeability. The structure for the map files is:

Record 1	ITIME, ITIME, DELT, TIME, TEXT, NC, NR, KK
Record 2	((A(J,I), J=1,NCOL), I=1,NROW)

where

ITIME	is the time step number (i.e. KSTP in MODFLOW)
DELT	is the time step size (PERTIM)
TIME	is the elapsed simulation time (TOTIM)
TEXT	is the 16 character description of the dependent variable (TEXT) [Declared CHARACTER TEXT(4)*4]
NC	is the number or columns or x-increments (NC)
NR	is the number of rows or y-increments (NR)
KK	is a slice index in SWIFT, but refers the layer number in MODFLOW (ILAY) For areal maps KK is the layer, counting downwards from the top most. For cross-sectional maps, KK is the slice index, e.g. for an X-Z map, KK refers to the y-index slice number.

The matrix file is written in ASCII or unformatted (binary) mode as controlled by LMAPIT on the M-2 or M-7 record. In the case of an ASCII file (LMAPIT=1), the format is:

Record 1 (2I10, 2E10.3, 4A4, 3I10)

Record 2 (1PG12.5)

There is no format specification for the unformatted file.

10.6 MASS BALANCE SUMMARY

It is convenient to have the mass balance at each time step summarized in a separate table. At each time step the program writes a record to UNIT 17 including the time step number, elapsed simulation time, time step and mass balances for pressure, heat, brine, unleached nuclide, leached but not dissolved nuclide, dissolved nuclide and nuclide in the matrix subsystem. The output is controlled by LMBAL on record M-2.

10.7 HETEROGENEOUS RESERVOIR SPECIFICATION

The heterogeneous reservoir specifications allows for a separate file to control the hydraulic parameters and grid definition otherwise input on record R1-21. The heterogeneous reservoir file in a binary file which contains the block-by-block values of hydraulic conductivity, porosity, depth, thickness and heat capacity. This option is preferred over the record-based R1-21 for situations in which values vary from block to block. The R1-21 is best suited for zonal-based applications.

The heterogeneous reservoir file can be created through contouring or Kriging of site data. This file is substantially more compact than using the formatted R1-21 style which can reach several megabytes. Furthermore, the file is stored separately thus allowing easier editing of the primary data input file.

The heterogeneous reservoir option is invoked by entering a negative value (i.e., -1) for I1 in the R1-21 record. The code then requests the file name containing the heterogeneous reservoir data. The contents of this file are:

<u>Record Type 1</u>

Version [Character *12] "VERSION 2.54"

Record Type 2

ICONST [Interger *8]

followed by:

VALUE [Real *8] if ICONST=0

or

ARRAY(NB) [Real *8] if ICONST=1

There is one Record Type 1 and seven Record Type 2 sets for the following arrays:

KX (M), M = 1, NB /x-Hydraulic conductivity
KY (M), M = 1, NB /y-Hydraulic conductivity
KZ (M), M = 1, NB /z-Hydraulic conductivity
PHI (M), M = 1, NB /Porosity
UH (M), M = 1, NB /Depth (positive downwards)
UTH (M), M = 1, NB /Block Thickness
UCPR (M), M = 1, NB/Heat capacity

There is no error checking on the length or contents of the arrays. While this provides a convenient means to include heterogeneity, the user should verify the contents of the binary file (i.e., KOUT=0, M-3; IIPRT = 12, R2-13). The use of a window option is recommended (M-3 and R2-16).

10.8 NUCLIDE MONITOR BLOCK

The radionuclide concentration at selected block (see Section 7) are written to UNIT 9 at each time step for postprocessing. This provides a time series of the nuclide mass fraction. The calculated concentration values may, for example, be multiplied by the water mass flux rate leaving a particular block to obtain the nuclide mass discharge rate. This would be appropriate for risk assessment or possibly evaluating the performance of a remediation strategy.

The format of the nuclide monitor file is one record for the elapsed time followed by one record for each nuclide at each time step. In the case of multiple components, the concentrations follow sequentially on the record starting with component number 1. The format for each record is:

TIME

I(1), DI(1), DI(2,), (CC(J), J=1, NDSC)

where:

TIME is the elapsed simulation time (G11.4)

I is the component (I3)

DI() is component label (2A4)

CC(J) is the concentration mass fraction (G11.4).

10.9 AQUIFER INFLUENCE SUMMARY

The values of flux of water, heat and brine at aquifer influence function boundary blocks are written to UNIT 18. This facilitates post processing of boundary fluxes where the user has specified prescribed values for the pressure (at elevation), temperature and brine. The output is controlled by parameter LAIF on Record M-2. At each time step the values of flux are written to the file. Auxiliary programs or spreadsheets may be used to integrate or sum the data.

The output file is in ASCII. A header record is written followed by the transient data. The format of the header record is:

Record	Format	Variables
1	A80	TITLEIT(I), I = 1, 80
2	A80	TITLEIT(I), I = 81, 160
3	4I5, 4E10.3	JABL, I, J, K, VABB(JABL) PIN(JABL), TIN(JABL), CIN(JABL) (Total of NABL records)
4	E10.3	TIME
5	10E10.3	QWSW(L), QHSW(L), QGIS(L), (CC(L+I) *QWSW(L), I=1, NCP) (Total of NABL records)

Note: Records 4 and 5 are repeated for each time step. The CC array is printed only if radionuclides are present. The term QWSW*CC is the mass flux of radionuclide, i.e., lb/day of water times radionuclide mass fraction concentration.

11 CONSIDERATIONS FOR EFFICIENT MODEL USAGE

This chapter is intended for both expert and non-expert model users alike. Section 11.1 contains suggestions for creating conceptual and mathematical models that adequately represent the subject site. Section 11.2 contains suggestions for avoiding hardware and software problems. Many of the suggestions in this chapter are general in nature and may seem obvious, but experience shows that even experienced modelers make basic errors at times. This chapter will also help those new to the SWIFT model troubleshoot errors.

11.1 CREATING AND DEBUGGING SWIFT MODELS

1. The conceptual model must include sufficient details of the field in order to adequately represent the real world system. A model (conceptual and mathematical) is inherently a simplification of reality. The degree to which a model adequately represents the physical system depends on the level of detail incorporated into the model.

2. Adequate vertical and horizontal discretization should be provided. This point cannot be stressed enough. This is one of the most common model usage errors because of the number of factors tied to grid discretization. Grid discretization should be based on the model application, not on available hardware. Grids that are too coarse may result in odd-looking (diamond-shaped) contours. These grid orientation effects can occur when the ratio of increments, i.e., length-to-width exceeds 10. Grids should also be graded smoothly in which the length increases by no more than a factor of 2 in any direction from one block to the next. Poor discretization also results in slow execution and/or simulation termination. This is because discretization directly effects the values that are used for dispersion and other coefficients in the model. Grid dimensions are provided on records R1-17, 18, 19.

3. The model user should include reasonable time steps recognizing the Courant number. This consideration is almost as important as grid design. Unreasonably large time steps may cause the model to perform many non-linear iterations or to "blow up". Also note that excessively small time steps may cause misleading mass balance calculations. At early time steps, there may be insufficient boundary fluxes which result in poor mass balance results. Time stepping information is entered on records R2-12. To check the values, specify IIPRT = 12 on R2-13.

4. The model user should use reasonable Peclet numbers for transport simulations. If the Peclet number (grid dimension/dispersion coefficient) is too large, the model will oscillate when using centered-in-space (R2-2). A large Peclet number will also unrealistically smear the spread of the concentration via numerical dispersion when using backward-in-space. Based on truncation analysis of one-dimensional systems, Peclet numbers greater than 4 may cause problems. However, a value of 10 or more is sometimes acceptable for multidimensional problems. The dimensions are provided in records R1-17, 18, 19. Dispersion coefficients are provided on record R1-2, R1-2.5. Check the values by specifying IIPRT = 12 on R2-13.

5. Accurate calibration should be performed. This is one of the most important aspects of model development, but continues to be overlooked by model users. Without sensitivity analyses demonstrating model results vs. observed data, predictive simulation are questionable.

6. Odd-looking results may indicate flaws in the system conceptualization, the application of model input or postprocessing. This includes stray contours, wavy-looking contours and diamond shaped contours in grids that are fairly well discretized. Make sure that all input data (especially R1-21) and grid conversions (Chapter 13) are correctly applied.

7. Wells should not be placed in zero pore volume blocks. This is a fairly harmless common error. Error codes are written to the output and are discussed in Appendix F. Zero pore volume blocks are entered in the R1-26 records. Well rates and locations are entered in the R2-6 and the R2-7 records, respectively.

8. Long term-simulations with weak regional groundwater gradients require special attention. If a long-term (5,000 - 10,000 year) simulation is performed, one may notice that, for certain geologic structures, the gradient will tend to dissipate. The gradient may not be maintained during a transient flow simulation when INAT (I-1 Record) is utilized. If this occurs, one may need to apply the regional gradient upon the modeled area by using: (1) a combination of perimeter injection and pumping wells (R2-6 & R2-7), or (2) pressure differential boundary conditions (R1-28).

9. If the model has an abnormal termination or "crashes", check the error codes written to the output file. These error codes are referenced in the Data Input Guide (Appendix F).

10. If the model application is small enough, use the direct solver. This will avoid all uncertainty associated with the iterative solver.

11. The model user should not casually use the default iteration and convergence parameters when using the indirect L2SOR solver (METHOD = ±2).

Convergence and mass balance should be monitored to check for correct application. Generally the solver requires a minimum of 3 or 5 iterations for variable density analysis. For steady-state water-table conditions, the number of outer iterations required is often between 10 and 20. When in doubt, print full diagnostics (KOUT = 0, IIPRT = 13, LMBAL = 1).

12. Labelling input data records in columns 71-80 should be utilized in order to improve QA, communication and transferability. Also, unused fields can also be used to enter comments and rationale for input parameters. For example, boundary conditions and perimeter wells can be identified to reduce confusion.

11.2 HARDWARE AND SOFTWARE CONSIDERATIONS

1. SWIFT for Windows is NOT written in ANSI standard FORTRAN. The majority of the code is ANSI compatible, but many of the I/O routines are not. If one modifies the code, it may not behave correctly in every instance. More importantly, if one modifies the code, these changes are NOT supported by HSI GeoTrans. Also note that the only compiler supported for use with SWIFT for Windows is the Lahey 95 FORTRAN compiler. Other compilers may not work without substantial conversion.

2. Provide adequate hardware for the model that you are running. It is always a good idea to have as much RAM as possible on a machine that is running simulations. The RAM requirements for each SWIFT simulation are printed by the code. If one doesn't have sufficient RAM available and have disk paging enabled, the model will run, but data will be written to the hard disk. This slows model execution considerably as the hard disk is much slower than RAM chips are. The use of a fast processor (P233, 266, 300 450 or better) is also recommended. This version of SWIFT is optimized for use on the Intel Pentium II or III, and runs best on it.

3. Array sizes must be realistically represented. Failure to dimension the array sizes in MAIN.FOR will result in abnormal model termination. The arrays should be dimensioned slightly larger than required by the problem.If not, the model may provide unreasonable results and eventually "bomb". The necessary array sizes are printed to the output file. Therefore, one may check the output file and edit the array sizes in MAIN.FOR accordingly. Please note that there are four primary arrays and each must be the correct size. Suggested sizes for 32, 64, 128 MB computers are included in MAIN.FOR.

12 SPECIAL TOPICS

In this chapter, special topics on input variables for SWIFT are discussed. For example, the definitions of permeability and compressibility are not always familiar to many hydrogeologists. These and other topics are briefly discussed to aid users in addressing the overlapping jargon of hydrogeologists and reservoir engineers.

12.1 CONVERSION OF COMPRESSIBILITY

Using nomenclature from the SWIFT model, the capacity of a geologic formation results from the compressibility of water, c_w, and the rock compressibility, c_r or total compressibility, c_t. These parameters may be combined with the formation porosity, ϕ; water density, ρ; formation thickness, b; and the gravitational constant, g/g_c to form the storativity, S as follows:

$$S = \rho\phi\,(c_w + c_r)b\,\frac{g}{g_c}$$

$$= \rho\phi(c_w + c_r)b\left(\frac{1}{144}\right) = \rho\phi\,(c_t)b\left(\frac{1}{144}\right)$$

where the English units are:

S = dimensionless

ρ = [lb/ft^3]

ϕ = dimensionless

c_w = [psi^{-1}]

c_r = [psi^{-1}]

c_t = [psi^{-1}]

b = [ft]

g = [ft/sec^2] 32.2 (approximately)

g_c = [ft-lbm/lbf - sec^2] 32.2

Hydrogeologists typically define storativity in terms of the fluid compressibility, β, and the compressibility of the porous media, α, as follows:

$$S = \rho\phi\ (\alpha/\phi + \beta)\ b\ \frac{g}{g_c}$$

in which terms are related by

$\alpha = \phi\ C_r$

$\beta = C_w$

Exceptions to the above include J. Bear (1992) and DeWiest (1966). Note the differences and avoid confusing conventions.

Thus, if you know the storativity for an application and assume a value for water compressibility, the compressibility of rock can be calculated as:

$$C_r = (144\ S/b - \rho\phi C_w)/\rho\phi$$

12.2 CONVERSION OF PERMEABILITY UNITS

The SWIFT for Windows model requires input in the form of hydraulic conductivity. The code uses the reference condition (viscosity, and fluid density) and internally stores the permeability. It is convenient to convert formation permeability to hydraulic conductivity based on standard conditions of fresh water at ground surface conditions (fluid density equal to 62.4 lb/ft^3). The conversion factor used is:

2.7 ft/day per d

where d is darcy and md is millidarcy.

Under variable density conditions one needs to include the effects of fluid density and viscosity. A more appropriate conversion is:

$$K = k * 0.00274 * (sp.gr.) / \mu$$

where

k = permeability (md)
K = hydraulic conductivity (ft/day)
sp.gr. = specific gravity, and
μ = fluid viscosity (cp)

12.3 DEVELOPMENT OF PRESSURE AT DATUM

The SWIFT for Windows code uses the dependent variable pressure-at-elevation, or fluid pressure to calculate the groundwater flow under variable fluid density conditions. Intercell fluxes between adjacent finite-difference grid blocks are evaluated using the equations for the continuity of mass and Darcy's law for groundwater flow. The resulting partial differential equation is second order in space, wherein the intercell flow is defined by the harmonic mean to describe the flow transmissibility. This definition preserves mass flux and weights the intercell flows with the appropriate fluid density as well as the grid block dimensions, permeability and fluid viscosity.

Between two grid blocks, ground water flow is evaluated using the difference in the pressure at elevation (i.e., the difference in fluid pressure) and the difference in the block centroid elevation (i.e., the difference in elevation potential). Simply stated, the code evaluates the total potential difference, as composed of the fluid pressure and elevation potential.

The pressure at datum is a scheme to represent the equivalent total potential and can be defined in several ways. The datum plane is defined at a reference elevation, often taken as the ground surface or the top of the aquifer model. Pressure at elevation in each grid block is converted to a common basis, the datum plane, in order to create a display (i.e., isopleths of pressure or potentiometric surfaces) the potential field. The definition of pressure correction depends on the interpretation of the potential integral:

$$\Phi = gz + \int_{p}^{p_o} \left(\frac{dp}{\rho}\right)$$

Reference: (Freeze and Cherry, 1979, equation 2.9, page 20)

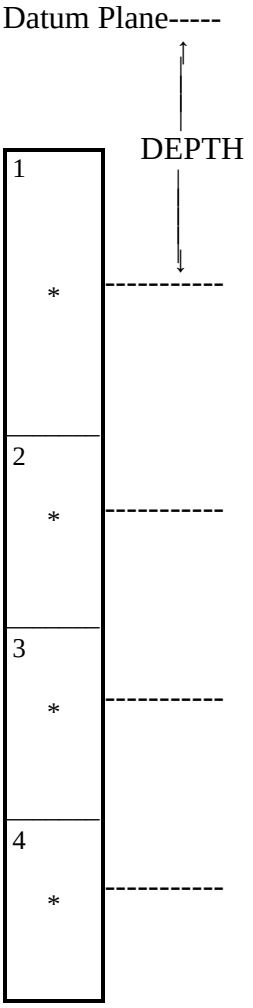
where:

Φ	=	fluid potential,
dp	=	fluid pressure derivative,
g	=	gravitation constant,
z	=	elevation,
ρ	=	fluid (water) density,
p	=	fluid pressure, and
p_o	=	reference pressure.

The first term is the elevation potential and the second is the fluid pressure recognizing that there is work involved in raising the fluid pressure from $p = p_o$ to $p = p$. In the SWIFT for Windows model, the integral is defined by examining the columns of blocks and performing the integral as a summation using the block under consideration and all of the overlying grid blocks.

The following figures detail these methods of calculating the pressure.

PRESSURE AT DATUM CALCULATION



$$Pd_4 = p_4 + \rho_o \cdot g \cdot DEPTH$$

$$+ \tfrac{1}{2}(\rho_1+\rho_2)\cdot g \cdot \tfrac{1}{2}(\Delta Z_1+\Delta Z_2)$$

$$+ \tfrac{1}{2}(\rho_2+\rho_3)\cdot g \cdot \tfrac{1}{2}(\Delta Z_2+\Delta Z_3)$$

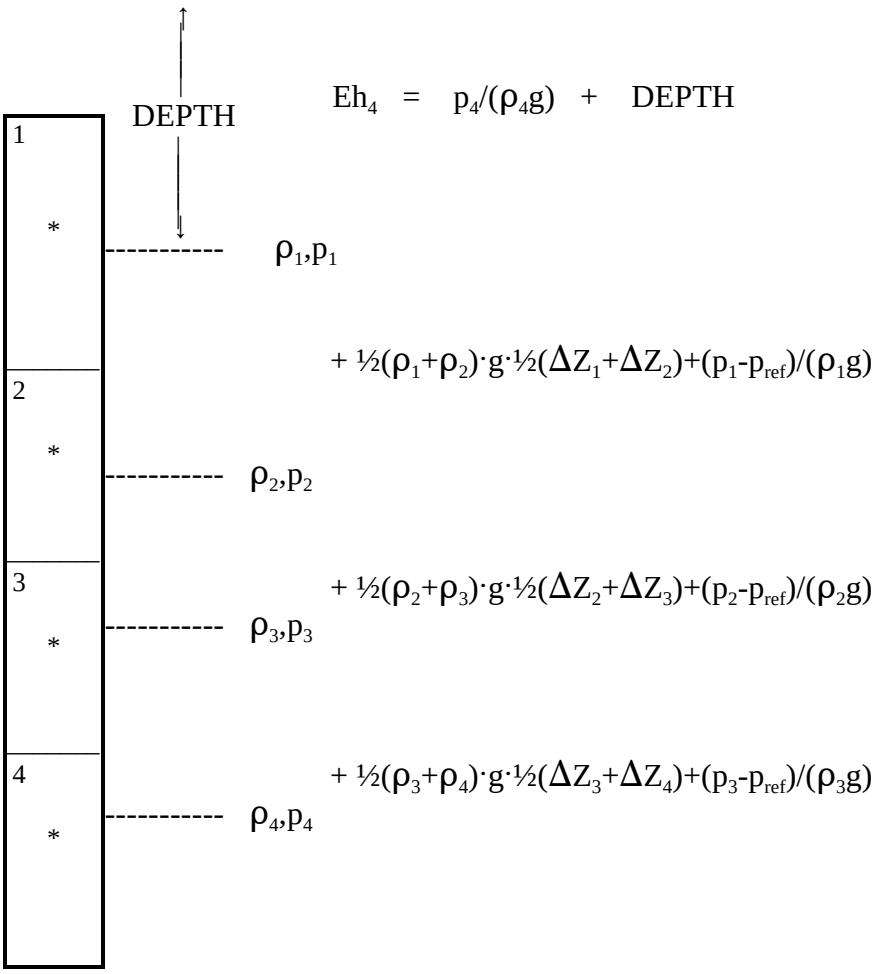
$$+ \tfrac{1}{2}(\rho_3+\rho_4)\cdot g \cdot \tfrac{1}{2}(\Delta Z_3+\Delta Z_4)$$

$$Pd_i = \sum_{k=i}^{NZ} [\![\ 1/4(\rho_k+\rho_{k-1})g(\Delta Z_i+\Delta Z_{i-1})]\!]$$
$$+ \ \rho_o\ g\ DEPTH \ + \ p_i$$

where:

ρ_o	Reference fluid (water) density,
ρ_i	Fluid (water) density of block i,
p_i	Pressure at elevation (fluid only) of block i,
ΔZ_i	Vertical grid block size of block i,
Pd_i	Pressure at datum (total) of block i,
g	Gravitational constant, and
DEPTH	Distance from datum plane to centroid elevation of layer 1 (top most) grid block, and
*	Centroid of grid block.

