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User's Manual for the Sandia Waste-Isolation Flow and Transport Model (SWIFT) Release 4.81

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Mark Reeves, Robert M. Cranwell

Prepared for
U. S. NUCLEAR REGULATORY COMMISSION

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USER'S MANUAL FOR THE SANDIA WASTE-ISOLATION
FLOW AND TRANSPORT MODEL (SWIFT)
RELEASE 4.81

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and

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November 1981

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Albuquerque, New Mexico 87185
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for the
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ABSTRACT

This report describes a three-dimensional finite-difference model (SWIFT) which is used to simulate flow and transport processes in geologic media. The model was developed for use by the Nuclear Regulatory Commission in the analysis of deep geologic nuclear waste-disposal facilities. This document, as indicated by the title, is a user's manual and is intended to facilitate the use of the SWIFT simulator. Mathematical equations, submodels, application notes, and a description of the program itself are given herein. In addition, a complete input data guide is given along with several appendices which are helpful in setting up a data-input deck.

ACKNOWLEDGMENTS

Much of the text of Chapters 2 through 5 has been presented previously in short courses given to staff members of Sandia National Laboratories and the Nuclear Regulatory Commission. The helpful comments of those who attended is gratefully acknowledged. However, this document would not have been possible without the tireless efforts of two members of the INTERA secretarial staff, Ms. Mary G. Michaux and Ms. Joyce A. Chavers, to whom we extend our sincere appreciation.

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CHAPTER 1

INTRODUCTION

1.1 BRIEF DESCRIPTION OF THE SWIFT MODEL

Computer code SWIFT (Sandia Waste Isolation, Flow and Transport Model) is a fully transient, three-dimensional model which solves the coupled equations for transport in geologic media. The processes considered are:

- (1) fluid flow
- (2) heat transport
- (3) dominant-species^a miscible displacement
- (4) trace-species^b miscible displacement

The first three processes are coupled via fluid density and viscosity. Together they provide the velocity field on which the fourth process depends.

1.2 APPLICATIONS OF SWIFT

Because of their generality, these models have many applications. They include, but are not limited to, the following:

- nuclear waste isolation in various geologic formations
- injection of industrial wastes into saline aquifers
- heat storage in aquifers
- in-situ solution mining
- migration of contaminants from landfills
- disposal of municipal wastes
- salt-water intrusion in coastal regions
- brine disposal from petroleum-storage facilities
- brine disposal as a byproduct of methane production from geopressured aquifers
- determination of aquifer transport parameters from well-test data

^a Hereafter referred to as "brine".

^b Hereafter referred to as "radionuclides".

1.3 DEVELOPMENT OF SWIFT

The first phase in the evolution of these codes began in 1975 when the U. S. Geological Survey (USGS) awarded a contract to INTERCOMP Resource Development and Engineering, Inc., a company with international experience in oil-reservoir simulation and, at that time, the parent company of INTERA Environmental Consultants. The objective of this contract was to develop a general model to simulate waste injection in deep saline aquifers. The result of this effort was a simulator for singlephase fluid flow, heat transport both through the rock and the fluid media, and fluid compositional changes for a dominant miscible component. The work is discussed in the reference INTERCOMP [1976].

The second phase in the development of SWIFT began in 1977 at Sandia Laboratories of Albuquerque, New Mexico. This organization, under contract to the U. S. Nuclear Regulatory Commission (NRC), sought to acquire, in the form of a computer simulator, a waste-isolation methodology to treat coupled three-dimensional transport of fluid, brine in nondilute concentrations, heat, and chains of radionuclides in dilute concentrations for periods of time approaching one million years. After examining the then existing technology at several national laboratories in the U. S. and within the USGS, Sandia scientists concluded that no computer model existed which included all the necessary features for a nuclear waste-isolation model. They also concluded that, among the available models, INTERA's waste-injection program represented the state of the art for geosphere simulation. Consequently, INTERA was engaged under subcontract to Sandia to add the transport of radionuclide chains to the existing code. The resulting computer model, i.e., the original version of the SWIFT simulator, is discussed in the report by Dillon, Lantz, and Pahwa [1978]. Since that time, various submodels have been added and improvements in efficiency have been made.

1.4 PURPOSE OF THIS DOCUMENT

The purpose of this document is to describe the SWIFT model itself. Thus the theoretical underpinning, the program structure, and an input data guide are presented. Some general guidance on application of the model is also given. However, detailed instruction on application are reserved for a companion document by Finley and Reeves [1981]. There eleven sample problems are thoroughly discussed and the corresponding input and output of the SWIFT model are presented. This document, thus, is one of two which are designed to enable the analyst to effectively use the SWIFT computer model. The discussion begins with the basic transport equations.