ENVIRONMENTAL HEAD CALCULATION

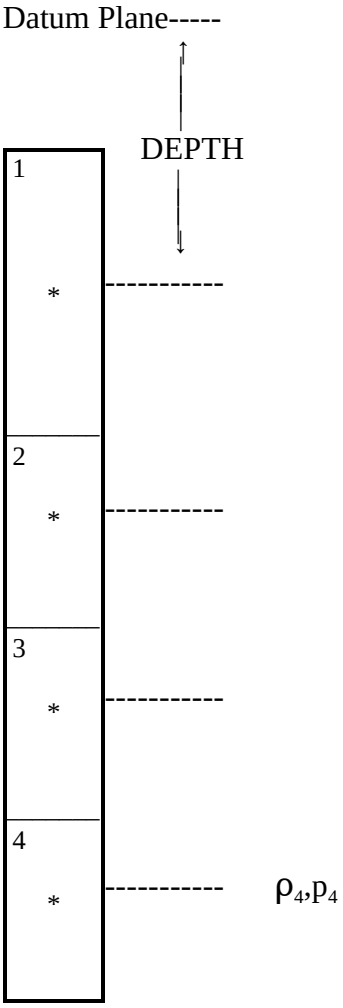


$$Eh_i = \sum_{k=i}^{NZ} [\![\ 1/4(\rho_k+\rho_{k-1})g(\Delta Z_i+\Delta Z_{i-1})]\!] + DEPTH + (p_i - p_{ref})/(\rho_i\, g)$$

where:

ρ_o	Reference fluid (water) density,
ρ_i	Fluid (water) density of block i,
p_i	Pressure at elevation (fluid only) of block i,
p_{ref}	Reference pressure (14.7 psi or 101325 Pa),
ΔZ_i	Vertical grid block size of block i,
Eh_i	Environmental head of block i,
g	Gravitational constant, and
DEPTH	Distance from datum plane to centroid elevation of layer 1 (top most) grid block, and
*	Centroid of grid block.

FRESHWATER HEAD CALCULATION



$$Fw_i = \left(\rho_i - \rho_{ref} \right) g \, DEPTH$$

where:

Fw_i	Freshwater head at block i,
ρ_{ref}	Reference freshwater fluid density (62.4 lb/ft^3, or 1000 Kg/m^3),
p_{ref}	Reference pressure (14.7 psi or 101325 Pa),
DEPTH	Distance from datum plane to centroid elevation of layer 1 (top most) grid block, and
*	Centroid of grid block.

12.4 MASS FRACTION VS DENSITY VS SPECIFIC GRAVITY

The relation between mass fraction *vs* fluid density *vs* specific gravity if often misunderstood. The relationship between specific gravity and fluid density is linear. Mass fraction used in SWIFT is almost, but not quite linear. Thus care should be taken in examining the results from simulations using SWIFT.

The definition of mass fraction is:

mass of brine divided by mass of water

where:

"water" is a fluid with the density defined by "BWRN".
Often this is the formation fluid, but more importantly this is the density where C = 0.0

"brine" is a fluid with the density defined by "BWRI".
For most injection well models, we define brine as the injectate. By convention, this is the fluid where the mass fraction, C = 1.0

The SWIFT model solves for conservation of mass and the fluid density is allowed to vary linearly. The density is a linear function of pressure (compressibility of water), temperature (coefficient of thermal expansion) and chemical composition (as defined by the two fluid densities BWRN and BWRI).

On the next page is an example set of calculations, based on the above definition. Note that the middle specific gravity 1.08 = 1/2 (1.00 +1.16), the scaled mass fraction is 0.537, not 0.500.

SPECIFIC GRAVITY	DENSITY AT 170 DEGREES	POUNDS SALT INJECTED	MASS FRACTION	SCALED FRACTION
1.00	61.00	0.00	0.0000	0.0000
1.01	61.61	0.61	0.0099	0.0718
1.02	62.22	1.22	0.0196	0.1422
1.03	62.83	1.83	0.0291	0.2112
1.04	63.44	2.44	0.0385	0.2788
1.05	64.05	3.05	0.0476	0.3452
1.06	64.66	3.66	0.0566	0.4104
1.07	65.27	4.27	0.0654	0.4743
1.08	65.88	4.88	0.0741	0.5370
1.09	66.49	5.49	0.0826	0.5986
1.10	67.10	6.10	0.0909	0.6591
1.11	67.71	6.71	0.0991	0.7185
1.12	68.32	7.32	0.1071	0.7768
1.13	68.93	7.93	0.1150	0.8341
1.14	69.54	8.54	0.1228	0.8904
1.15	70.15	9.15	0.1304	0.9457
1.16	70.76	9.76	0.1379	1.0000

13 UNSWIFT POSTPROCESSING

The UNSWIFT program written by HSI GeoTrans converts map files (UNIT 13) to regularly-spaced grid for SURFER® using bilinear interpolation in order to create contour plots. SURFER® is a registered trademark of Golden Software, Inc.

The UNSWIFT program is written in FORTRAN 77 and is currently operational on a Pentium Win 95/98 PC using the Lahey LF90, Version 4.5 compiler. The program can read pressure, temperature, brine or nuclide concentration data from a SWIFT map, and prepare a grid file compatible with SURFER®.

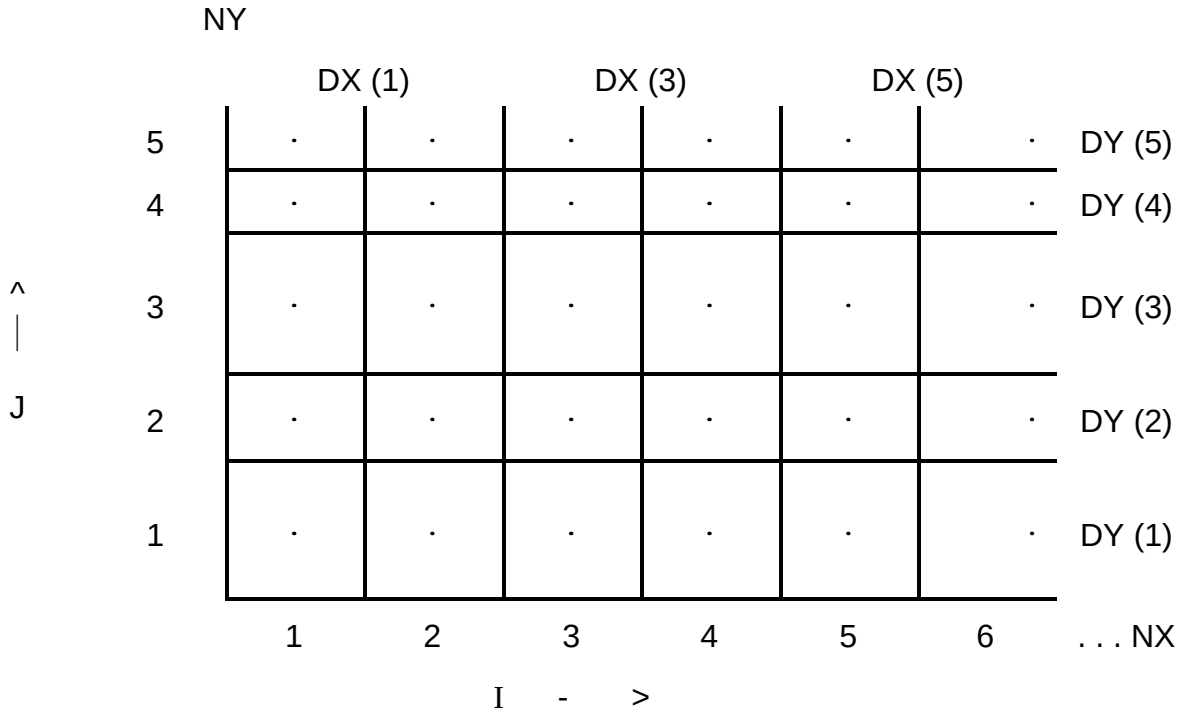
13.1 OVERVIEW

SWIFT for Windows produces results for block-centered, variably-spaced finite difference grids. Plotting software such as SURFER® however, work with uniformly-spaced, node-centered grids in order to contour given data. Therefore, without UNSWIFT, results from SWIFT would have to be read as "randomly-distributed" data for contouring.

Gridding randomly-distributed data is time-consuming and may introduce error. While the distribution pattern of the data points is regular and known, it cannot used by SURFER®. UNSWIFT converts this "regular" data from the model to the contouring package using bilinear interpolation. Note that it is not guaranteed to work in all situations. Sometimes, head or concentration results from a model require a more sophisticated interpolation approach.

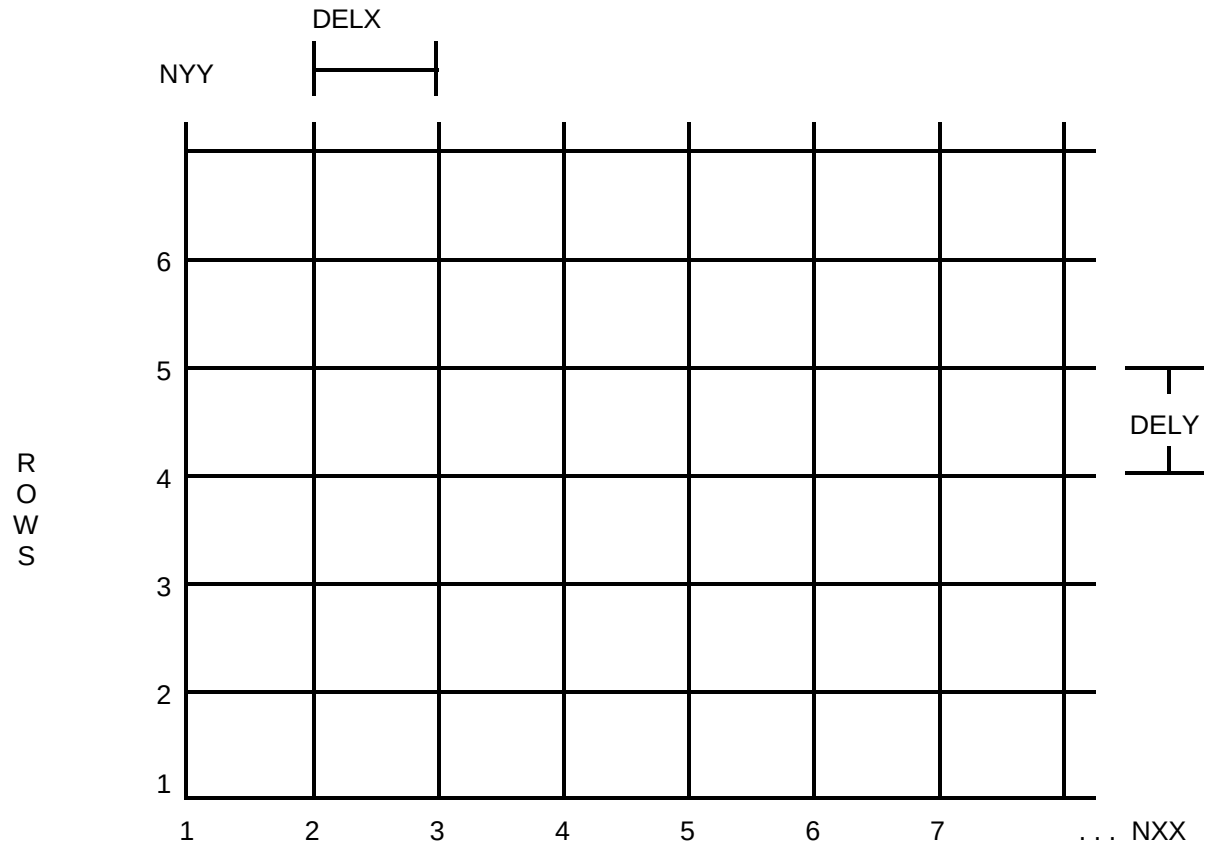
Thus, UNSWIFT provides a convenient and accurate means to prepare contour plots by preserving the lattice nature of the map data. This is done expediently and without the introduction of erroneous contours.

An example of a SWIFT grid for a layer is shown below.



Values are calculated at block centers. The grid increments are nonuniform.

UNSWIFT converts array data from the above grid to the one shown below.

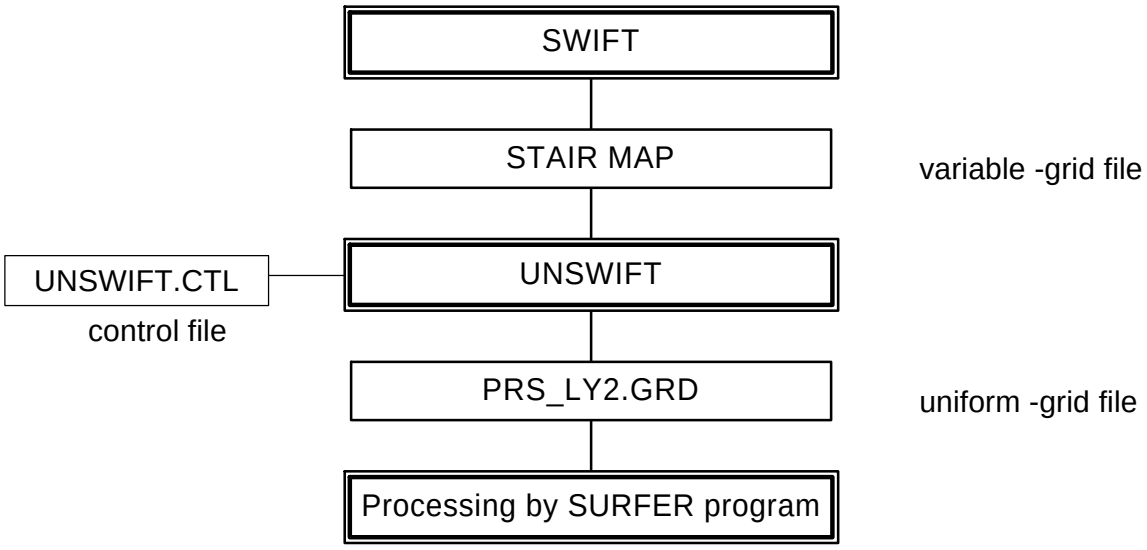


Note the changes in coordinate system and the node-centered data on the resulting grid.

The outer boundary of the resulting grid should be within the original grid, as UNSWIFT does not extrapolate beyond one grid cell. A bilinear interpolation technique is used to convert the data.

13.2 OPERATION

The operation of UNSWIFT is illustrated below.



STAIR.MAP is an unformatted map file generated by SWIFT. The map writing option is invoked by setting MAP > 0 in R2-13. UNSWIFT.CTL is a control file for UNSWIFT which contains information necessary for the conversion of SWIFT data. PRS_LY2.GRD is the uniform grid file generated by UNSWIFT which is ready for contouring. The uniform grid file can be in formatted or binary form.

For a typical problem with SWIFT, the control file will remain the same. The map file STAIR.MAP will change with each run. The map file may contain data for many stress periods, time steps, and layers. UNSWIFT lets one look at each array interactively and process only those needed for gridding.

13.3 INPUT DATA GUIDE FOR THE CONTROL FILE

Each record in the input data file is preceded by a record header line containing the names of variables for that record. The variable names are placed in the header line aligned with the columns where the input data is expected for the variable. For illustration, header line and sample data are shown below for Record 2.

NX NY ICODE IDEBUG<)))FMTGRD)))))))))))))))) Record 2

19 51 0 1(8G10.0)

NOTE: DO NOT DELETE THE HEADER LINES IN THE CONTROL FILE!

The following records are to be used to create the UNSWIFT control file.

RECORD 1: TITLE RECORD (A60, A10)

Title record is only for documenting the control file. It is ignored by UNSWIFT.

Col

1-60: TITLE: Problem title.

61-70: FILEC: Name of this control file. As a convention, use CTL as the type name for control files (eg. UNSWIFT.CTL).

RECORD 2: INPUT GRID SIZE, FORMAT OPTIONS (4I10, A20)

Col

1-10: NX: Number of columns dimensioned in SWIFT.
Maximum allowed is 250.

11-20: NY: Number of rows dimensioned in SWIFT.
Maximum allowed is 250.

21-30: ICODE: 0 = Variable to uniform translation (SWIFT to SURFER).
[Common Usage]
1 = Uniform to variable translation (SURFER to SWIFT).

31-40: IDEBUG: 0 = No action
1 = Create extra output to check control file input.

41-60: FMTGRD: Format for the DELR, DELC grid spacing given in Records 8 and 9. Example: **(8E10.0)**. If the List-Directed option is used to input R1-17, 18 or 19, then a ***** can be used for FMTGRD and portions of the SWIFT input file can be used directly.

RECORD 3: VARIABLY-SPACED GRID PARAMETERS (I10, A30, I10, 2G10.0)

Col

1-10: IFMTH: Type of file:
0 = binary
1 = formatted (as per FMTH, see cols 11-40 of this record).

11-40: FMTH: Format of the variably-spaced file. Example:'**(8E12.3)**'. If IFMTH=0, leave blank.

41-50: ILOG: Log (base 10) transformation of variably-spaced data.
0 = no transformation.
1 = yes, perform transformation.
The log transformation is appropriate for concentration plots with data ranging in many orders.

51-60: HCUT: Lower cut-off or truncation value for variably-spaced data. In the same units as head or concentration.

61-70: IGRID: Option to create finite difference grid using SURFER.bln format.
0 = No, do not create a grid file
1 = Yes, do create a grid. The program will prompt for the file name. Usually this option is only necessary for the first execution of UNSWIFT. For production runs, set IGRID=0.

RECORD 4: UNIFORMLY-SPACED GRID PARAMETERS (I10, A30)

Col

1-10: IFMTZ: File format:
0 = binary (only SURFER)
1 = formatted (as per FMTZ, see cols. 21-40 of this record).

11-40: FMTZ: Format for the uniformly-gridded file. Example: **(8E10.3)**.
If IFMTZ=0, leave blank.

RECORD 5: WINDOW OPTION (4I10)

Specify all the parameters. Enter a blank or a zero for IL, IR, IT, IB if window option is not used.

Col

1-10: IL: Column index of left-most column of window. Use the consistent convention of the SWIFT data. The default is a top-left origin. For Cartesian simulations, the SWIFT model can be set with either top-left or bottom-left for the X-Y plane. The output from SWIFT is controlled by PRT (Record M-3). Because

the window can be a X-Y, X-Z or Y-Z grid, the input options offers significant flexibility.

21-30: IR: Column index of right-most column of window.

31-40: IT: Row index of top-most row of window.

41-50: IB: Row index of bottom-most row of window.

Note: To invert the grid from top-left origin to bottom-left origin, enter a negative value for IB.

RECORD 6: UNIFORM GRID DESIGN (2I10, 4E10.0)

Col

1-10: NXX: Number of columns of the uniform mesh. Note that the mesh is node-centered.

11-20: NYY: Number of rows of the uniform mesh.

21-30: DELX: Grid spacing along x-direction in distance units.

31-40: DELY: Grid spacing along y-direction in distance units.

41-50: X0: Offset in the x-direction for the origin of uniform mesh. Origin is at lower-left corner.

51-60: Y0: Offset in the y-direction. Origin is at lower-left corner.

For example, the total x-distance of a model is 5000 ft, and the total y-distance is 4000 ft.

DELX is equal to 5000/(NXX-1), and likewise
DELY is equal to 4000/(NYY-1).

RECORD 7: NO-FLOW AND DRY CELL CODING (2E10.0)

SWIFT for Windows has special values meaning no-flow and dry cells.

Col

1-10: HNOFLO: Head value which stands for a zero pore volume block, no-flow cell or a cell outside the model boundary. For SWIFT for Windows, enter -9999.0.

11-20: HDRY: Coding scheme the model uses to specify cells that are desaturated during simulation. For SWIFT for Windows, enter 1.0D-30.

RECORD 8: MODEL GRID SPACING in X-DIRECTION (see FMTGRD on RECORD 1)

Provide the array DELC(NX) in the format specified in RECORD 2 parameter FMTGRD. For large grids, one may just want to transfer the grid spacing from the model input data. The parameter FMTGRD provides a flexible way of reading this data. For an areal x-y system, the DELC() corresponds to the x-grid spacing DELX() on Record R1-17 for SWIFT. Similarly the DELR() below corresponds the DELY() on Record R1-18. For Y-Z, the DELC() would correspond to DELY() and DELR() on Record 9 would correspond to DELZ().

RECORD 9: MODEL GRID SPACING in Y-DIRECTION (see FMTGRD on RECORD 1)

Similar to Record 8, provide the array DELR(NY).

13.4 RUNNING UNSWIFT

The code UNSWIFT is available for the Lahey 90 compiler. Listed below are the steps to translate a variable-spaced grid (SWIFT) to a uniformly-spaced grid (SURFER®).

1. Prepare data input such that SWIFT produces map files at the appropriate times. This would include setting MAP > 0 and KMP13 = 0. The SWIFT problem should then be run. The results will be placed in a .MAP file. Note that SWIFT can produce maps for as many time steps as are necessary. Also one can create different maps from previously created restart files.

2. Prepare a control file for UNSWIFT. Start with a copy of the supplied sample control file. Copy this sample file to one's control file by typing

   COPY SAMPLE.CTL yourfile.CTL

3. Modify the control file as per the input data instruction in this manual. Using the convention illustrated in this manual and the input data guide, prepare the control data file for UNSWIFT.

   3.1 Specify ICODE=0 for translating from SWIFT to SURFER.

   3.2 Determine whether the window option will be used. Determine the size of the input window in distance units.

   3.3 Utilize the grid spacing in the SWIFT input data file (R1-16 - 18) for Records 8 and 9 in the control file. Make sure that the record headers are still present. The input for SWIFT is list-directed.

   3.4 Maximum X and Y distance is obtained by summing the grid input for SWIFT (Records 8 & 9 in UNSWIFT.) Use these numbers (if the window

option is not specified) to design NXX and DELX. Similar steps should be followed for NYY and DELY.

3.5 IFMTH can be 0 or 1, as SWIFT 2.54 prepares only either formatted or binary map files. If a grid file from SWIFT output has been prepared, set IFMTH = 1, and supply a format string under FTMH.

3.6 IFMTZ should be left as zero, as it is the most efficient way of sending data to SURFER®. If it is necessary to inspect and edit certain array data, set IFMTZ=1 and supply a format such as **(8G12.5)** under FTMZ in Record 4.

3.7 If one is overlaying the contour line with a BLN file in SURFER, check the coordinate of the bottom-left corner of the BLN data. If it is non-zero, supply the (x,y) offset coordinates under X0 and Y0 in Record 6.

3.8 HNOFLO, HDRY, and HCUT have their origins from earlier versions of UNSWIFT for other finite-difference codes. Generally HNOFLO and HDRY are not used. Be careful with HCUT, especially if the pressure at datum extend into the negative range. Also avoid negative logs by setting HCUT to a small positive number when ILOG=1 (Record 3).

4. When running UNSWIFT (INTERACTIVELY), the user will be prompted for the control file name and the map file name. Upon successful reading of the control file, UNSWIFT proceeds to read the first header of the SWIFT map file. The example below shows typical inquiry by UNSWIFT:

```
F:\     UNSWIFT
        << UNSWIFT - Version 1.4 >>
              Control file name: UNSWIFT.CTL
        Variable grid input file: STAIR.MAP
        Time Step: 50   Time:  52.00  Data: HEAD
To process, enter uniform grid file name,
[Enter] to skip, or type END to stop: PRS_LY2.GRD
```

UNSWIFT reads the header record for each array in STAIR.MAP and displays it on the screen. The next prompt has three possible responses: (1) If you want to process the array, enter the name of the uniform grid file to be created, (2) if you want skip this array press **[Enter]** key, (3) if you want to terminate further reading of the map file and ignore this array, type **END**.

```
Time Step: 50   Time:  52.00  Data: CONC
To process, enter uniform grid file name,
      [Enter] to skip, or type END to stop: CON_LY2.GRD
```

5. RUNNING UNSWIFT IN BATCH: The version 1.3 of UNSWIFT accepts command line arguments which is convenient in running UNSWIFT through batch files. The example shown in step 4 may be run in batch by typing the following command:

UNSWIFT UNSWIFT.CTL STAIR.MAP PRS_LY2.GRD CON_LY2 END

The file names must be separated by a space character. The last parameter should be END to terminate processing the remaining arrays in the map file.

6. Execute SURFER® using the uniformly-spaced file created in the previous step as the input grid (eg. CON_LY2.GRD) file for contouring.

13.5 SOME COMMENTS ON CODE IMPLEMENTATION

1. This version must be compiled with the same compiler as that used for SWIFT. The Lahey LF95 compiler is required. This version is written specifically for operating on Pentium computers.

2. By default all non-ASCII files are "unformatted". A clever method is utilized in UNSWIFT by writing "unformatted direct access" file to appear like a "binary" file readable by SURFER®.

3. If problems arise in reading the binary map with UNSWIFT or reading the binary grid in SURFER®, change to ASCII format and examine the respective file contents for potential problems.

4. Note that the output file from UNSWIFT can be written in ASCII. This allows input into programs other than SURFER®, but note that the data have already been interpolated. Recontouring the data could produce misleading results depending on the method used. This is not true with SURFER® because the grid input file has been written in exactly the same format that SURFER® can read directly without recontouring. If one uses a different contouring package, the results should be checked against SURFER® output as this is the only package supported for use with UNSWIFT.

5. It is recommended that the window option be turned OFF initially so that the entire output may be checked.

6. List-directed input is recommended for use with UNSWIFT. This allows the grid dimensions to be imported directly from the SWIFT input file. This eliminates unnecessary input errors. To instruct UNSWIFT to use list-directed input, place an asterisk (*) in the first column of the FMTGRD input (Record 2, column 41).

7. Some confusion may arise over the design of the uniformly spaced grid. In order to determine the grid spacing, decide the number of grid blocks and divide the total axis distance by this number. Please note that the number of columns and rows (NXX and NYY) should be one more than the actual number of rows and columns. This is because the numbers that are being used are the number of grid lines not blocks. Please also note that the number of grid blocks in either direction should be sufficient to provide adequate resolution of your results.

8. While UNSWIFT can be used to map a relatively coarse SWIFT map onto a more refined SURFER® grid, use caution when interpreting the contours. For example, one can use the bilinear interpolation to UNSWIFT a 20 x 30 SWIFT map onto a 101 x 151 SURFER® grid. This will result in "smooth" contours, but may not properly reflect the trace model results. In general, the number of increments in the variable and uniform grid should be similar.

9. Great care should be taken in constructing the control file as an incorrect entry will produce misleading results.

10. The user should verify the times at which maps are produced by SWIFT. Make sure that the input data for SWIFT (R2-12, TCHG) specifies the correct time period for mapping. Producing a map at the incorrect elapsed simulation time will cause serious problems when interpreting the output data.

Table 13-1. Example Control File Listing.

```
Problem title ))))))))))))))))))))))))))))))))))))))))))))))))))))Q  File Name
card 1
SWIFT for Windows Sample test problem                          UNSWIFT.CTL
      NX       NY     ICODE    IDEBUG <))))Q FMTGRD ))))))))))))))))))Q   card 2
      39       29       0       1(8E10.0)
    IFMTH <)))))  FMTH ))))))))))))))))))Q     ILOG     HCUT     IGRID   card 3
      1(8E12.3)                        0       0       1
    IFMTZ <)))))  FMTZ ))))))))))))))))))Q                          card 4
      1(8E10.3)
      IL       IR       IT       IB                        card 5
      1       39        1       29
      NXX      NYY      DELX     DELY       X0       Y0           card 6
      51       31     219.0    240.0      0.0      0.0
    HNFLO     HDRY                                      card 7
     0.0      0.0
    DX(1)    DX(2)    DX(3)  ...  DX(i), i=1,NX                 card 8
     600.     600.     600.     600.     300.     300.     300.     300.
     300.     300.     300.     300.     150.     150.     150.     150.
     150.     150.     150.     150.     150.     150.     150.     150.
     150.     150.     150.     150.     150.     300.     300.     300.
     300.     300.     300.     300.     300.     600.     600.
    DY(1)    DY(2)    DY(3)  ...  DY(i), i=1,NY                 card 9
     600.     600.     400.     400.     200.     200.     200.     200.
     200.     200.     200.     200.     200.     200.     200.     200.
     200.     150.     150.     150.     150.     150.     150.     150.
     150.     200.     300.     400.     500.
```

14 STLINE PARTICLE TRACKING

14.1 INTRODUCTION

The STLINE streamline model provides an efficient and economical means of computing particle-movement trajectories, distances and times. The model uses a discrete steady-state velocity field or a series of velocity fields created from a previous flow simulation. After establishing initial particle locations, the program tracks the movement of individual particles through time. The trajectory (or streamline) of each particle may be displayed as a trace of discrete points as viewed in each of three orthogonal planes within an assumed Cartesian coordinate system. Any consistent set of units may be used.

The program is written with a flexible input format. Grid block dimensions, velocities and porosities are read as unformatted records from a previous flow simulation using SWIFT/486 (Reeves et al., 1986a and b; Ward et al., 1993).

14.2 STREAMLINE EQUATIONS

The grid is assumed to consist of a set of rectangular parallel pipes, or grid blocks, like the one shown in Figure 1. The SWIFT code calculates potentials at grid-block centers and then differences them to obtain interstitial fluid velocities at the grid-block edges. Thus, only the centers and edges of the individual cells are of concern. For particle tracking, however, intra-cell translations must be determined, and it is convenient to supplement the system, or global coordinates (X,Y,Z) with local grid-block coordinates (x,y,z) (see Figure 14.1).

Since velocities are known only at the grid-block edges, interpolation is used within individual cells. The program uses linear interpolation. Thus, for any local position (x,y,z), the x-component of velocity is given by

$$V_x = a_x + xb_x \tag{1}$$

where

$$a_x = V_{1x} \text{ and } b_x = (V_{2x} - V_{1x})/\Delta X \tag{2}$$

Here, and throughout this section, only relations for the x component are presented since comparable relations for the y and z components may be obtained easily by analogy. In Eqs. (1) and (2), V_{1x} and V_{2x} denote edge velocities and ΔX denotes a grid-block width, as shown in Figure 14.1.

The distance travelled (δx, δy, δz) in the time step δt may be determined analytically by integrating the equation

$$\delta t = \int_{x}^{x+\delta x} dx/V_x \tag{3}$$

for each coordinate. However, this yields exponential relations for the coordinate changes. Thus, it is more efficient to approximate the velocity by an average of the two end-point values, yielding

$$\delta x = \bar{V}_x \, \delta t \tag{4}$$

where

$$\bar{V}_x = a_x + b_x x + b_x \delta x/2 \tag{5}$$

Solving Eqs. (4) and (5) for Δx yields the result

$$\delta x = (a_x + b_x x) \, \delta t/(1 - b_x \delta t/2) \tag{6}$$

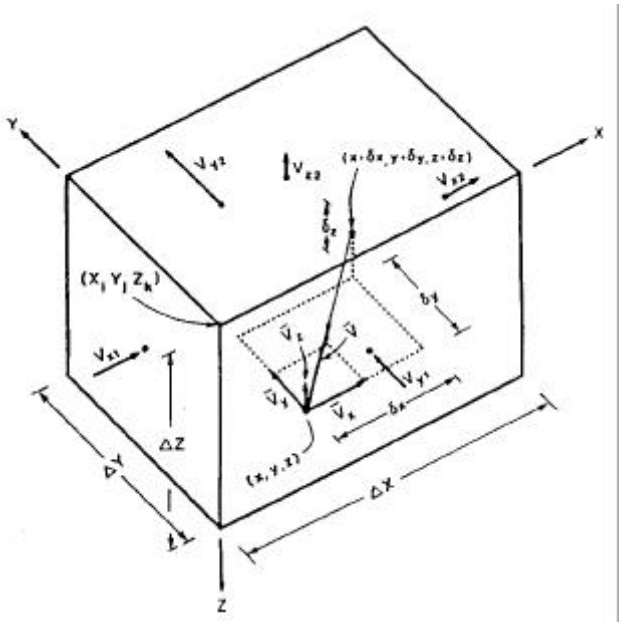
From the coordinate increments, as determined from equations of the form of Eq. (6), the incremental path length is obtained from

$$\delta s = (\delta x^2 + \delta y^2 + \delta z^2)^{1/2} \tag{7}$$

In applying Eq. (6) and its counterparts in the y and z directions, two inaccuracies can occur. One of them may be described as an inter-cell error, which results from a particle crossing a cell boundary. In such an event, the particle velocity is determined by extrapolation of Eqs. (1) and (2) for the source cell rather than using velocities appropriate for the receiver cell. To minimize such errors, it is necessary that

$$\delta x \ll \Delta x \quad \text{or} \quad \delta t \ll \Delta x/[V_x] \tag{8}$$

Figure 14-1. Intra-cell translation of a particle. The local coordinate system (x,y,z) for grid-block (I,J,K) is imbedded within a global system (X,Y,Z).



where the angle brackets denote the grid-cell average

$$[V_x] = (V_{1x} + V_{2x})/2 \tag{9}$$

The other error may be described as an intra-cell error resulting from the approximation of Eq. (4). There the error term of least order is given by

$$E(\delta x) \approx [V_x] (V_{2x} - V_{1x})^2 \delta t^3/12 \tag{10}$$

assuming a linear variation in velocities within the grid block. Both Eqs. (8) and (10) imply a limitation on the time step. Analytical application of these equations is somewhat difficult due to their grid-cell dependence and the uncertainty of the particle paths. Practical application of the error relations of Eqs. (7) and (9), however, may be implemented easily by making a very rough estimate of the time step from Eq. (8).

$$X_p^n = X_p^o + \sum_{i=1}^{n} \delta x_p^i \tag{11}$$

In order to determine particle trajectories and, hence, the streamlines of the flow field, the STLINE code accumulates global position coordinates for each particle using the increments as defined in Eq. (6). Adding a subscript to indicate particle identity and a superscript to indicate the time step, the resulting coordinate may be expressed as

$$S_p^n = \sum_{i=1}^{n} \delta s_p^i \tag{12}$$

with comparable relations for Y_p^n and Z_p^n. For each trajectory, the program also accumulates a global path length from the path length increments defined in Eq. (7):

14.3 COMPUTER IMPLEMENTATION

The STLINE program consists of a main program and several subroutines. The input consists of input/output control parameters; grid-structure values; flow information, i.e., Darcy velocities and porosities; initial particle positions; time-increment variables; and plotting specifications. The output consists of three-dimensional arrays of Darcy velocities, and porosities in one file and files of particle trajectories, or streamlines.

Initial particle locations (X_p^0, Y_p^n, Z_p^0) within the global grid system are specified in input record R11 (see next section) by real numbers of the form (I.i, J.j, K.k). Integers I, J and K denote the grid block, and the remaining fractions i, j, and k correspond to the fractional distance across that grid block in the x, y, and z directions, respectively. An example is the centroid of the first grid-block (1,1,1), which is specified with the coordinates (1.5, 1.5, 1.5).

The tracking of the individual particles as they move from their initial locations is accomplished by means of the five parameters TMAX, TOLXY, TOLZ, FRACDXY, and FRACDZ, which are input on record R5. These parameters determine the automatic time stepping for each particle with special attention for horizontal and vertical movement. The parameter TMAX is the total desired simulation time. Particles will be translated up to a value TMAX unless limited by the maximum number of time steps. The automatic time steps are controlled by the allowable fractional block distance. The parameters FRACDXY and FRACDZ define the fractional (i.e., distance normalized with respect to block increment dimension) movement desired. The fractional movement in turn is used to determine the desired time step. This scheme allows for automatic updating of the time step as a particle experiences changes in the velocity field from block to block. The code seeks to provide stability in Courant ratio ($V\delta t/\Delta X$).

Streamlines are calculated with individual time stepping. The time step is chosen based on the minimum travel time for horizontal (x or y) and vertical (z) directions. The control parameters FRACDXY and FRACDZ may be tuned to best fit a streamline. A zero value can be entered for FRACDZ in order to skip vertical projection calculations. This would be appropriate for many three-dimensional applications where horizontal translation control the time step criteria. In many hydrologic applications, FRACDXY will be most useful.

Streamlines which pass through perimeter or boundary grid blocks will be sensitive, of course, to the boundary velocities. Unfortunately, such velocities typically are not defined by block-centered finite-difference codes, for which STLINE has been designed. Consequently, option parameters IBCX, IBCY, and IBCZ have been provided in input record R6. These parameters permit one either to specify a no-flow boundary or to set the velocity to that of the adjacent block edge for each of the three coordinate directions i.e., if the flow model has a discharge boundary such as a river or prescribed head boundary.

Transient velocity fields may be used by creating a series of velocity records with SWIFT/486. Values are written to the file each time they are printed as controlled by variable IIPRT on Record R2-13 of the SWIFT/486 data file. The transient velocity fields are read (variable ITRANS, Record R2) and linear interpolation is used between epocs. If the first velocity is written at times other than zero, the first velocity field is held constant between time zero and when the first velocity is written. Thereafter interpolation between two velocity fields is performed.

The final topic to be discussed in this section is, appropriately, that of termination of the particle tracking. As indicated above, a maximum simulation time is specified within the input. However, the code is made more efficient by three additional termination criteria. Particle tracking is terminated whenever one (or more) of the following conditions is met:

1. The maximum allowable simulation time is exceeded;

2. The maximum number of allowable calculation time steps (ITMAX, Record R2) is exceeded;

3. All of the particles have exited from the flow field i.e., at a river or prescribed head boundary; and

4. The minimum bound, or tolerance (TOLXY or TOLZ, Record R5), on particle movement is reached by all of the particles.

An example of Item (3) is provided by the converging flow field of a production well in which all particles leave the system. An example of Item (4) is provided by the diverging flow field of an injection well. In the extremities of this field, interstitial velocities would be sufficiently small such that additional tracking of particles would be unnecessary. In addition to controlling the calculation as a whole, the tolerance conditions of Item (4) is also applied on a particle-by-particle basis. Thus, if the fractional movement, as defined in terms of grid block dimensions (i.e., $\delta x/\Delta X$), is less than that specified by the TOLXY or TOLZ variable for any particular particle, the particle is "frozen" in place, and further calculations are eliminated for that particle.

14.4 DATA FILES

The STLINE program requires:

1. Input data file to define the particle location and print options.

2. Velocity file from a previous SWIFT/486 simulation.

3. Screen input to define the above files.

The input data file is a set of records, created via a text editor. The individual records are defined in Section 14.4.1. The velocity file may contain one or more velocity fields from a flow simulation. The file format is binary or unformatted and the contents described in Section 14.4.2. In executing the STLINE program, the above mentioned file names are prompted for on the screen or may be entered directly on the command line, i.e.,

RUN77 STLINE INSTL SW_RUN1

where:

INSTL.DAT is the input data file for STLINE and

SW_RUN1.VL is the output velocity from the SWIFT/486 simulation using SW_RUN1.DAT.