CHAPTER 2

MATHEMATICAL MODEL

2.1 TRANSIENT FLUID FLOW AND HEAT, BRINE AND RADIONUCLIDE TRANSPORT

The transport equations used here are obtained by combining the appropriate continuity and constitutive relations and have been derived by several authors (e.g., see Cooper [1966]; Reddell and Sunada [1970]; Bear [1979]; and Aziz and Settari [1979]). The resulting relations may be stated as follows:

Fluid:

$$\nabla \cdot (\rho \mathbf{u}) - q + R_s' = \frac{\partial}{\partial t} (\phi \rho) \quad (2-1)$$

conduction production salt accumulation
dissolution

Heat:

$$\begin{aligned}
 -\nabla \cdot (\rho \underline{H} \underline{u}) + \nabla \cdot (\underline{\underline{E}}_H \cdot \nabla T) - q_L \\
 \text{convection} \quad \text{conduction/} \quad \text{heat loss to} \\
 \text{dispersion} \quad \text{under/overburden} \\
 - q_H \quad - q_H \\
 \text{injected} \quad \text{produced} \quad (2-2) \\
 \text{enthalpy*} \quad \text{enthalpy} \\
 = \frac{\partial}{\partial t} [\phi \rho \underline{u} + (1-\phi) \rho_R c_{pR} T] \\
 \text{accumulation in fluid and rock}
 \end{aligned}$$

+ All terms are defined in the notation section.

* This is a source term since, via the sign convention adopted here, the rate of fluid injection is inherently negative.

Brine:

$$\begin{array}{l} -\nabla \cdot (\rho \hat{C} \underline{u}) + \nabla \cdot (\rho E_C \cdot \nabla \hat{C}) - q\hat{C} \\ \text{convection} \quad \text{dispersion/} \quad \text{injected} \\ \text{diffusion} \quad \text{brine*} \end{array} \quad (2-3)$$
$$\begin{array}{l} -q_C + R_s = \frac{\partial}{\partial t} (\phi \rho \hat{C}) \\ \text{produced} \quad \text{salt-} \quad \text{accumulation} \\ \text{brine} \quad \text{dissolution} \end{array}$$

Radionuclide (component i):

$$\begin{array}{l} -\nabla \cdot (\rho C_i \underline{u}) + \nabla \cdot (\rho E_C \cdot \nabla C_i) - qC_i - q_{ci} \\ \text{convection} \quad \text{dispersion/} \quad \text{injected} \quad \text{produced} \\ \text{diffusion} \quad \text{components*} \quad \text{components} \end{array} \quad (2-4)$$
$$\begin{array}{l} + q_{oi} + \sum_{j=1}^N k_{ij} \lambda_j K_j \phi \rho C_j - \lambda_i K_i \phi \rho C_i \\ \text{waste} \quad \text{generation of} \quad \text{decay of} \\ \text{leach} \quad \text{component i by} \quad \text{component i} \\ \text{decay of j} \end{array}$$
$$= \frac{\partial}{\partial t} (\phi \rho K_i C_i)$$

accumulation

Several quantities in Eqs. (2-1) - (2-4) require further definition in terms of the basic parameters. The tensors in Eqs. (2-2), (2-3) and (2-4) are defined as sums of dispersion and molecular terms:

* This is a source term since, via the sign convention adopted here, the rate of fluid injection is inherently negative.

$$\underline{\underline{\epsilon}}_C = \underline{\underline{D}} + D_m \underline{\underline{I}} \quad (2-5)$$

and

$$\underline{\underline{\epsilon}}_H = \underline{\underline{D}} \rho c_{pw} + K_m \underline{\underline{I}} \quad (2-6)$$

where

$$D_{ij} = \alpha_T u \delta_{ij} + (\alpha_L - \alpha_T) u_i u_j / u \quad (2-7)$$

in a cartesian system. Also, adsorption of radionuclides is included via an assumption of a linear equilibrium isotherm. This yields the distribution coefficient k_{di} and the retardation factor of Eq. (2-4):

$$K_i = 1 + \rho_R k_{di} (1-\phi) / \phi \quad (2-8)$$

Equations (2-1) - (2-4) are coupled by four auxiliary relations for Darcy flux:

$$\underline{\underline{u}} = -(\underline{\underline{k}} / \mu) (\nabla p - \rho \frac{\underline{\underline{g}}}{g_c} \nabla z) \quad (2-9)$$

porosity:

$$\phi = \phi_0 [1 + c_R (p - p_0)] \quad (2-10)$$

fluid density:

$$\rho = \rho_0 [1 + c_w (p - p_0) + c_T (T - T_0) + c_s \hat{C}] \quad (2-11)$$

fluid viscosity:

$$\mu = \mu_R (\hat{C}) \exp [B(\hat{C}) (T^{-1} - T_R^{-1})] \quad (2-12)$$

where parameter c_s is defined in terms of an input density range ($\rho_I - \rho_N$) and the reference density ρ_0 :

$$c_s = (\rho_I - \rho_N) / \rho_0 \quad (2-13)$$

2.2 STEADY-STATE SPECIALIZATION OF THE FLOW AND BRINE-TRANSPORT EQUATIONS

In safety evaluations for nuclear-waste depositories quite often the frame of interest may extend over many thousands of years. Typically the assumption of time-invariant flow, heat and brine conditions is justified in such cases due to the lack of specific data for such a long period of time. For the fluid flow, the overall effect of transient rainfall boundary conditions may have a minor effect on radionuclide transport. Duguid and Reeves [1976] have shown this for a combined saturated-unsaturated simulation of tritium transport over a period of only one month. For the heat transport, a geothermal gradient or even a constant temperature may be adequate and can be prescribed as an initial condition for the SWIFT code. For the brine transport, a relatively simple stratigraphy will sometimes permit a hand-calculation of the steady-state brine distribution. Such a case may also be included in the SWIFT calculation by the use of an initial condition. More complex stratigraphies, however, may require solution of the steady-state brine equation to give the brine distribution relative to the location of the salt formation(s).

To treat such safety evaluations most efficiently, two steady-state options have been included in the SWIFT code. The first option permits solution of the time-independent flow equation:

Fluid (steady state):

In both options the accumulation term is set to zero, as shown explicitly in Eq. (2-14). For the steady-state fluid flow option, however, the salt-dissolution term is also set to zero, and the presence of brine and heat are included via the mechanisms of a variable density and a variable viscosity.

The second option permits a coupled time-independent solution for both fluid flow, Eq. (2-14), and brine transport:

Brine (steady state):

$$\begin{array}{l} -\nabla \cdot (\rho \hat{C} \mathbf{u}) + \nabla \cdot (\rho \mathbf{E}_C \cdot \nabla \hat{C}) - q\hat{C} \\ \text{convection} \quad \text{dispersion/} \quad \text{injected} \\ \text{diffusion} \quad \text{brine*} \\ \\ -q_C + R_s = 0 \\ \text{produced} \quad \text{salt-} \\ \text{brine} \quad \text{dissolution} \end{array} \quad (2-15)$$

In this case, in addition to a variable density and a variable viscosity, the salt-dissolution term is non-zero, in general.

2.3 SOLUTION TECHNIQUES

Equations (2-1) to (2-4) including steady-state variation in Eqs. (2-14) and (2-15) form a set of coupled parabolic equations. The equations for flow, Eqs. (2-1) or (2-14), heat, Eq. (2-2), and brine, Eqs. (2-3) or (2-15), are relatively strongly coupled through Eqs. (2-9) - (2-12) and must be solved iteratively. However, the transport equations for the radionuclides, i.e. Eq. (2-4), are relatively weakly coupled to the others. This fact arises from the assumption of trace concentrations for the radionuclides. Thus, Darcy velocity, porosity, density and viscosity are determined independently of radionuclide concentrations, and, for a given time step, there is no need to iterate the radionuclide solution procedure.

The numerical algorithm is discussed thoroughly in Appendix A of INTERCOMP [1976]. Here only a general overview is presented. Very briefly, then, the region of interest is divided into grid blocks, and finite differencing is invoked in both space and time domains. Either centered or upwind-weighting schemes may be used in the spatial differencing, and either centered or fully implicit schemes may be used in the temporal differencing. The primary difference between transient and steady-state algorithms is the choice of dependent variables. In the latter, the variables are p and \hat{C} rather than δp and $\delta \hat{C}$. Such a choice permits direct calculation of the steady-state without any intermediate steps. One rather unique feature of the algorithm is a formal gaussian elimination between the discretized flow, heat, and brine equations for the purpose of minimizing coupling. Also, transmissibilities, which control grid-block transfers and which arise from the conduction and dispersion terms, are lagged by one time step, again for the purpose of minimizing the deleterious effects of the nonlinear coupling.