The program optionally writes several files:

1. Output listing which echoes the input and provides tabular listings of particle locations.

2. SURFER® boundary line files where line segments are concatenated, one boundary line for each particle.

3. MODPATH pathline file, similar to boundary line file, but formatted the same as output created by MODPATH (Pollock, 1989). MODPATH is the pathline post processor for MODFLOW (McDonald and Harbaugh, 1988).

4. SURFER® posting file to allow posting of symbols or time display in conjunction with the boundary line file.

A summary of the files is presented in Table 14-1. Each file type is discussed in detail, followed by a sample problem.

14.4.1 INPUT DATA

The following data define the parameters used in the particle tracking program. This includes the control variables, the simulation option and initial particle location are defined. This is read from UNIT 5 and is an ASCII formatted file.

RECORD R1 (A65) *COMMENTS*

LIST: TITLE

TITLE One record of alphanumeric data for a title.

RECORD R2 (8I5) *CONTROL PARAMETERS*

LIST: NX, NY, NZ, NP, NTM, ITRANS, IDBUG, IREVS

NX, NY, NZ Number of grid blocks in x, y and z directions (col. 1-5, 6-10, 11-15).

NP Number of particles to be tracked (col. 16-20).

NTM Maximum number of time increments (col. 21-25).

ITRANS Index for transient velocity field input (col. 26-30):
0 = Steady-state velocity
1 = Transient velocity

IDBUG Index for diagnostic output control (col. 31-35):
0 = No printing
1 = Partial diagnostic
2 = Complete diagnostic

IREVS Control on direction of particle tracking (col. 36-40):
0 = Forward tracking
1 = Reverse tracking

Table 14-1. Data files, unit numbers, and file suffix.

UNIT	FUNCTION	FILE SUFFIX
*	Screen Display	---
5	Input File	.DAT
6	Output (80 col.) Listing	.OUT
7	SWIFT/486 Input Velocity (Binary)	.VL
8	SURFER® Boundary Line	.BLN
9	MODPATH Pathline	.TRK
10	SURFER® Posting Data	.DPS

RECORD R3 (12I5) *PRINT OPTIONS*

LIST: IDX, IVX, IVY, IVZ, IPHI, KPNT, ISUR, IELEV, KSUR, KPST, IMOD, KMOD

The print options include control parameter prefixed with I or K. The I indicates yes/no, i.e.,

0 = No print
1 = Print

The K indicates frequency where

0 or 1 = every time step
n = every n'th time step

IDX — Control parameters for printing (.OUT) the grid-block increment arrays DX, DY and DZ (col. 1-5).

IVX, IVY, IVZ — Control parameters for printing (.OUT) Darcy-velocity arrays UX, UY and UZ, (cols. 6-10, 11-15, 16-20), respectively.

IPHI — Control parameter for printing (.OUT) the porosity array PHI (col. 21-25).

KPNT — Frequency control parameter for printing (.OUT) particle locations at the end of each timestep (col. 26-30). [A zero or one means every time step]

ISUR — Control parameter for writing SURFER® boundary line file (.BLN) and posting file (.DPS) where (col. 31-35):
0 = No file
1 = X-Y coordinates are listed
2 = Y-Z coordinates are listed
3 = X-Z coordinates are listed

IELEV — Control parameter for SURFER® orientation where (col. 36-40):
0 = Z is elevation
1 = Z is in depth

KSUR — Frequency control for writing SURFER® boundary line (.BLN) records, i.e., write every KSUR'th timestep (col. 41-45). [A zero or one means every time step]

KPST — Frequency control for writing SURFER® posting (.DPS) records, i.e., write every KPST'th timestep (col. 46-50). [A zero or one means every time step]

IMOD Control parameter for writing MODPATH (.TRK) particle location file (col. 51-55).

KMOD Frequency control for writing MODPATH (.TRK) records, i.e., write every KMOD'th timestep (col. 56-60).

RECORD R4 (3E10.0) *INITIAL LOCATION*

LIST: (XI(I), YI(I), ZI(I), I = 1, NP)

XI, YI ZI Initial or starting particle coordinates (cols. 1-10, 11-20, 21-30).

NOTE: Particle locations are specified here as (I.i, J.j, K.k). Two examples of this notation are the following:

(1.5, 1.5, 1.5) is the centroid of block (1,1,1)
(1.0, 1.0, 1.0) is a top outside corner of the system

NOTE: A total of NP records are required here.

RECORD R5 (7E10.0) *TIME STEP CONTROL*

LIST: TMAX, TOLXY, TOLZ, FRACDXY, FRACDZ, TSCLSR, HDAT

TMAX Maximum simulation time limit (col. 1-10).

TOLXY Minimum tolerance of particle movement in the x or y direction (Default = 0.005). [Tolerance is defined as the smallest allowable coordinate change, relative to the local block dimension. To terminate calculations sooner, enter a larger value. To allow more or continued calculations enter a smaller value. In sink blocks, a particle may overshoot the "exit" if given an inappropriate value.] (col. 11-20).

TOLZ Minimum tolerance of particle movement in the z-direction (col. 21-30).

FRACDXY Fractional block distance (fraction of ΔX or ΔY) allowed in either the x or y direction per time increment (col. 31-40). [Values range from $1x10^{-20}$ to 0.5, typically 0.05]

FRACDZ Fractional block distance allowed (fraction of ΔZ) in the z-direction per time increment (col. 41-50). Enter a zero to force horizontal FRACDXY control. [Values range from $1x10^{-20}$ to 0.5, typically 0.05]

TSCLSR Scale factor for the printed values of time on output files (col. 51-60). [For example to list values in years, enter 0.0239 (1/365) to convert SWIFT output in days]

HDAT Value to override HDATUM in SWIFT velocity file (col. 61-70). Enter a zero to use the SWIFT value directly.

RECORD R6 (6I5) *BOUNDARY VELOCITY*

LIST: IBCX1, IBCX2, IBCY1, IBCY2, IBCZ1, IBCZ2

IBCX1, IBCX2, IBCY1, IBCY2, IBCZ1, IBCZ2 Control parameters for specifying boundary conditions on all sides of system in each coordinate direction (col. 1-5, 6-10, 11-15).

The following values apply to each parameter:

0 = Boundary velocities are set equal to zero
1 = Adjacent block velocities in the specified direction are used at the boundary edge

14.4.2 VELOCITY FILE

The velocity file from the execution of the SWIFT/486 code is an unformatted file containing the grid, the components of velocity and the value of time.

RECORD V1 (Unformatted) *VERSION*

LIST: NUM

NUM A 12-character string containing "Version 2.54"

RECORD V2 (Unformatted) *DATUM ELEVATION*

LIST: HDATUM

HDATUM Datum depth measured relative to reference plane (REAL*8, see SWIFT Record R1-16).

RECORD V3 (Unformatted) *GRID*

LIST: NXX, NYY, (DX(I), I=1, NXX), (DY(J), J=1, NYY)

NXX, NYY Number of grid blocks in x and y-directions (Integer*4).

DX, DY Arrays of grid-block increments for x and y coordinates (Real*8).

NOTE: The program checks to see that NXX = NX and NYY = NY

RECORD V4 (Unformatted) *DEPTH*

LIST: (H(M), M=1, NB)

H Depth to grid block center measured positively downward starting from top-most layer of blocks (Real*8).

NOTE: Indices M and NB represent the grid-block index and the number of grid blocks. The latter is defined in terms of the dimensions:

NB = NX*NY*NZ

The former is defined in terms of the indices (I,J,K) by

M = I + (J-1)*NX + (K-1)*NX*NY

RECORD V5 (Unformatted) *THICKNESS*

LIST: (DZ(M), M=1, NB)

DZ Saturated grid block thickness starting with top most layer (Real*8).

RECORD V6 (Unformatted) *PORE VOLUME*

LIST: (PHI(M), M=1, NB)

PHI Array of saturated grid-block pore volumes (Real*8).

NOTE: PHI = DX*DY*DZ*porosity*saturation, where saturation is the fractional water level elevation in a block.

RECORD V7 (Unformatted) *VELOCITY*

LIST: (UX(M), M=1, NB), (UY(M), M=1, NB), (UZ(M), M=1, NB)

UX, UY, UZ Darcy-velocity arrays (Real*8).

NOTE: According to the indexing convention UX(M) = UX (I,J,K) is the x-component of Darcy velocity at the interface between blocks (I-1,J,K) and (I,J,K). A similar convention holds for UY and UZ.

RECORD V8 (Unformatted) *PRESSURE*

LIST: (P(M), M=1, NB)

P Pressure at elevation (Real*8). This data is read in from SWIFT output but not used directly in particle travel calculations.

RECORD V9 (Unformatted) *FLUID DENSITY*

LIST: (BW(M), M=1, NB)

BW Fluid density (Read *8)

RECORD V10 (Unformatted) *TIME*

LIST: RDTIME

RDTIME Time at which preceding velocity file was calculated (Real*8). This has units of days for English, or seconds for metric. See SWIFT/486 input record IUNIT on Record M-2.

14.4.3 BOUNDARY LINE FILE

The boundary line file (with .BLN extension) format is designed for direct input into SURFER® as follows:

NPTSI	ZERO
X(1)	Y(1)
X(2)	Y(2)
X(3)	Y(3)

```
.                    .
.                    .
X(NPTS1)    Y(NPTS1)
NPTS2       ZERO
X(1)        Y(1)
X(2)        Y(2)
X(3)        Y(3)
.                    .
.                    .
X(NPTS2)    Y(NPTS2)
        etc.
```

where NPTS1 is the number of points to define the first particle (i.e., particle A). Zero has a value of 0. The second particle (i.e., particle B) follows directly. There is one set of paired vectors for each of the particles. Because STLINE is three-dimensional and SURFER® is two-dimensional, the user must select the orientation for the SURFER® boundary line file. On Record R3, variable ISUR in the STLINE input control file, the user identifies the orientation of slice as:

1 for X-Y plane,
2 for Y-Z plane,
3 for X-Z plane.

Also on Record R3, variable IELEV, the user selects the SURFER® orientation for Z as follows:

0 for elevation,
1 for depth.

14.4.4 PATHLINE FILE

The pathline file (with .TRK extension) for defined by MODPATH (Pollock, 1989) contains the following:

1. Particle index number, (col. 1-15)
2. Global coordinate in the x-direction, (col. 16-35)
3. Global coordinate in the y-direction, (col. 37-56)
4. Local coordinate in the z-direction within the cell, (col. 58-77)
5. Global coordinate in the z-direction, (col. 79-98)
6. Cumulative travel time, (col. 100-119)
7. J index of cell containing the point, (col 121-123)

8. I index of cell containing the point, (col 125-127)
9. K index of cell containing the point (col. 129-131).

The output is ASCII using the format (Fortran):

FORMAT (I15,1X,5(E20.12,1X),2(I3,1X),I3).

Note that in the MODPATH convention J refer the column or the x-direction in SWIFT and I refers to the y-direction. Other existing software used to present MODPATH output may then be used to display pathlines from STLINE.

14.4.5 POSTING FILE

The SURFER® posting file (with .DPS extension) is an ASCII file contains:

X(1)	Y(1)	T(1)	ALF(1)	P(1)
X(2)	Y(2)	T(2)	ALF(2)	P(2)
X(3)	Y(3)	T(3)	ALF(3)	P(3)
.		.	.	.
.		.	.	.
X(N)	Y(N)	T(N)	ALF(N)	P(N)

where: X( ) is the first ordinate,
Y( ) is the second ordinate,
T( ) is the elapsed travel time,
ALF( ) is the velocity vector angle, measured counterclockwise relative to the x-axis, and
P( ) is the one character identification, i.e., A, B, C etc.

There are N records depending on the number of time steps for each particle and the frequency of writing (Record R3, variable KPST on the control input file). It is recommended that the value of KPST be a multiple of KSUR. This would result in selecting posting of the symbol or value of time along each of the path lines.

14.5 VERIFICATION PROBLEM

In order to illustrate the use of the streamline program, the problem of an injection well in a uniform flow field is presented. The flow field is generated by a steady-state flow simulation using SWIFT/486, and then several streamlines are generated via the particle-tracking method of STLINE. In addition, a comparison is made between the numerical model and analytic results. The sample problem constitutes a verification of the SWIFT-STLINE combination.

14.5.1 DESCRIPTION OF THE PROBLEM

Two of the most important features of the problem of steady-state injection into a uniform flow field are: (1) the existence of a groundwater divide which separates aquifer fluid from injected fluid; and (2) the existence of a stagnation point. Figure 14-2 shows this point for the sample problem under consideration here. Also, the analytic streamline differs only insignificantly from the groundwater divide.

These two points may be examined more carefully by considering the analytic solution. Using the notation of Bear (1979, p. 367), this solution may be written in two different forms. First, the piezometric head is given by:

$$\phi = -q_o x/K - Q_w [\ln (x^2+y^2)]/4\pi KB \qquad (13)$$

and secondly, the stream function is given by:

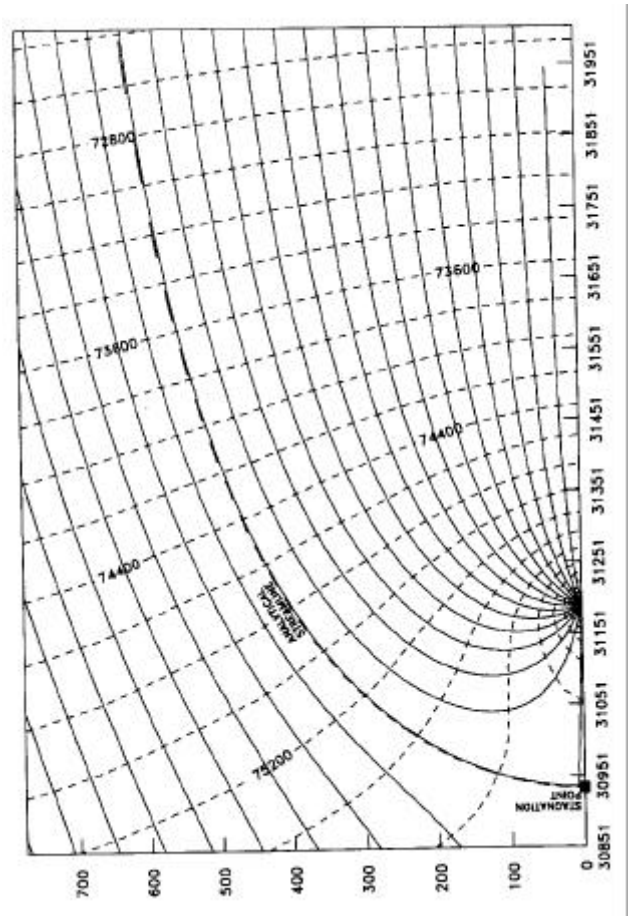
$$X = -q_o y/K - Q_w[\tan^{-1} (y/x)]/2\pi KB \qquad (14)$$

where:

ϕ = piezometric head,
X = stream function,
q_o = ambient Darcy velocity (specific discharge),
K = hydraulic conductivity,
B = aquifer thickness, and
Q_w = flow rate ($Q_w > 0$ for injection).

The second equation is more important because constant values of the stream function characterize different streamlines.

Figure 14-2. Analytic streamlines for an injection well in a uniform flow field.



The groundwater divide is defined by Eq. (14) with the conditions y 0 and $\tan^{-1}$ (y/x) π, as discussed by Bear (1972, p. 324). The resulting equation for the divide streamline is:

$$y = \pm|x| \tan (2\pi q_o By/Q_w) \quad (15)$$

where the signs denote the two branches for $y < 0$ and $y > 0$. This curve has the asymptotes:

$$y_z = \pm Q_w/2q_oB \quad (16)$$

The second noteworthy feature of the analysis is the existence of a stagnation point. Equation (15) is undefined for y=0. However, the abscissa of this point may be obtained through a limiting process, and is given by

$$x_s = Q_w/2\pi Bq_o \quad (17)$$

The point (x_s, 0) represents that point at which the flow diverges at right angles to the x axis. This is therefore a null point for which there is not flow, i.e., a point of stagnation.

14.5.2 INPUT DATA

The hydrological data for the sample problem is shown in Table 14-2. In addition, grid information is required by both SWIFT and STLINE. Fine gridding is used in the vicinity of the well in order to resolve numerically the logarithmic behavior of the fluid pressure, Eq. (13). Increments are chosen to vary from 5 m to 10,000 m in both x and y directions as they emanate from the well, as may be inferred from the limited region shown in Figure 14-3 and Table 14-3. Numerical streamlines are quite sensitive to the width of the system L_y. For the analytical model, an infinite system is used, whereas for the numerical model, a finite system is used of necessity. For comparison with analytic results, this width is:

$$L_y = 31{,}192 \text{ m} = 38.9\, y_z \quad (18)$$

Equation (18) shows the system width (for the numerical simulation) in terms of a fundamental unit of the physical system, namely the asymptote of the groundwater divide, Eq. (16).

The initial particle locations are specified in Card R4. As indicated, STLINE uses the representation M.m for definition of initial coordinates where M is the value of the block index I,

Table 14-2. Characteristic Parameters of the Aquifer and the Injection Well for the Sample Problem.

Parameter	Value
Ambient Darcy Velocity	1.5×10^{-8} m/s
Hydraulic Conductivity	4.0×10^{-6} m/s
Porosity	0.1
Aquifer Thickness	125 m
Injection Rate	1.5×10^{-3} m^3/s

Figure 14-3. Initial particle and well locations in SWIFT, STLINE, and well-centered coordinates systems. All distances are in meters.

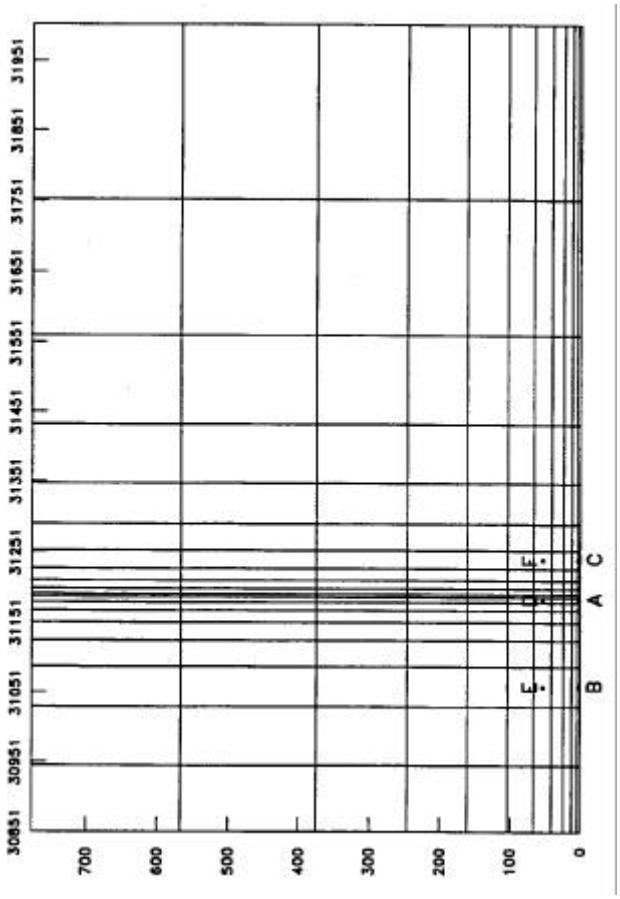


Table 14-3. Coordinates (meters) of Initial Particle Locations.

Point	SWIFT (X,Y)		STLINE (I.i, J.j)
A	31,183	2.5	20.5, 1.5
B	31,059	2.5	15.5, 1.5
C	31,240	2.5	25.5, 1.5
D	31,183	53.3	20.5, 5.5
E	31,059	53.3	15.5, 5.5
F	31,240	53.3	25.5, 5.5
WELL	31,189	0.0	21.5, 1.0

J, or K, and m is the fractional distance across the block, in the direction of increasing M. Initial locations are shown in Figure 14-3. They are also given in STLINE and SWIFT coordinates in Table 14-2.

14.5.3 RESULTS

Results of the sample problem are given in Figure 14-4. Six streamlines are shown using the SURFER® output of STLINE. As shown, there is a small discrepancy between numeric and analytic data. This circumstance could result from a difference in the treatment of the injection well. For the analytic model, this well is located precisely at one point. However, for the numeric model, the injection rate is spread uniformly over one 5x5 m grid block. (For pictorial purposes, only the well is located at the grid-block centroid in Figure 14-3.) A more likely source of the discrepancy, however, is the total region size, particularly in the lateral y direction. For the analytical solution, an infinite region was used whereas, of necessity, a finite region was used for the numerical solution.

Improvements could be achieved by further increases in region size and modifications of the grid. However, such refinements are not necessary here since the primary objective is to demonstrate the use of the streamline program, and for that purpose, the present calculation is quite adequate.

14.6 EXAMPLE APPLICATION

This problem demonstrates the application of stream lines with STLINE. The example application utilizes a three-dimensional flow system composed of variable thickness and variable elevation grid blocks to simulate a typical valley-fill aquifer transversed by a river. The three-dimensional, SWIFT grid, Figure 14-5, is composed of 39 x 29 x 3 blocks ranging 150 to 600 feet horizontally. Thicknesses vary from 5 to 90. Model boundary conditions include a head-dependent condition for the river and constant head conditions for the upgradient and downgradient edges of the model. Water table conditions are instituted for the top layer of the model.

To demonstrate the movement of particles, three pumping wells are simulated causing local cones of depression. The steady-state potentiometric surface for model layer 2 is shown in

Figure 14-4. STLINE plots of streamlines generated by tracking Particles A-F using SURFER® command file INJSTL.CMD.

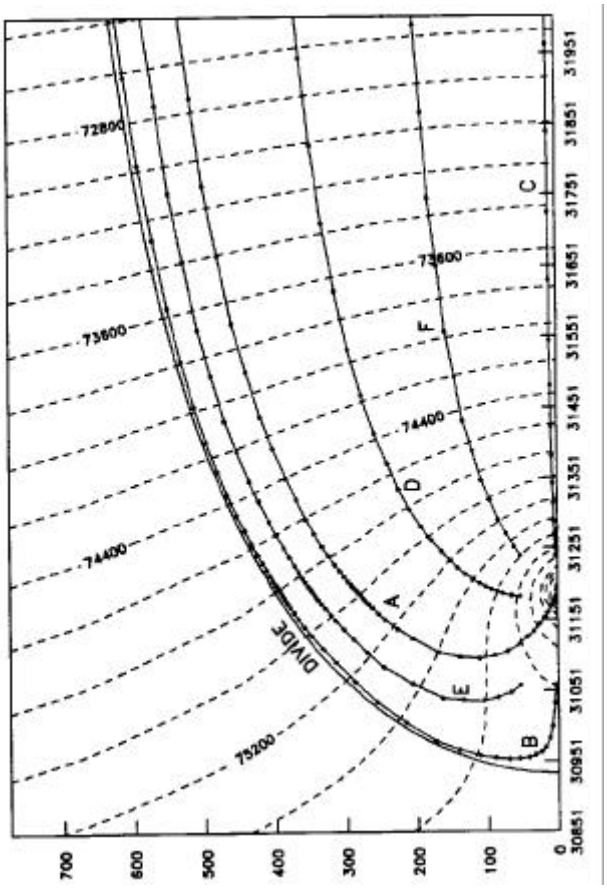


Figure 14-5. Finite difference grid and potentiometric surface for model layer 2.

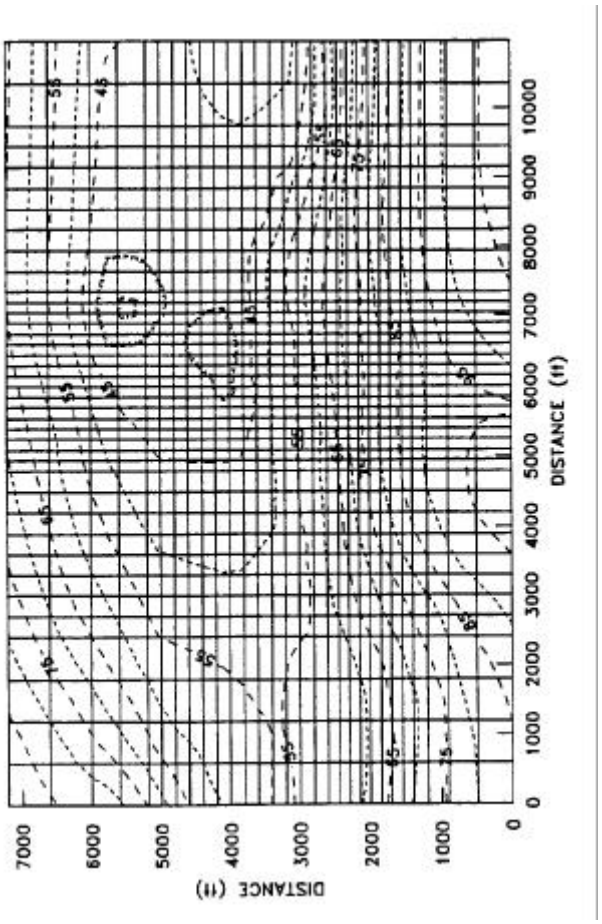


Figure 14-5. Five stream lines are evaluated (A-E). Groundwater flow converges towards the river and the pumping wells. The streamlines are presented in areal and vertical sections in Figures 14-6 and 14-7. The vertical section in Figure 14-7 is a Y-Z slice along model column 25. The block centers of the model grid are also posted in Figure 14-7 demonstrating the variable thicknesses. The particle location, denoted by an asterisk, is printed at each n'th time step. Note the slower particle movement along streamline E where the gradient is less pronounced. Streamlines A, B, and C terminate at the pumping wells, while D and E terminate at the river, Figure 14-6.

14.7 NOTATION

Roman Symbols

a_x, b_x	Linear interpolation parameters for velocity component, V_x.
S_p^n	Total path length of particle p at time step n.
t	Time.
V_x,V_y,V_z	Components of the interstitial fluid velocities at any position (x,y,z).
V_{1x}, V_{2x}	Velocity components at X and X + ΔX.
$\bar{V}_x$	Arithmetic average of velocities at time t and t + δt.
$\{V_x\}$	Arithmetic average of velocity components at X and X + ΔX.
X,Y,Z	System, or global, coordinates of a typical particle.
X_p^n,Y_p^n,Z_p^n	Global coordinates of particle p at time step n.
x,y,z	Grid-block, or local, coordinates
y_z	Asymptotic width between streamlines of injection well in a uniform flow field.

Greek Symbols

ΔX,ΔY,ΔZ	Dimensions of a typical grid-block.
δs	Incremental increase in path length occurring during δt.
δt	Computational time step.
δx,δy,δz	Positional changes of a reference particle occurring during time step δt.

Figure 14-6. Areal (x-y) view of streamlines in stair-cased grid.

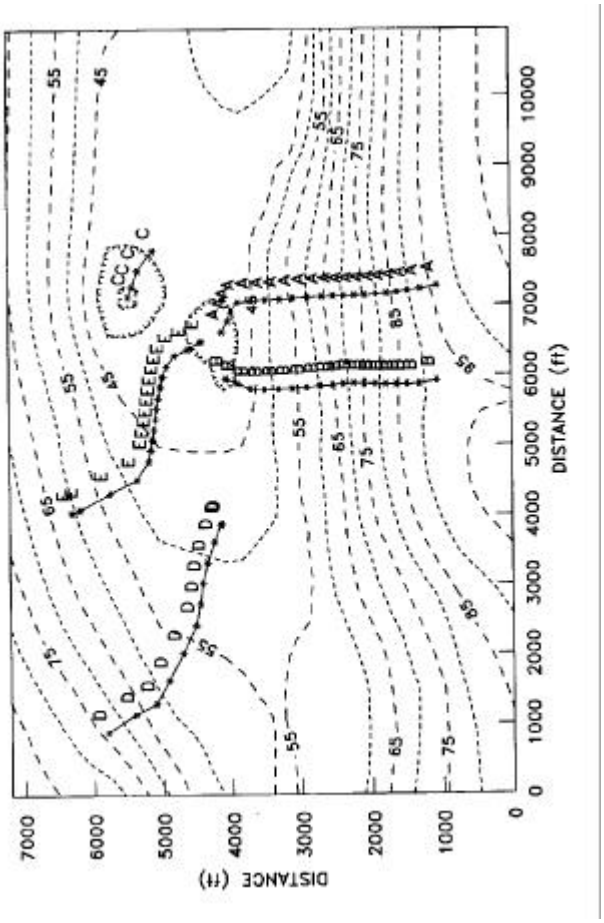
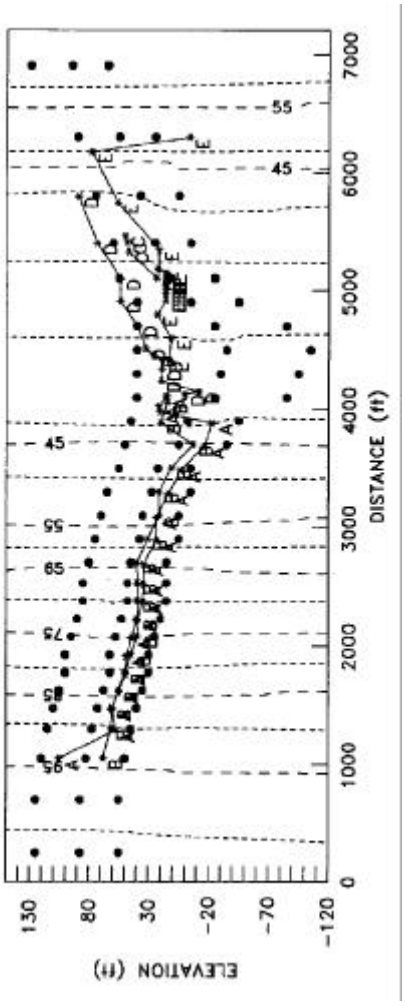


Figure 14-7. Vertical (y-z) view of streamlines and block centroids along column 25.



15 CHRONOLOGY

The SWIFT/486 code is the result of work performed by several related consulting firms. Funding has principally been through government contracts. This section reviews the chronology and evolution of the code.

Listed below are the significant benchmark versions of the code used in the development of SWIFT/486.

CODE	CODE DEVELOPER	SOURCE OF FUNDING	REFERENCE
SWIP	Intercomp, Inc.	USGS	Intercomp, 1976
SWIPR	Intera, Inc.	USGS	Intera, 1979
SWIFT	Intera, Inc.	NRC	Dillon et al., 1978 Reeves and Cranwell, 1981 Finley and Reeves, 1981 Ward et al., 1984
SWIFT II	GeoTrans, Inc.	NRC	Reeves et al., 1986a Reeves et al., 1986b Reeves et al., 1987
SWIFT III	GeoTrans, Inc.	GeoTrans	Ward, 1987
SWIFT/386	GeoTrans, Inc.	GeoTrans	Ward, 1991
SWIFT/486	GeoTrans, Inc.	GeoTrans	Ward, Harrover, and Vincent, 1992
SWIFT-98	HSI GeoTrans	HSI GeoTrans	Ward and Benegar, 1998

The following paragraphs summarize the evolution of each version.

SWIP - 1976 (SURVEY WASTE INJECTION PROGRAM)

Under funding by the U.S. Geological Survey, Intercomp developed the three-dimensional model intended for assessing the effects of deep well injection of wastes into saline aquifers. The code is a hybrid of hydrologic and petroleum technology. Capabilities include the coupled solution of equations for groundwater flow, heat and brine transport. Additional features include: variable density, viscosity, well bore friction and heat loss. The report contains several verification and validation problems. The code is also referred to Deep Well Disposal Model (DWDM).

SWIPR - 1979 (SURVEY WASTE INJECTION PROGRAM REVISED)

Under contract to the USGS, Intera, a former division of Intercomp, extended the model to include: a freewater surface, sorption and decay for contaminant transport. Both SWIP and SWIPR are stagnant, that is, updates have not been issued. Both codes are designed for Control Data mainframes with Fortran 4. The SWIPR code is also referred to as SWIP2.

SWIFT - 1981 (SANDIA WASTE-ISOLATION FLOW AND TRANSPORT)

Under contract to the U.S. Nuclear Regulatory Commission, Intera extended the code to simulate transport of chains of radionuclides. In contrast to the brine equation, nuclides are assumed to be of trace quantifies, that is the concentration does not affect the fluid density. A steady-state flow option was included. The code is intended for performance assessment of high-level nuclear waste repositories. In support of the code two other documents were prepared. The SWIFT self-teaching curriculum (Finley and Reeves, 1981) document 11 application problems. The verification and field comparison document (Ward et al., 1984) details 11 more problems, demonstrating that the code compares favorably with analytical and field data. Data input instructions are given in Reeves and Cranwell, 1981.

SWIFT II - 1986 (SANDIA WASTE-ISOLATION FLOW AND TRANSPORT FOR FRACTURED MEDIA)

Under contract to NRC, GeoTrans, a former subsidiary of Intera, extended the code to include: fractured media, enhanced freewater surface and extended boundary conditions. To provide the use with complete information a document on the theory and implementation was prepared (Reeves et al., 1986a). Mathematical development is fully detailed in this 200 page report. Data input instructions are given in Reeves et al., 1986b. In a supplemental document eight problems and data sets were prepared for self-instruction (Reeves et al., 1986c).

SWIFT III - 1987 (SANDIA WASTE-ISOLATION FLOW AND TRANSPORT FOR FRACTURED MEDIA)

GeoTrans extended the code to comply with ANSI Fortran 77. Additional refinements in user options, mapping facilities and auxiliary files were performed. The data input instructions by Ward, 1989 reflect these changes.

SWIFT/386 - 1991 (SANDIA WASTE-ISOLATION FLOW AND TRANSPORT FOR FRACTURED MEDIA)

GeoTrans further extended the code for use on personal computers. Additional features include multiple values of rock-type compressibility. The primary change is the addition of a run-time monitor to improve user friendliness.

SWIFT/486 - 1993 (SANDIA WASTE-ISOLATION FLOW AND TRANSPORT FOR FRACTURED MEDIA)

The code is further extended to utilize the 80486 processor. Added options including: stair-cased grid input HTOP (R1-19.1), environmental and fresh water head, improved mass balance, Peclet and Courant number diagnostic, matrix printing control using L2SORP (M-2), maps of all radionuclide concentration, summary output for aquifer influence function (LAIF).

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APPENDIX A

DEFINITION OF INPUT VARIABLES

DEFINITION OF INPUT VARIABLES

ACS(NRT)	Product of the rate of salt dissolution and the mass fractions of solubles to total dry mass, d^{-1} (s^{-1}).
AKSD(NRTD)	Hydraulic conductivity of the local subsystem, ft/d (m/s).
ALCH	Leach time for radioactive waste within the repository boundaries, d (s).
ALPD(NRTD)	Dispersivity within the local subsystem, ft (m).
ALPHAL(NRT)	Longitudinal dispersivity within the global system, ft (m).
ALPHAT(NRT)	Transverse dispersivity within the global system, ft (m).
ALPHL	Longitudinal dispersivity within the global system, ft (m).
ALPHT	Transverse dispersivity within the global system, ft (m).
AMAX	Maximum contour value in plotting submodel.
AMIN	Minimum contour value in plotting submodel.
AP	Fraction of parent component KP that decays to the component I.
ARHLD(NTIME)	Areal density of the repository heat source, Btu/ft^2-d (J/m^2-s).
BHP	Bottom-hole pressure for a well, psi (Pa).
BLCH	Lag time for initiation of leaching of waste from repository, d (s).
BROCK	Rock density of the solid particle, lb/ft^3 (kg/m^3).
BWRI	Density of the contaminated fluid ($\hat{C} = 1$) at PBWR and TBWR, lb/ft^3 (kg/m^3).
BWRN	Density of the natural reservoir fluid ($\hat{C} = 0$) at PBWR and TBWR, lb/ft^3 (kg/m^3).
CINIT	Initial concentration (brine or radionuclide) of each of the blocks within a defined region, mass fraction.
CINJ	Brine concentration in the injection fluid, mass fraction.

CMN	Lower limit on the brine concentrations to be plotted, mass fraction.
CMX	Upper limit on the brine concentrations to be plotted, mass fraction.
CNAME(2)	Identification of the radioactive component.
CNDUM(NTIME)	Radionuclide concentrations within the unleached repository wastes, expressed as mass per unit volume of wastes (see CTIME), lb/ft^3 (kg/m^3).
COC	Observed concentrations to be plotted, mass fraction.
CONV	Conversion factor for the thermal conductivities to obtain units of Btu/ft-d-°F (J/m-s-°C).
CONVC	Conversion factor for the waste concentrations to obtain units of lb/ft^3 (kg/m^3).
CONVH	Conversion factor for the repository heat densities to obtain units of Btu/m^2-d (J/m^2-s).
CONVL	For canistered wastes, CONVL multiples SDRIFT, SCNSTR, DCNSTR, and HCNSTR to convert them to ft (m). For uncanistered wastes CONVL multiplies only DCNSTR to convert it to ft^3 (m^3) of wastes per bulk ft^3 (m^3).
CONVT	Conversion factor for the interpolation times to obtain units of d (s).
CPOB	Heat capacity of the overburden, Btu/ft^3-°F (J/m^3-°C).
CPR	Heat capacity of the fluid-saturated global medium, Btu/ft^3-°F (J/m^3-°C).
CPRKD(NRTD)	Heat capacity of the fluid-saturated local medium, Btu/ft^3 °F (J/m^3-°C).
CPR1(NZ)	Heat capacity of the fluid-saturated global medium with cylindrical geometry, Btu/ft^3-°F (J/m^3-°C).
CPUB	Heat capacity of the underburden, Btu/ft^3-°F (J/m^3-°C).
CPW	Heat capacity of the reservoir fluid, Btu/lb-°F (J/kg-°C).
CR, CRR	Compressibility of pore structure within the global system, psi^{-1}, (Pa^{-1}).
CRD	Compressibility of the pore structure within the local subsystems, psi^{-1} (Pa^{-1}).

CRTDST	Time-dependent values of pore structure compressibility, psi^{-1} (Pa^{-1}).
CS(NCP)	Solubility limit, mass fraction.
CTIME(NTIME)	Interpolation time for concentrations within the unleached waste and/or heat density in the repository (see CNDUM and ARHLD), d (s).
CTW	Coefficient of thermal expansion of the reservoir fluid, $°F^{-1}$ ($°C^{-1}$).
CW	Compressibility of the reservoir fluid, psi^{-1} (Pa^{-1}).
C1	Boundary brine concentration of the global system, mass fraction.
DAMPX	Damping factor used in the wellbore calculations, dimensionless.
DCMX	Maximum change desired per time step in the trace-component concentration, mass fraction.
DCNSTR	For canistered wastes, the diameter of each canister in ft (m). For uncanistered wastes, the volumetric waste density, volume of waste/bulk volume.
DEC(NCP)	Component half life in years.
DELPW	For the wellbore submodel, the incremental value of pressure used in wellbore integrations, psi (Pa).
DELX(NX)	Length of each column of blocks in the x direction, ft (m).
DELY(NY)	Length of each column of blocks in the y direction, ft (m).
DELZ(NX)	Thickness of each vertical layer, ft (m).
DEPTH	Depth to center of grid-block (1,1,1) from the reference plane, ft (m).
DI(2,NCP)	Identification of the radioactive component I.
DIS(NCP)	Adsorption coefficient κ for a Freundlich isotherm in the global system, $(ft^3/lb)^{\eta}$ or $(m^3/kg)^{\eta}$.
DIS(2*NCP)	Adsorption coefficient η for a Freundlich isotherm in the global system, dimensionless.
DISD(NCP)	Adsorption distribution coefficient for the local system, ft^3/lb (m^3/kg).

DMEFD(NRTD)	Molecular diffusivity for the local subsystem, ft/d (m^2/s).
DMEFF, DMEFFR	Molecular diffusivity in the global subsystem, m^2/d (m^2/s).
DMFD1(NRTD)	Coefficient of thermal increase in diffusivity for the local subsystem, $°F^{-1}$ ($°C^{-1}$).
DPMX	For automatic time stepping, the maximum pressure change (over the grid) desired per time step, psi (Pa).
DS(NSD)	Separation of nodes I and I+1 in the local subsystems, a function of rock type, ft (m).
DSD(NRTD)	Local increment at the system interface, ft (m).
DSDO(NRTD)	Local increment at the outer extremity of the subsystem, ft (m).
DSMX	For automatic time stepping, the maximum change in brine concentration (over the grid) desired per time step, mass fraction.
DT	Time-step specification, d (s).
DTMAX	For automatic time stepping, the maximum time step allowed, d (s).
DTMIN	For automatic time stepping, the minimum time step allowed, d (s).
DTPMX	For automatic time stepping, the maximum temperature change desired per time step, °F (°C).
DW	Inside wellbore diameter, ft (m).
DZOB	Thickness of each overburden block, ft (m).
DZUB	Thickness of each underburden block, ft (m).
ED	Inside tubing roughness, ft (m).
EPS	Tolerance on the calculation of temperature within the wellbore, °F (°C).
FAB	Factor by which the aquifer-influence coefficient VAB will be modified, dimensionless.
FAMD	Modification factor for cross-sectional area of dual porosity block, dimensionless.

FPHI	Modification factor by which porosity (as used in heat storage calculation) will be modified, dimensionless.
FPV	Modification factor for the pore volume, dimensionless.
FTUX	Modification factor for x-direction Darcy velocity, heat and solute dispersion coefficients, dimensionless.
FTUY	Same as FTUX, but for y-direction.
FTUZ	Same as FTUX, but for z-direction.
FTX	Modification factor for the x-direction transmissibility, dimensionless.
FTY	Same as FTX, but for y direction.
FTZ	Same as FTX, but for z direction.
HADD	Depth modification factor, ft (m).
HCNSTR	Canister height for the waste-leach model, ft (m).
HDATUM	Datum depth measured relative to the reference plane, ft (m).
HINIT	Depth used for setting up initial pressure condition (see PINIT), ft (m).
HTOP	Depth to top of block, ft (m).
HTG	Geometry/heterogeneity control parameter.
I	Dummy index.
IAQ	Control parameter for aquifer-influence functions and boundary conditions.
IBUD	Number of L2SOR iteration sweeps.
IICL	Control parameter for changing the mode of solution of the primary equations.
ICOMP	Control parameter for initializing the brine concentrations.
ID	Title of the plots for a specific well.
IDSC	Nuclide monitor block, I index.

IFD	Position and orientation control for the local subsystems.
IFREE	Control parameter for free-water surface.
IIC1	Uppermost layer in which the well is completed.
IIC2	Lowermost layer in which the well is completed.
IINDW1	Well specification option.
IIPRT	Printing control for intermediate variables in the global system.
IIPRTD	Printing control for intermediate variables in local subsystems.
IIS	I-index location of a source block for fluid, heat or radionuclides.
IIW	I-index location of a grid cell containing a well.
IJS	J-index location of a source block for fluid, heat or radionuclides.
IJW	J-index location of a grid cell containing a well.
IKS	K-index location of a source block for fluid, heat or radionuclides.
ILEVEL	Indicator for specifying either canistered-waste storage or uncanistered waste storage.
IMETH	Control parameter for reading the method of solution.
IMPG	Number of time steps after which the optimum parameters for the inner iterations are recalculated for the two-line successive overrelaxation method.
IMPT	Time-step number at which maps are desired.
INAT	Control parameter for entering the initial fluid velocity.
INDQ	Control parameter for reading well rates.
INDT	Control parameter for iteration data for the reservoir solution.
IOPT	Control parameter for reading iteration data for the wellbore solution.
IO1	Frequency control parameter for output of the time-step summaries.

IO2	Frequency control parameter for output of the well summaries.
IO3	Control parameter for entering printing specifications of the grid-block values for the primary variables.
IO4	Control parameter for listing layer allocations of the injection/production rate.
IO5	Control parameter for listing the grid-block values of radionuclide concentrations for the global system.
IO5D	Control parameter for listing the grid-block values of the radionuclide concentrations for the local subsystems.
IO6	Control parameter for listing the aquifer-influence rates.
IO8	Control parameter for selectively listing the grid-block values of the primary variables for the global system.
IO8D	Control parameter for selectively listing the grid-block values of the primary variables for the local subsystems.
IPROD	Control parameter for reading wellbore data.
IRCH	Control parameter for reading recharge data.
IRD	Control parameter for initializing the concentrations of the radioactive trace components.
IRSS	Control parameter for reading source data for fluid, heat and radioactive components.
IRT,IR	Rock-type indicators for the global system and for the local subsystems.
ISURF	Control parameter for the wellbore calculations.
ITHRU	Run termination control and pressure-at-datum option parameter.
IUNIT	Units control parameter specifying either the English Engineering system or the SI system.
IWELL	Control parameter for reading well-definition data.
IXYZ	Control parameter for directional sweep of L2SOR.

I1	Parameter used several times to specify the lower limit on the I index of a region.
I1A	Same as I1.
I1B	Same as I2.
I2	Parameter used several times to specify the upper limit on the I index of a region.
JDSC	Nuclide monitor block, J index.
J1	Parameter used several times to specify the lower limit on the J index of a region.
J1A	Same as J1.
J1B	Same as J2.
J2	Parameter used several times to specify the upper limit on the J index of a region.
KAQ	Control parameter for setting boundary conditions on the heat-flow equation.
KBC(NRTD)	Local boundary-condition control.
KCNVD	Convection/dispersion control for the local subsystems.
KDSC	Nuclide monitor block, K index.
KGDP(NRTD)	Local geometry control.
KGRD(NRTD)	Local grid control.
KH	Conductivity-thickness of the aquifer, m^2/d (m^2/s).
KHEAT	Control parameter for the areal repository heat source.
KHL	Layer-allocation factor for the well, dimensionless.
KMP6, KMP10, KMP13	Control parameter for auxiliary map filed for units 6, 10 and 13.
KOB	Vertical thermal conductivities of the overburden, Btu/ft-d-°F (J/m-s-°C).

KOUT	Output control parameter for the global system.
KOUTD	Output control for the local subsystems.
KP(NP)	Parent component number.
KPB(NRTD)	Pressure-boundary control for the local subsystems.
KSLVD	Local control parameter for solution of both primary and radionuclide equations.
KSWB(NRTD)	Brine boundary control for the local subsystems.
KTPB(NRTD)	Temperature boundary control for the local subsystems.
KUB	Vertical thermal conductivities of the underburden, Btu/ft-d-°F (J/m-s-°C).
KW	Well number identifying a well for plots.
KX(NB)	Hydraulic conductivity in the x direction for the global system, ft/d (m/s).
KY(NB)	Same as KX, but in the y direction.
KYY(NZ)	Hydraulic conductivity in the radial direction for cylindrical coordinates, ft/d (m/s).
KZ(NB)	Same as KX, but in the z direction.
KZZ(NZ)	Same as KYY, but in the z direction.
K1	Parameter used several times to specify the lower limit on the K index of a region.
K1A	Same as K1.
K1B	Same as K2.
K2	Parameter used several times to specify the upper limit on the K index of a region.
LADJ(NCP)	Lambda index for adjustment of the rate constant of a radioactive component.
LAIF	Control parameter for aquifer influence function output.

LBI0	Control option for nuclide monitor blocks.
LMAPIT	Control parameter on map matrix output.
LMBAL	Control parameter for mass balance summary output.
L2SORP	Control parameter for frequency of printing L2SOR output.
MAP	Control parameter for selectively printing contour maps for the dependent variables.
MASS(NCP)	Mass number of a radioactive component.
MAXITN	Maximum number of outer nonlinear iterations in the solution of the primary equations.
MDAT	Control parameter for entering the mapping specifications.
METHOD	The method-of-solution indicator.
MINITN	Minimum number of outer nonlinear iterations in the solution of the primary equations.
NABLMX	Storage allocation for the number of boundary-condition blocks and aquifer-influence function blocks.
NCALC	Control parameter for the Carter-Tracy aquifer coefficients.
NCALL	Control parameter for selecting the primary partial differential equations to be solved.
NCP	Number of radioactive/trace components in the system.
NCV	Number of entries in the table of viscosity versus concentrations.
NDT	Number of entries in the table of depth versus temperature.
NITQ	Maximum number of outer iterations in the wellbore calculations.
NI1,NI2,NJ1, NJ2,NK1,NK2	Lower and upper indices on windowing output.
NORNXY, NORNXZ, NORNYZ	Control parameters for map orientation.

NOUT	Output control parameter for wellbore results.
NP(NCP)	Number of parent components for a radionuclide.
NPLC	Control parameter for plotting concentrations for the wells.
NPLP	Control parameter for plotting pressures for the wells.
NPLT	Control parameter for plotting temperatures for the wells.
NPT	Number of points in the table of influence-function versus dimensionless time.
NPTDST	Number of points in the table of time versus pore structure compressibility.
NRCHMX	Storage allocation for the number of recharge blocks.
NREPB	Number of respository blocks.
NRT	Number of global rock types.
NRTD	Number of local rock types.
NSD(NRTD)	Number of local grid blocks.
NSMAX	Storage allocation for the number of radioactive trace components that will be used during the run.
NSS	Number of source blocks for fluid, heat and radionuclides.
NTIME	Number of entries in the table of concentration (CNDUM) versus time (CTIME) for the unleached radioactive components and/or heat density (ARHLD) versus time (CTIME) for the repository blocks.
NTVI	Number of entries in the table of viscosity (VISI) versus temperature (TI) for the contaminated fluid.
NTVR	Number of entries in the table of viscosity (VISR) versus temperature (TR) for the resident reservoir fluid.
NWT	Total number of wells.
NX	Number of grid blocks in the x direction.
NY	Number of grid blocks in the y direction.

NZ	Number of grid blocks in the z direction.
NZOB	Number of overburden blocks.
NZUB	Number of underburden blocks.
OD	For the wellbore model, the outside diameter of the casing, ft (m).
PBASE	Atmospheric or reference pressure at the well head, psi (Pa).
PBD	Pressure boundary condition for the local subsystem, psi (Pa).
PBWR	Reference pressure for the input fluid densities, BWRN and BWRI, psi (Pa).
PDT	Terminal rate function.
PHI(NB)	Porosity of the global system, volume fraction.
PHID(NRTD)	Porosity of the local subsystems, volume fraction.
PHIH	Porosity-thickness product for the aquifer, ft (m).
PINIT	Initial pressure at the depth HINIT and at the standard pressure PO = PINIT for the density calculations, psi (Pa).
POROS(NZ)	Porosity for cylindrical coordinates, volume fraction.
POS	Observed surface pressure used for plotting, psi (Pa).
POW	Observed bottom-hole pressure used for plotting, psi (Pa).
PRT	Orientation control for the output arrays.
PRTAB	Print control key for the aquifer-influence coefficients.
PRTIF	Print control key for the influence-function table.
PSMN	Lower limit on the well-head pressures to be plotted, psi (Pa).
PSMX	Upper limit on the well-head pressures to be plotted, psi (Pa).
PTD(NPT)	Terminal-rate influence function, dimensionless.
PWMN	Lower limit on the bottom-hole pressures to be plotted, psi (Pa).

PWMX	Upper limit on the bottom-hole pressures to be plotted, psi (Pa).
P1	Boundary pressure of the global system, psi (Pa).
Q(NWT)	Well production rate, ft^3/d (m^3/s).
QCC(NSS,NCP)	Radioactive-component discharge rate, lb/d (kg/s).
QHH(NSS)	Heat discharge rate, Btu/d (J/s).
QRCH	Recharge rate, ft/d (m/s).
QWELL	Well production rate, ft^3/d (m^3/s).
QWW(NSS)	Fluid discharge rate, lb/d (kg/s).
RAQ	Internal radius of the aquifer, ft (m).
RCHG	Recharge rate, ft/d (m/s).
RE	External radius of the aquifer, ft (m).
RR(NX)	Radius of the grid-block centers, ft (m).
RSTRT	Control parameter for restarting a calculation.
RSTWR	Control parameter for writing a restart record.
RWW	Well radius, ft (m).
R1	For radial coordinates, the center of the first grid-block, ft (m).
SAD(NRTD)	Length of the prismatic local units or radius of the spherical local units, ft (m).
SC(NCV)	Concentrations for the table of viscosity (VCC) versus concentration, mass fraction.
SCNSTR	Center-to-center waste-canister separation within each row for the waste-leach model, ft (m).
SDRIFT	Separation of rows of waste canisters for the waste-leach model, ft (m).
SINX	Sine of the reservoir dip angle along the x-axis, dimensionless.

SINY	Sine of the reservoir dip angle along the y-axis, dimensionless.
SWBD(NRTD)	Brine boundary condition for the local subsystems, ft (m).
TBWR	Reference temperature for the input densities BWRN and BWRI, °F (°C).
TBOTW	For the wellbore model, the initial rock temperature at the bottom-hole depth, °F (°C).
TBUD	Convergence for L2SOR (units depend on equation solved).
TCHG	Time at which the next set of recurrent data will be read, d (s).
TD(NDT)	Temperature in the table of temperature versus depth (see PTD), °F (°C).
TD(NPT)	Time in the table of influence function versus time (see ZT), dimensionless.
TDIS	Thermal diffusivity of the rock surrounding the wellbore, m^2/hr (m^2/s).
THADD	Additive thickness modifier for a grid-block, ft (m).
THETA	Angle of deviation of the wellbore from the vertical direction, degrees.
THETAQ	Angle of influence of the aquifer-influence functions, degrees.
THP(NWT)	For the wellbore model, the tubing-hole or surface pressure, psi (Pa).
TI(NTVI)	Temperatures for the table of viscosity (VISI) versus temperature for the contaminated fluid, °F (°C).
TIMTDST	Interpolation time for pore structure compressibility, d(s).
TINJ	Temperature of the injected fluid, °F (°C).
TIR	Reference temperature for the viscosity (VISIR) of the contaminated fluid, °F (°C).
TITLE(160)	Title for the run.
TMN	Lower limit on the times to be plotted, d (s).
TMX	Upper limit on the times to be plotted, d (s).
TO	Standard temperature for calculating fluid density, °F (°C).

TOLDP	Tolerance on the pressure used in the wellbore calculations, psi (Pa).
TOLX	Tolerance on the fractional change in pressure used in the wellbore calculations, dimensionless.
TOS	Observed surface temperatures to be plotted, °F (°C).
TOW	Observed bottom-hole temperature to be plotted, °F (°C).
TOX	Observed times for data to be plotted, d (s).
TPARAM	Under or over-relaxation parameter for L2SOR.
TPBD(NRTD)	Temperature boundary condition for the local subsystems, °F (°C).
TR(NTVR)	Temperatures for the table of viscosity (VISR) versus temperature for the resident fluid, °F (°C).
TRR	Reference temperature for the viscosity (VISRR) of the resident fluid, °F (°C).
TSMN	Lower limit on the surface temperatures to be plotted, °F (°C).
TSMX	Upper limit on the surface temperatures to be plotted, °F (°C).
TTOPW	For the wellbore model, the initial rock temperature at well-head level, °F (°C).
TWMN	Lower limit on the bottom-hole temperatures to be plotted, °F (°C).
TWMX	Upper limit on the bottom-hole temperatures to be plotted, °F (°C).
T1	Boundary temperature of the global system, °F (°C).
T2	For a radiation boundary condition, the temperature of the surrounding media, °F (°C).
T3	For a radiation boundary condition, the coefficient of surface heat transfer, Btu/d-ft-°F (J/s-m-°C).
UCOEF	For the wellbore model, the heat-transfer coefficient between the inner surface of the tubing and the outer surface of the casing, Btu/m^2-°F-hr (J/m^2-°C-s).
UCRP	Modified heat capacity of the rock, Btu/ft^3-°F (J/m^3-°C).

UH	Modified depth of the center of the grid-block relative to the top of the reference plane, ft (m).
UKTD(IR)	Thermal conductivity of the fluid-saturated local medium, Btu/ft-°F-d (J/m-°C-s).
UKTX	Thermal conductivity of the fluid-saturated global medium in the x direction, Btu/ft-°F-d (J/m-°C-s).
UKTY	Same as UKTX, but for the y direction.
UKTZ	Same as UKTX, but for the z direction.
UTCX(NRT)	Thermal conductivity of the fluid-saturated global media in the x direction, Btu/ft-°F-d (J/m-°C-s).
UTCY(NRT)	Same as UTCX, but for the y direction.
UTCZ(NRT)	Same as UTCX, but for the z direction.
UTH	Modified grid-block thickness, ft (m).
VAB	Parameter used to specify both boundary conditions and aquifer-influence functions. The dimensions depend on the option chosen.
VCC(NCV)	Viscosities in the table for viscosity versus concentration (SC), cp (Pa-s).
VEL	Initial velocity of the resident reservoir fluid in the x direction, ft/d (m/s).
VISI(NTVI)	Viscosities in the table of viscosity versus temperature (TI) for the contaminated fluid, cp (Pa-s).
VISIR	Reference viscosity of the contaminated fluid at the reference temperature (TIR), cp (Pa-s).
WI	Well index, m^2/d, (m^2/s).
WTFAC	Weight factor for finite differencing in space.
X	For the wellbore model, the length of the tubing from the surface to the top of the perforations.
XYXL, XYYL	Length of the areal computer-output maps in the x and y directions, inches.

XZXL, XZZL	Length of the vertical computer-output maps in the x/r and z direction, inches.
YZYL, YZZL	Length of the vertical computer-output maps in the y and z directions, inches.
ZT(NDT)	Depths in the table of temperature (TD) versus depth, ft (m).

APPENDIX B

VARIABLE INDEX

VARIABLE INDEX

Variable	Cards	Format	Column	Dimensions
ACS(NRT)	R1A-2	7E10.0	1-70	d^{-1} (s^{-1})
AKSD(IR)	R1D-2	E10.0	31-40	ft/d (m/s)
ALCH	R2-10.5	E10.0	1-10	d (s)
ALPD(IR)	RID-2(List 1)	E10.0	41-50	ft (m)
ALPHAL(NRT)	R1-2.5(List 2)	7E10.0	1-70	ft (m)
ALPHAT(NRT)	R1-2.5(List 2)	7E10.0	1-70	ft (m)
ALPHL	R1-2	E10.0	41-50	ft (m)
ALPHT	R1-2	E10.0	51-60	ft (m)
AMAX	R2-15	E10.0	41-50	+
AMIN	R2-15	E10.0	31-40	+
AP(NP)	R0-1(Card 2)	E10.0	11-20,	*
ARHLD(NTIME)	R1A-8.5	7E10.0	1-70	Btu/ft^2-d (J/s-m^2)
BHP	R2-7(List 2)	E10.0	11-20	psi (Pa)
BLCH	R2-10.5	E10.0	11-20	d (s)
BROCK	R1-3	E10.0	1-10	lb/ft^3 (kg/m^3)
BWRI	R1-3	E10.0	41-50	lb/ft^3 (kg/m^3)
BWRN	R1-3	E10.0	31-40	lb/ft^3 (kg/m^3)
CINIT	I-2	E10.0	31-40	*
CINJ	R2-7(List 2)	E10.0	31-40	*
CMN	P-3(Card 2)	E10.0	41-50	*
CMX	P-3(Card 2)	E10.0	51-60	*
CNAME(2)	R1A-8	2A4	1-8	**
CNDUM(NTIME)	R1A-8	6E10.0	11-70	*
COC	P-4	E10.0	51-60	*
CONV	R1-2	E10.0	31-40	+
	R2-2.5	E10.0	31-40	+
CONVC	R1A-5	E10.0	11-20	+
CONVH	R1A-5	E10.0	31-40	+
CONVL	R1A-5	E10.0	1-10	+
CONVT	R1A-5	E10.0	21-30	+
CPOB	R1-13	E10.0	11-20	Btu/ft^3-°F (J/m^3-°C)
CPR	R1-1	E10.0	41-50	Btu/ft^3-°F (J/m^3-°C)
CPRKD(NRTD)	R1D-2(List 1)	E10.0	61-70	Btu/ft^3-°F (J/m^3-°C)
CPR1(NZ)	R1-23	E10.0	41-50	Btu/ft^3-°F (J/m^3-°C)
CPUB	R1-13	E10.0	31-40	Btu/ft^3-°F (J/m^3-°C)
CPW	R1-1	E10.0	31-40	Btu/lb-°F (J/kg-°C)
CR	R1-1	E10.0	11-20	psi^{-1} (Pa^{-1})

Variable	Cards	Format	Column	Dimensions
CRR	R1-2.5	E10.0	21-30	psi^{-1} (Pa^{-1})
	R2-2.6	E10.0	6-15	psi^{-1} (Pa^{-1})
CRD	R1D-1	E10.0	1-10	psi^{-1} (Pa^{-1})
CRTDST	R1-1.5	E10.0	11-20	psi^{-1} (Pa^{-1})
CS(NCP)	R1A-9	7E10.0	1-70	*
CTIME(NTIME)	R1A-7	7E10.0	1-70	d (s)
CTW	R1-1	E10.0	21-30	$°F^{-1}$ ($°C^{-1}$)
CW	R1-1	E10.0	1-10	psi^{-1} (Pa^{-1})
C1	R1-28(List 2)	E10.0	31-40	*
DAMPX	R2-3	E10.0	26-35	*
DCMX	R2-1	E10.0	21-30	*
DCNSTR	R1A-4	E10.0	21-30	ft (m)
DEC(NCP)	R0-1(List 1)	E10.0	31-40	yr
DELPW	R1-5	E10.0	11-20	psi (Pa)
DELX(NX)	R1-17	***		ft (m)
DELY(NY)	R1-18	***		ft (m)
DELZ(NZ)	R1-19, R1-19.1	***		ft (m)
	R1-23	E10.0	1-10	ft (m)
DEPTH	R1-20	E10.0	61-70	ft (m)
	R1-22	E10.0	31-40	ft (m)
DI(2,NCP)	R0-1(List 1)	2A4	4-11	**
DIS(NCP)	R0-2(List 1)	7E10.0	1-70	$(ft^3/lb)^{\eta}$ or $(m^3/kg)^{\eta}$
DIS(2*NCP)	R0-2(List 2)	7E10.0	1-70	*
DISD(NCP)	R1D-4	7E10.0	1-70	ft^3/lb (m^3/kg)
DMEFD(NRTD)	R1D-2(List 1)	E10.0	1-11	ft^2/d (m^2/s)
DMEFF	R1-2	E10.0	61-70	ft^2/d (m^2/s)
DMEFFR	R1-2.5(List 2)	E10.0	21-30	ft^2/d (m^2/s)
DMFD1(NRTD)	R1D-2(List 1)	E10.0	11-20	$°F^{-1}$ ($°C^{-1}$)
DPMX	R1-12	E10.0	41-50	psi (Pa)
DS(NSD)	R1D-2(List 3)	7E10.0	1-70	ft (m)
DSD	R1D-2(List 2)	E10.0	21-30	ft (m)
DSDO	R1D-2(List 2)	E10.0	31-40	ft (m)
DSMX	R2-12	E10.0	31-40	*
DT	R2-12	E10.0	11-20	d (s)
DTMAX	R2-12	E10.0	61-70	d (s)
DTMIN	R2-12	E10.0	71-80	d (s)
DTPMX	R2-12	E10.0	51-60	°F (°C)
DW	R2-7(List 3)	E10.0	11-20	ft (m)
DZOB(NZOB)	R1-14	7E10.0	1-70	ft (m)

Variable	Cards	Format	Column	Dimensions
DZUB(NZUB)	R1-15	7E10.0	1-70	ft (m)
D1	P-3(Card 1)	E10.0	21-30	d (s)
ED	R2-7(List 3)	E10.0	21-30	ft (m)
EPS	R2-3	E10.0	36-45	°F (°C)
FAB	R1-33(List 2)	E10.0	1-10	*
FAMD	R1D-5(List 2)	E10.0	1-10	*
FPHI	R1-26(List 2)	E10.0	41-50	*
FPV	R1-26(List 2)	E10.0	31-40	*
FTUX	R1-26(List 3)	E10.0	1-10	*
FTUY	R1-26(List 3)	E10.0	11-20	*
FTUZ	R1-26(List 3)	E10.0	21-30	*
FTX	R1-26(List 2)	E10.0	1-10	*
FTY	R1-26(List 2)	E10.0	11-20	*
FTZ	R1-26(List 2)	E10.0	21-30	*
HADD	R1-26(List 2)	E10.0	51-60	ft (m)
HCNSTR	R1A-4	F10.0	31-40	ft (m)
HDATUM	R1-16	E10.0	31-40	ft (m)
HINIT	R1-16	E10.0	21-30	ft (m)
HTG	M-3(Card 1)	I5	16-20	++
HTOP	R1-19.1	***	-	ft (m)
I	R0-1(Card 1)	I5	16-20	++
	R2-6	I5	1-5	++
	R2-7(List 1)	I5	1-5	++
	R2-10(List 1)	I5	1-5	++
IAQ	R1-27	I5	1-5	++
IBUD	R2-11.1	I5	6-10	++
ICHCR	R2-1	I5	51-55	++
ICLL	R2-1	I5	41-45	++
ICOMP	I-1	I5	1-5	++
ID	P-2	10A4	11-50	**
IDSC	N-1	I5	1-5	++
IFD	ROD-3	I5	36-40	++
IFREE	M-2	I5	16-20	++
IIC1	R2-7(List 1)	I5	16-20	++
IIC2	R2-7(List 1)	I5	21-25	++
IINDW1	R2-7(List 1)	I5	26-30	++
IIPRT	R2-13	I5	51-55	++
IIPRTD	R2-13	I5	66-70	++
IIS	R2-10(List 1)	I5	6-10	++

Variable	Cards	Format	Column	Dimensions
IIW	R2-7(List 1)	I5	6-10	++
IJS	R2-10(List 1)	I5	11-15	++
IJW	R2-7(List 1)	I5	11-15	++
IKS	R2-10(List 1)	I5	16-20	++
ILEVEL	R1A-3	I5	1-5	++
IMETH	R2-1	I5	11-15	++
IMPG	R2-11	I5	11-15	++
IMPT	M-6	I5	1-5	++
INAT	I-1	I5	6-10	++
INDQ	R2-1	I5	1-5	++
INDT	R2-1	I5	36-40	++
IOPT	R2-1	I5	31-35	++
IO1	R2-13	I5	1-5	++
IO2	R2-13	I5	6-10	++
IO3	R2-13	I5	11-15	++
IO4	R2-13	I5	16-20	++
IO5	R2-13	I5	21-25	++
IO5D	R2-13	I5	56-60	++
IO6	R2-13	I5	26-30	++
IO8	R2-13	I5	31-35	++
IO8D	R2-13	I5	61-65	++
IPROD	R2-1	I5	26-30	++
IR	ROD-3	I5	31-35	++
	R1D-3(List 1)	I5	1-5	++
	R2-2.6(List 2)	I5	1-5	++
IRCH	R2-1	I5	46-50	++
IRD	I-1	I5	11-15	++
IRSS	R2-1	I5	21-25	++
IRT	R1A-1	I5	31-35	++
ISURF	M-2	I5	11-15	++
ITHRU	R2-1	I5	16-20	++
IUNIT	M-2	I5	36-40	++
IWELL	R2-1	I5	6-10	++
IXYZ	R2-11.1	I5	1-5	++

Variable	Cards	Format	Column	Dimensions
I1	R1-21(List 1)	I5	1-5	++
	R1-26(List 1)	I5	1-5	++
	R1-28(List 1)	I5	1-5	++
	R1-30(List 1)	I5	1-5	++
	R1-33(List 1)	I5	1-5	++
	I-2	I5	1-5	++
	I-4	I5	6-10	++
	R2-2.5	I5	6-10	++
	R2-15	I5	1-5	++
	R1D-5(List 1)	I5	1-5	++
I1A	ROD-3	I5	1-5	++
	R1A-1	I5	1-5	++
	R1A-6	I5	1-5	++
I1B	ROD-3	I5	6-10	++
	R1A-1	I5	6-10	++
	R1A-6	15	6-10	++
I2	R1-21(List 1)	I5	6-10	++
	R1-26(List 1)	I5	6-10	++
	R1-28(List 1)	I5	6-10	++
	R1-30(List 1)	I5	6-10	++
	R1-33(List 1)	I5	6-10	++
	I-2	I5	6-10	++
	I-4	I5	6-10	++
	R2-2.5	I5	6-10	++
	R2-15	I5	6-10	++
	R1D-5(List 1)	I5	6-10	++
JDSC	N-1	I5	6-10	
J1	R1-21(List 1)	I5	11-15	++
	R1-26(List 1)	I5	11-15	++
	R1-28(List 1)	I5	11-15	++
	R1-30(List 1)	I5	11-15	++
	R1-33(List 1)	I5	11-15	++
	I-2	I5	11-15	++
	I-4	I5	6-10	++
	R2-2.5	I5	6-10	++
	R2-15	I5	11-15	++
	R1D-5(List 1)	I5	11-15	++

Variable	Cards	Format	Column	Dimensions
J1A	ROD-3	I5	11-15	++
	R1A-1	I5	11-15	++
	R1A-6	I5	11-15	++
J1B	ROD-3	I5	16-20	++
	R1A-1	I5	16-20	++
	R1A-6	I5	16-20	++
J2	R1-21(List 1)	I5	16-20	++
	R1-26(List 1)	I5	16-20	++
	R1-28(List 1)	I5	16-20	++
	R1-30(List 1)	I5	16-20	++
	R1-33(List 1)	I5	16-20	++
	R2-2.5	I5	6-10	++
	I-2	I5	16-20	++
	I-4	I5	6-10	++
	R2-15	I5	16-20	++
	R1D-5	I5	16-20	++
KAQ	R1-28(List 1)	I5	31-35	++
KBC	R1D-3	I5	6-10	++
KCNVD	ROD-1	I5	1-5	++
KDSC	N-1	I5	11-15	++
KGDP(NRTD)	R1D-2(List 2)	I5	1-5	++
KGRD(NRTD)	R1D-2(List 2)	I5	6-10	++
KH	R1-31	E10.0	1-10	ft^2/d (m^2/s)
KHEAT	M-3(Card 3)	I5	66-70	++
KHL(IIC2)	R2-7(List 4)	E10.0	1-10,	**
			11-20,	
			21-30...	
KMP6	R2-14	I5	16-20	++
KMP10	R2-14	I5	21-25	++
KMP13	R2-14	I5	26-30	++
KOB	R1-13	E10.0	1-10	Btu/ft-d-°F (J/m-s-°C)
KOUT	M-3(Card 1)	I5	31-35	++
KOUTD	M-3(Card 2)	I5	16-20	++
KP(NP)	R0-1(List 2)	I5	1-5,	
			21-25...	
KPB	R1D-3(List 1)	I5	11-15	++
KSLVD	M-3(Card 2)	I5	6-10	++
KSWB	R1D-3(List 1)	I5	21-25	++
KTPB	R1D-3(List 1)	I5	16-20	++

Variable	Cards	Format	Column	Dimensions
KUB	R1-13	E10.0	21-30	Btu/ft-d-°F (J/m-s-°C)
KW	P-2	I5	1-5, 6-10	++
KX	R1-20	E10.0	1-10	ft/d (m/s)
	R1-21(List 2)	E10.0	1-10	ft/d (m/s)
KY	R1-20	E10.0	11-20	ft/d (m/s)
	R1-21(List 2)	E10.0	21-30	ft/d (m/s)
KYY(NZ)	R1-23	E10.0	11-20	ft/d (m/s)
KZ	R1-20	E10.0	21-30	ft/d (m/s)
	R1-21(List 2)	E10.0	21-30	ft/d (m/s)
KZZ(NZ)	R1-23	E10.0	21-30	ft/d (m/s)
K1	R1-21(List 1)	I5	21-25	++
	R1-26(List 1)	I5	21-25	++
	R1-28(List 1)	I5	21-25	++
	R1-30(List 1)	I5	21-25	++
	R1-33(List 1)	I5	21-25	++
	I-2	I5	21-25	++
	R2-15	I5	21-25	++
	R10-5	I5	21-25	++
K1A	ROD-3	I5	21-25	++
	R1A-1	I5	21-25	++
	R1A-6	I5	21-25	++
K1B	ROD-3	I5	26-30	++
	R1A-1	I5	26-30	++
	R1A-6	I5	26-30	++
K2	R1-21(List 2)	I5	26-30	++
	R1-26(List 2)	I5	26-30	++
	R1-28(List 2)	I5	26-30	++
	R1-30(List 2)	I5	26-30	++
	R1-33(List 2)	I5	26-30	++
	I-2	I5	26-30	++
	R2-15	I5	26-30	++
	R10-5	I5	26-30	++
LADJ(NCP)	R0-1(List 1)	I5	26-30	++
LAIF	M-2	15	56-60	
LBI0	M-2	I5	41-45	++
LMAPIT	M-2	I5	46-50	++
	M-7	I5	6-10	++
LMBAL	M-2	I5	51-55	++
L2SORP	M-2	I5	61-65	++

Variable	Cards	Format	Column	Dimensions
MAP	R2-13	I5	41-45	++
MASS(NCP)	R0-1(List 1)	I3	1-3	++
MAXITN	R2-11	I5	6-10	++
MDAT	R2-13	I5	46-50	++
METHOD	M-3(Card 1)	I5	56-60	++
	R2-2	I5	1-5	++
MINITN	R2-11	I5	1-5	++
NABLMX	M-3(Card 1)	I5	46-50	++
NCALC	R1-29	I5	1-5	++
NCALL	M-2	I5	1-5	++
	R2-11.5	I5	1-5	++
NCP	M-3(Card 1)	I5	21-25	++
NCV	R1-6	I5	1-5	++
NDT	R1-6	I5	16-20	++
NITQ	R2-3	I5	1-5	++
NI1	M-4	I5	1-5	++
	R2-16	I5	1-5	++
NI2	M-4	I5	6-10	++
	R2-16	I5	6-10	++
NJ1	M-4	I5	11-15	++
	R2-16	I5	11-15	++
NJ2	M-4	I5	16-20	++
	R2-16	I5	16-20	++
NK1	M-4	I5	21-25	++
	R2-16	I5	21-25	++
NK2	M-4	I5	26-30	++
	R2-16	I5	26-30	++
NORNXY	R2-14	I5	1-5	++
NORNXZ	R2-14	I5	6-10	++
NORNYZ	R2-14	I5	11-15	++
NOUT	R1-4	I5	1-5	++
NP(NCP)	R0-1(List 1)	I5	21-25	++
NPLC	M-2	I5	31-35	++
NPLP	M-2	I5	21-25	++
NPLT	M-2	I5	26-30	++
NPT	R1-29	I5	6-10	++
NPTDST	R1-1.5(List 1)	I5	1-5	++
NRCHMX	M-3(Card 1)	I5	51-55	++
NREPB	M-3(Card 2)	I5	1-5	++

Variable	Cards	Format	Column	Dimensions
NRT	M-3(Card 1)	I5	26-30	++
NRTD	M-3(Card 2)	I5	11-15	++
NSD(NRTD)	ROD-2	14I5	1-70	++
NSMAX	M-3(Card 1)	I5	41-45	++
NSS	R2-9	I5	1-5	++
NTIME	M-3(Card 1)	I5	61-65	++
NTVI	R1-6	I5	11-15	++
NTVR	R1-6	I5	6-10	++
NWT	R2-4	I5	1-5	++
NX	M-3(Card 1)	I5	1-5	++
NY	M-3(Card 1)	I5	6-10	++
NZ	M-3(Card 1)	I5	11-15	++
NZOB	R1-12	I5	1-5	++
NZUB	R1-12	I5	6-10	++
OD	R2-7(List 3)	E10.0	31-40	ft (m)
PBASE	R1-5	E10.0	1-10	psi (Pa)
PBD(NRTD)	R1D-3(List 2)	E10.0	1-10	psi (Pa)
PBWR	R1-3	E10.0	11-20	psi (Pa)
PHI	R1-20	E10.0	31-40	*
	R1-21(List 2)	E10.0	31-40	*
PHID(NRTD)	R1D-2(List 1)	E10.0	21-30	*
PHIH	R1-31	E10.0	11-20	ft (m)
PINIT	R1-16	E10.0	11-20	psi (Pa)
POROS(NZ)	R1-23	E10.0	31-40	*
POS	P-4	E10.0	21-30	psi (Pa)
POW	P-4	E10.0	11-20	psi (Pa)
PRT	M-3(Card 1)	I5	36-40	++
PRTAB	R1-27	I5	6-10	++
PRTIF	R1-29	I5	11-15	++
PSMN	P-3(Card 1)	E10.0	51-60	psi (Pa)
PSMX	P-3(Card 1)	E10.0	61-70	psi (Pa)
PTD(NPT)	R1-32	E10.0	11-20,	*
			31-40...	
PWMN	P-2(Card 1)	E10.0	31-40	psi (Pa)
PWMX	P-2(Card 2)	E10.0	41-50	psi (Pa)
P1	R1-28(List 2)	E10.0	11-20	psi (Pa)
Q(NWT)	R2-5	7E10.0	1-70	ft^3/d (m^3/s)
QCC(NSS,NCP)	R2-10(List 2)	6E10.0	21-80	lb/d (kg/s)
QHH(NSS)	R2-10(List 2)	E10.0	11-20	Btu/d (J/s)

Variable	Cards	Format	Column	Dimensions
QRCH	R2-2.5	E10.0	21-30	ft/d (m/s)
QWELL	R2-6	E10.0	6-16	ft^3/d (m^3/s)
QWW(NSS)	R2-10(List 2)	E10.0	1-10	lb/d (kg/s)
RAQ	R1-31	E10.0	21-30	ft (m)
RCHG	R2-2.5	E10.0	21-30	ft/d (m/s)
RE	R1-22	E10.0	21-30	ft (m)
RR(NX)	R1-24	7E10.0	1-70	ft (m)
RSTRT	M-2	I5	6-10	++
RSTWR	R2-13	I5	36-40	++
RWW	R1-22	E10.0	1-10	ft (m)
R1	R1-22	E10.0	11-20	ft (m)
SAD(NRTD)	R1D-2(List 2)	E10.0	11-20	ft (m)
SC(NCV)	R1-8	E10.0	1-10,	*
			21-30...	
SCNSTR	R1A-4	E10.0	11-20	ft (m)
SDRIFT	R1A-4	E10.0	1-10	ft (m)
SINX	R1-20	E10.0	41-50	*
SINY	R1-20	E10.0	51-60	*
SWBD(NRTD)	R1D-3(List 2)	E10.0	21-30	*
TBWR	R1-3	E10.0	21-30	°F (°C)
TBOTW	R2-7(List 3)	E10.0	51-60	°F (°C)
TBUD	R2-11.1	E10.0	11-20	+
TCHG	R2-12	E10.0	1-10	d (s)
TD(NDT)	R1-11	E10.0	11-20,	°F (°C)
			31-40...	
TD(NPT)	R1-32	E10.0	1-10,	*
			21-30...	
TDIS	R1-5	E10.0	21-30	ft^2/hr (m^2/s)
THADD	R1-26(List 2)	E10.0	61-70	ft (m)
THETA	R2-7(List 3)	E10.0	71-80	°
THETAQ	R1-31	E10.0	31-40	°
THP(NWT)	R2-8	7E10.0	1-70	psi
TI(NTVI)	R1-10	E10.0	1-10,	°F (°C)
			11-20,...	
TINJ	R2-7(List 2)	E10.0	21-30	°F (°C)
TIMTDST	R1-1.5	E10.0	1-10	d (s)
TIR	R1-7	E10.0	21-30	°F (°C)
TITLE	M-1	A80/A80	1-80	**
TMN	P-3(Card 1)	E10.0	1-10	d (s)

Variable	Cards	Format	Column	Dimensions
TMX	P-3(Card 1)	E10.0	11-20	d (s)
TO	R1-16	E10.0	1-10	°F (°C)
TOLDP	R2-3	E10.0	16-25	psi (Pa)
TOLX	R2-3	E10.0	6-15	*
TOS	P-4	E10.0	41-50	°F (°C)
TOW	P-4	E10.0	31-40	°F (°C)
TOX	P-4	E10.0	1-10	d (s)
TPARM	R2-11.1	E10.0	21-30	*
TPBD(NRTD)	R1D-3(List 2)	E10.0	11-20	°F (°C)
TR(NTVR)	R1-9	E10.0	1-10,	°F (°C)
			21-30...	
TRR	R1-7	E10.0	1-10	°F (°C)
TSMN	P-3(Card 2)	E10.0	21-30	°F (°C)
TSMX	P-3(Card 2)	E10.0	31-40	°F (°C)
TTOPW	R2-7(List 3)	E10.0	41-50	°F (°C)
TWMN	P-3(Card 2)	E10.0	1-10	°F (°C)
TWMX	P-3(Card 2)	E10.0	11-20	°F (°C)
T1	R1-28(List 2)	E10.0	21-30	°F (°C)
T2	R1-28(List 2)	E10.0	41-50	°F (°C)
T3	R1-28(List 2)	E10.0	51-60	Btu/d-ft-°F (J/m-s-°C)
UCOEF	R2-7(List 3)	E10.0	61-70	Btu/ft^3-°F-hr (J/m-s-°C)
UCPR	R1-21(List 2)	E10.0	61-70	Btu/ft^3-°F (J/m^3-°C)
UH	R1-21(List 2)	E10.0	41-50	ft (m)
UKTX	R1-2	E10.0	1-10	Btu/ft-°F-d (J/m-s-°C)
UKTY	R1-2	E10.0	11-20	Btu/ft-°F-d (J/m-s-°C)
UKTZ	R1-2	E10.0	21-30	Btu/ft-°F-d (J/m-s-°C)
UTCX(NRT)	R1-2.5(List 1)	E10.0	1-10	Btu/ft-°F-d (J/m-s-°C)
UTCY(NRT)	R1-2.5(List 1)	E10.0	11-20	Btu/ft-°F-d (J/m-s-°C)
UTCZ(NRT)	R1-2.5(List 1)	E10.0	21-30	Btu/ft-°F-d (J/m-s-°C)
UTH	R1-21(List 2)	E10.0	51-60	ft (m)
VAB	R1-28(List 2)	E10.0	1-10	+
	R1-30(List 2)	E10.0	1-10	*
VCC(NCV)	R1-8	E10.0	11-20,	cp (Pa-s)
			31-40...	
VEL	I-3	E10.0	1-10	ft/d (m/s)
VISI(NTVI)	R1-10	E10.0	11-20,	cp (Pa-s)
			31-40...	
VISIR	R1-7	E10.0	31-40	cp (Pa-s)

Variable	Cards	Format	Column	Dimensions
VISR(NTVR)	R1-9	E10.0	11-20,	cp (Pa-s)
			31-40....	
VISRR	R1-7	E10.0	11-20	cp (Pa-s)
WI	R2-7(List 2)	E10.0	1-10	ft^2/d (m^2/s)
WTFAC	R2-2	E10.0	6-15	*
X	R2-7(List 1)	E10.0	1-10	ft (m)
XYXL	R2-14.5	E10.0	1-10	in
XYYL	R2-14.5	E10.0	11-20	in
XZXL	R2-14.5	E10.0	21-30	in
XZZL	R2-14.5	E10.0	31-40	in
YXYL	R2-14.5	E10.0	41-50	in
YZZL	R2-14.5	E10.0	51-60	in
ZT(NDT)	R1-11	E10.0	1-10,	ft (m)
			21-30...	

* Dimensionless
** Alphanumeric
*** List-directed
\+ Depends on Input
++ Indicates a program flag, switch, option indicator or other indicator for which dimensions do not apply.

APPENDIX C

ENGLISH AND SI UNITS

ENGLISH AND SI UNITS

Variable	English	SI
Area	ft^2	m^2
Compressibility	1/psi	1/Pa
Component mass flow rate	lb/d	kg/s
Component transmissibility	lb/d	kg/s
Concentration	fraction	fraction
Darcy velocity	ft/d	m/s
Density	lb/ft^3	kg/m^3
Diffusivity	ft^2/d	m^2/s
Dispersivity	ft	m
Distribution coefficient	ft^3/lb	m^3/kg
Enthalpy	Btu	J
Fluid transmissibility	lb/d	kg/s
Fluid heat capacity	Btu/lb-°F	J/kg-°C
Fluid mass flow rate	lb/d	kg/s
Half-life	yr	yr
Heat flow rate	Btu/d	J/s
Hydraulic conductivity	ft/d	m/s
Length	ft	m
Mass	lb	kg
Porosity	fraction	fraction
Pressure	psi	Pa
Rock heat capacity	Btu/ft^3-°F	J/m^3-°C
Salt dissolution product	1/d	1/s
Temperature	°F	°C
Thermal conductivity	Btu/ft-d-°F	J/m-s-°C
Thermal expansion	1/°F	1/°C
Thermal transmissibility	Btu/d-°F	J/s-°C
Time	d	s
Viscosity	cp (centipoise)	Pa-s
Volume	ft^3	m^3
Waste concentration	lb/ft^3	kg/m^3
Well flow rate	ft^3/d	m^3/s
Well index	ft^2/d	m^2/s

APPENDIX D

CONVERSION OF ENGLISH TO METRIC UNITS OR THE SWIFT MODEL*

CONVERSION OF ENGLISH TO METRIC UNITS OR THE SWIFT MODEL*

MULTIPLY	BY	TO OBTAIN
1/psi	1.4504E-4	1/Pa
1/°F	1.800	1/°C
Btu/lbm-°F	4185.0	J/kg-°C
Btu/ft^3-°F	67037.	J/m^3-°C
Btu/ft-d-°F	.07208	J/m-s-°C
ft	.3048	m
ft^2/d	1.0753E-6	m^2/s
lbm/ft^3	16.018	kg/m^3
psi	6894.6	Pa
°F	.5556-17.78	°C
cp (centipoise)	.001	Pa-s
Btu/lbm	2325.0	J/kg
ft/d	3.5278E-6	m/s
lbm	.45359	kg
ft^3	.028317	m^3
Btu	1054.6	J
ft^3/d	3.2774E-7	m^3/s
d	86400.	s
lb/d	5.2498E-6	kg/s

* To facilitate data input conversions, the order of this table follows closely the order of input to the code.

APPENDIX E

ACCURACY AND NUMERICAL LIMITATIONS

ACCURACY AND NUMERICAL LIMITATIONS

When using SWIFT for Windows the question of accuracy arises. This is the particular concern for modeling waste concentrations which typically vary over many orders of magnitude. To address this issue an interpretation scale is defined. The brine and nuclide equations are formally defined in terms of mass fraction, that is, mass of constituent per mass of water. A consistent scale can be defined using the largest value of concentration and normalizing all other values. Readers should use the interpretation as guidance in model application. Inherent to developing the scale is the computer precision. Double precision variables are used consistently in SWIFT for Windows. This provides at least 15 significant figures for all real numbers.

In the Figure E-1, several limitations of model application are shown. At the lower end, the computer capable of only 15 significant figures, thus "normalized" concentrations less than 10^{-15} are meaningless. In the next range, 10^{-14} to 10^{-12} we encountered numerical error. In this range results are accurate only to an order of magnitude. In using a numerical model, the code imposes further restrictions on the results. The numerical model solves a set of partial differential equations by matrix inversion. This process of repetitive additions, subtractions and multiplications requires at least six significant figures.

At the next higher level, 10^{-8}, the conceptual model limitation is defined. Based on modeling experience, the assumption inherent in the development of a conceptual model limit the range of defensible analysis.

In the defensible analysis, model results are highly reliable and accurate. The range is from 1 to approximately 10^{-7}. This range typically exceeds the observed in natural systems. For example a hazardous waste source may be 100,000 ug/L or ppb and the detection limit from laboratory analysis is only 1 ug/L (ppb). This range is only 10^{5}.

Figure E-1. Interpretation Scale.

	0	Normalized Concentration
L	-1	
O	-2	
G	-3	
	-4	Range of Defensible Analysis
C	-5	
O	-6	
N	-7	
C		
E	-8	Conceptual Model Limitations
N		
T	-9	
R	-10	Computer Code Accuracy Limitations
A	-11	
T		
I	-12	
O	-13	Numerical Error
N	-14	
	-15	Computer Precision Limits (i.e., double precision with 15 significant digits)

APPENDIX F

DATA INPUT ERRORS

DATA INPUT ERRORS

In order to facilitate its application, the SWIFT model performs a number of checks on the input data. If an error is detected, the code then converts to an error mode of operation. In this mode, the reading of data continues through the last recurrent data set. An error summary is then written, and the run is aborted. This appendix provides an explanation of the codes which appear in the summary.

Error	Explanation	Record
1	Increment numbers are incorrectly specified: NX < 2, NY < 1 or NZ < 1.	M-3
2	Number of aquifer influence function blocks (NABLMX) exceeds the total number of blocks (NB)	M-3
3	Compressibilities assume unphysical values: CW < 0 or CR < 0; or heat capacities are given unphysical values: CPW < 0 or CPR < 0.	R1-1
4	Thermal conductivities are given unphysical values: UKTX < 0 , UKTY < 0 or UKTZ < 0; dispersivities are incorrectly specified: ALPHL < 0 or ALPHT < 0; the diffusion is erroneously defined: DMEFF < 0; or the dimensions of ALPHL and ALPHT have exceeded the dimensions (NRTMAXM): NRT > NRTMAXM.	R1-2
5	Fluid or rock densities are incorrectly specified: BROCK $\leq$ 0, BWRN $\leq$ 0 or BWRI $\leq$ 0.	R1-3
6	Viscosities are given unphysical values: VISRR $\leq$ 0, VISIR $\leq$ 0, VCC $\leq$ 0, VISR $\leq$ 0 or VISI $\leq$ 0; brine concentrations are incorrectly specified: SCC < 0 the reference temperatures have been used a second time: TR = TRR or TI = TIR; or NCV > NCVMX, NTVR > NVRMX, NTVI > NVIMX, NDT > NDTMX.	R1-7 RI-8 R1-9 R1-10
7	The heterogeneity/geometry control is outside its permitted range: HTG < 1 or HTG > 3.	M-3
8	Initialization output is incorrectly specified: KOUT =/ 0, 1 or 3.	M-3

Error	Explanation	Record
9	The print orientation control is outside its permitted range: PRT < -1 or PRT > 2.	M-3
10	For the over/underburden, either the thermal conductivity is incorrectly stated: KOB < 0 with NZOB > 2; or KUB < 0 with NZUB > 2.	R1-13
11	Grid-block sizes are specified incorrectly: DELX $\leq$ 0, DELY $\leq$ 0 or DELZ $\leq$ 0.	R1-17 R1-18 R1-19
12	Homogeneous reservoir properties are prescribed incorrectly for the incorrectly for the permeabilities: KX < 0, KY < 0 or KZ < 0; for the porosity: PHI < 0; or for the reservoir dip angles: SINX < -1 or SINX > 1, SINY < -1 or SINY > 1.	R1-20
13	Heterogeneous reservoir properties are prescribed incorrectly for the grid-block indices: I1 < 1 or I2 > NX, J1 < 1 or J2 > NY, K1 < 1 or K2 > NZ, I1 > I2, J1 > J2 or K1 > K2; for the permeabilities: KX < 0, KY < 0 or KZ < 0; for the porosity: PHI < 0 or PHI > 1 or for the heat capacity of the saturated rock: UCPR < 0.	R1-21
14	For the gridding of the radial coordinate, the radii are incorrectly specified: R1 $\leq$ RWW with R1 > 0, R1 $\geq$ RE, or ln (RE/R1)/(NX-0.5) will cause overflow.	R1-22
15	For simulation in cylindrical coordinates, the value of the vertical increment is incorrect: DELZ $\leq$ 0; the values of the permeabilities are incorrect: KYY < 0 or KZZ < 0; or the value of the porosity is incorrect: POROS < 0 or POROS > 1.	R1-23
16	Radial block centers are erroneously prescribed: RR(I) > RE for 1 $\leq$ I $\leq$ NX.	R1-25

Error	Explanation	Record
17	Block edges are incorrectly specified for the reservoir modifications: I1 < 1 or I1 > NX, J1 < 1 or J1 > NY, K1 < 1 or K2 > NZ, I1 > I2, J1 > J2 or K1 > K2.	R1-26
18	Aquifer-influence conditions are in error for the option parameter: IAQ < 0 or IAQ > 4; or for the block edges: I1 < 1 or I2 > NX, J1 < 1 or J2 > NY, K1 < 1 or K2 > NZ I1 > I2, J1 > J2 or K1 > K2; or NPT > NPTMX.	R1-27 R1-28
19	The number of aquifer-influence functions (NABL) summed from the input specifications exceeds that allocated (NABLMX) in READ M-3 or the number of points in the table of influence function (NPT) exceeds that allocated (NPTMX).	R1-28
20	The number of recharge blocks (NRCH) summed from the input specifications exceeds that allocated (NRCHMX) in READ M-3.	R2-2.5
21	For initialization of the brine concentrations, the block indices are given incorrectly: I1 < 1 or I2 > NX, J1 < 1 or J2 > NY, K1 < 1 or K2 > NZ I1 > I2, J1 > J2 or K1 > K2; or for the concentration: CINIT < 0.	I-2
22	For initialization of the radionuclide concentrations, the block indices are given incorrectly, as specified for Error 21.	I-4
23	Some grid block, which has a nonzero pore volume also has a zero sum of transmissibilities over its surface.	R1-21 R1-26
24	A grid-block pore volume is negative.	R1-26
25	The number of wells is specified incorrectly: NWT < 1 or NWT > NWMAX where the latter parameter is defined internally within routine MAIN. Currently the value of this quantity is: NWMAX = 100.	R2-4
26	A well index I is out of range: I < 1 or I > NWT.	R2-6
27	Well locators IIW and IJW are outside the reservoir: IIW < 1 or IIW > NX, IJW < 1 or IJW > NY.	R2-7

Error	Explanation	Record
28	The well-completion zone lies outside of the system: IIC1 < 1 or IIC2 < 1, IIC1 > NZ or IIC2 > NZ, IIC1 > IIC2, or the top block of the completion interval has zero pore volume.	R2-7
30	The well-specification option is erroneously given: IINDW1 =/ 1, ±2, ±3, or ±4 or IINDW1 = 2, 3, 4 with NCALL greater than 4.	R2-7
32	Well index is incorrectly defined: WI $\leq$ 0 with IINDW1 $\neq$ 1.	R2-7
35	The completion interval contains only blocks having zero pore volumes.	R2-7
37	Layer-allocation factors are incorrectly prescribed: KHL < 0.	R2-7
38	All layer-allocation factors, KHL, are zero. At least one KHL factor must be nonzero.	R2-7
39	39A well identification number I is out of range: I < 1 or I > NWT.	R2-7
40	Differencing and matrix solution are improperly given: METHOD < -2 or METHOD > 2 or WTFAC > 1.	R2-2
41	The number of nonlinear iterations is incorrect: MINITN < 1 or MINITN > MAXITN.	R2-11
43	Recurrent time is specified incorrectly TCHG $\leq$ TIME where TIME is the current time.	R2-12
44	The time step is: DT = 0 for the first time step.	R2-12
45	The maximum time step is erroneous: DTMAX < DTMIN.	R2-12
46	Mapping is specified incorrectly in that one of the four digits of MAP is greater than unity.	R2-13
47	Maps are prescribed incorrectly: I1 < 1 or I2 > NX, J1 < 1 or J2 > NY, K1 < 1 or K2 > NZ, I1 > I2, J1 > J2 or K1 > K2, or for cylindrical geometry (HTG = 3, READ M-3) J2 $\neq$ 1.	R2-15
48	The number of nuclide monitor blocks encountered exceeds that allocated exceeds that allocated (NDSCMX).	R2-16

Error	Explanation	Record
50	Sink/source information contains error. The number of blocks of blocks containing sinks is greater than that allocated: NSS > NSMAX; the sink number is too large: I > NSS; or the block indices are incorrect: IIS < 1 or IIS > NX, IJS < 1 or IJS > NY, IKS < 1 or IKS > NZ.	R2-9 R2-10
51	Radioactive-component specification is incorrect. For the component number, I = 0 or I > NCP, or for the number of parents, NP < 0.	R0-1
52	The half-life is physically unreasonable: DEC < 0.	R0-1
53	Branching, as specified, is incorrect. For the parent index, KP < 1 or KP > NCP, or for the branching ratio, AP < 0.	R0-1
54	The Freundlich κ factor is given incorrectly: DIS(I) < 0, I $\leq$ NCP.	R0-2
55	For the rock-type modifications, the block numbers are out of range: I1A < 1 or I1B > NX, J1A < 1 or J1B > NY, K1A < 1 or K1B > NZ. I1A > I1B, J1A > J1B or K1A > K1B.	R1A-1
56	The salt-dissolution coefficient is prescribed erroneously: ACS < 0.	R1A-2
57	For canistered storage (ILEVEL = 1, READ R1A-3), the spacing parameters are given incorrectly: SDRIFT < 0, SCNSTR < 0, DCNSTR < 0, or HCNSTR < 0.	R1A-4
58	The specified location of the repository is unreasonable. A block number is out of range: I1A < 1 or I1B > NX, J1A < 1 or J1B > NY, K1A < 1 or K1B > NZ; I1A > I1B, J1A > J1B or K1A > K1B. or the allocated number of repository blocks, NREPB, is exceeded.	R1A-6
59	For the concentration of the unleached wastes or the repository heat load, the interpolation table is given incorrectly: CTIME $\leq$ 0, or the values are not in ascending order.	R1A-7

Error	Explanation	Record
60	For canistered storage (ILEVEL = 1 in READ R1A-3), the storage-parameter values are erroneous: SDRIFT > Max (DELX, DELY), SCNSTR > Max (DELX, DELY), or HCNSTR > DELZ.	R1A-4
61	Solubilities are given incorrectly: CS < 0.	R1A-9
62	The dual-porosity blocks are not specified correctly. Block indices are in error: I1A < 1 or I1B > NX, J1A < 1 or J1B > NY, K1A < 1 or K1B > NZ; I1A > I1B, J1A > J1B or K1A > K1B; the local rock-type indicator is outside its permitted range: IR > NRTD; or the position control for the local unit can not be interpreted: IFD < -3 or IFD > 3.	ROD-3
63	The properties of the local units have unphysical values. For the rock compressibility: CRD < 0; for auto mesh generation the length of the local units: SAD $\leq$ 0 or DSD $\leq$ 0; for double mesh generation: DSDO < 0; for user defined mesh: DS(I) $\leq$ 0; for permeability and porosity: AKSD < 0 or PHID < 0; for the dispersivity: ALPD < 0; or for the thermal conductivity and heat capacity: UKTD < 0 or CPRKD < 0.	R1D-1 R1D-2
64	Distribution coefficients are incorrect: D1SD < 0.	R1D-4
65	Mesh generation is prescribed incorrectly. For single mesh-generation (outer increment DSDO = 0), thee is an insufficient number of nodes (KGRD = 1): NSD $\leq$ 3; or for double-mesh generation (DSDO > 0), there is an insufficient number of nodes (KGRD = 2): NSD $\leq$ 4.	ROD-2 R1D-2
66	Grid block volume is less than pore volume in a dual porosity block. Avoid pore volume modification with dual porosity blocks.	R1-26

Error	Explanation	Record
67	Modifications to dual porosity blocks are not specified correctly. Block indices are in error: I1 < 1 or I1 > NX, J1 < 1 or J1 > NY, K1 < 1 or K1 > NZ, I1 > I1, J1 > J2, or K1 > K2.	R1D-5