One of the attractive features of the SWIFT code is the matrix-solution option which these codes offer. Either direct or two-line successive over-relaxation methods may be used. Typically, the former is preferable because of its efficiency. However, whenever core storage is a problem, the over-relaxation approach is available. In either case, sparseness methods are used to maximize computer efficiency. In addition, the method of Price and Coats [1973] is used to achieve an optimal band-width structure through a particular ordering of the grid-block numbers.

Another attractive feature of the code is that of dynamic storage allocation. The code has been written especially for storage efficiency by placing all variably dimensioned variables within one blank-common array. As a part of its initial setup procedure, the code then determines the maximum dimensions of these variables and allocates the required core. Such dynamic allocation is permitted by most of the Control Data installations on which the code is currently implemented. However, for other installations in which dynamic allocation is not permitted, only the main subprogram need be recompiled to optimize storage.

CHAPTER 3 SUBMODELS

The SWIFT model contains several submodels which have been implemented in order to broaden their ranges of applicability. Submodels for density, viscosity, wells, and the overburden/ underburden region were included in the original development for treatment of the waste-injection problem. Then, waste-leach and salt-dissolution submodels were added for assessing the transport of wastes within a bedded-salt formation, and a radiation boundary option was implemented to permit a more general treatment of the heat transport. The following sections present mathematical formulations and, when possible, validations and verifications of these submodels.

3.1 DENSITY

One of the unique features of the SWIFT model is that it permits variable densities and viscosities. The submodel for density is given in Eq. (2-11) :

$$\rho = \rho_0 [1 + c_w(p-p_0) + c_T (T-T_0) + c_s \hat{C}] \quad (3-1)$$

This relation has been investigated recently by Muller, Finley and Pearson [1980]. They conclude that the use of constant values for c_w and c_s are adequate for most simulations but that the constant c_T must be carefully chosen for the expected temperature range. They argue that since the variation of c_w is only 0.5 percent for a pressure change of 100 bars that the use of a constant value of c_w is adequate for most hydrological simulations. As for the brine coefficient c_s , they note that the experimentally observed variation of density with concentration is not linear for four different salts. However, using a linear relation introduces, at most, a two percent error in the density. Such an error would most likely be quite acceptable relative to other uncertainties in most simulations.

Parameter c_T is somewhat more variable than c_w and c_s . To show this, Muller, Finley and Pearson compare experimental data from Kennedy and Holser [1966] with the linear model of SWIFT and with a density model of Sorey [1978], which contains a quadratic term in

All terms are defined in the notation section.

temperature. Figure 3-1 shows density variations from a reference value at 20°C. As shown, Sorey's quadratic model compares quite favorably with the data. The linear model shows a rather sensitive dependence to the value chosen for c_T . If this value is taken from the slope of the data at 20°C, the predicted densities can vary from the data by as much as eight percent at elevated temperatures. However, if the value for c_T is chosen at 60°C, the variation is no more than about one percent.

The reference INTERCOMP [1976] examines parameters c_s and c_T as coupled functions of both brine concentration and temperature and makes similar observations. The conclusion is that a linear model is quite adequate for parameters c_w and c_s , but that to use the linear density model, one must choose c_T based on the expected temperature range.

3.2 VISCOSITY

The SWIFT model uses Eq. (2-12) to express the dependence of viscosity upon concentration and temperature, namely

$$\mu = \mu_R(\hat{C}) \exp [B(\hat{C}) (T^{-1} - T_R^{-1})] \quad (3-2)$$

Quantities μ_R and B are empirical functions which are determined from data. The relation in Eq. (3-2) is shown schematically by Figure 3-2. Data of varying amounts, depending on availability, are specified along Curves r , i , and c and are used to determine the empirical relations $\mu_R(\hat{C})$ and $B(\hat{C})$. Curves r and i are given by the extreme concentration values and are given as $\mu(0, T)$ and $\mu(1, T)$, respectively. Curve c , on the other hand, is defined by an intermediate value of temperature called the reference temperature T_R , and is given by $\mu(\hat{C}, T_R)$. From the data given for Curves r and i , the following four values of the empirical constants are determined: $\mu_R(0)$, $\mu_R(1)$, $B_r = B(0)$ and $B_i = B(1)$. From the latter two, function $B(\hat{C})$ is determined by linear interpolation. From the former two, and from such additional data given along Curve c as may be available, function $\mu_R(\hat{C})$ is determined either by linear interpolation or by power-law interpolation, depending on the amount of additional data. Very briefly, then, Eq. (3-2) and the above-mentioned techniques for determining empirical functions $\mu_R(\hat{C})$ and $B(\hat{C})$ constitute the viscosity submodel of the SWIFT programs.

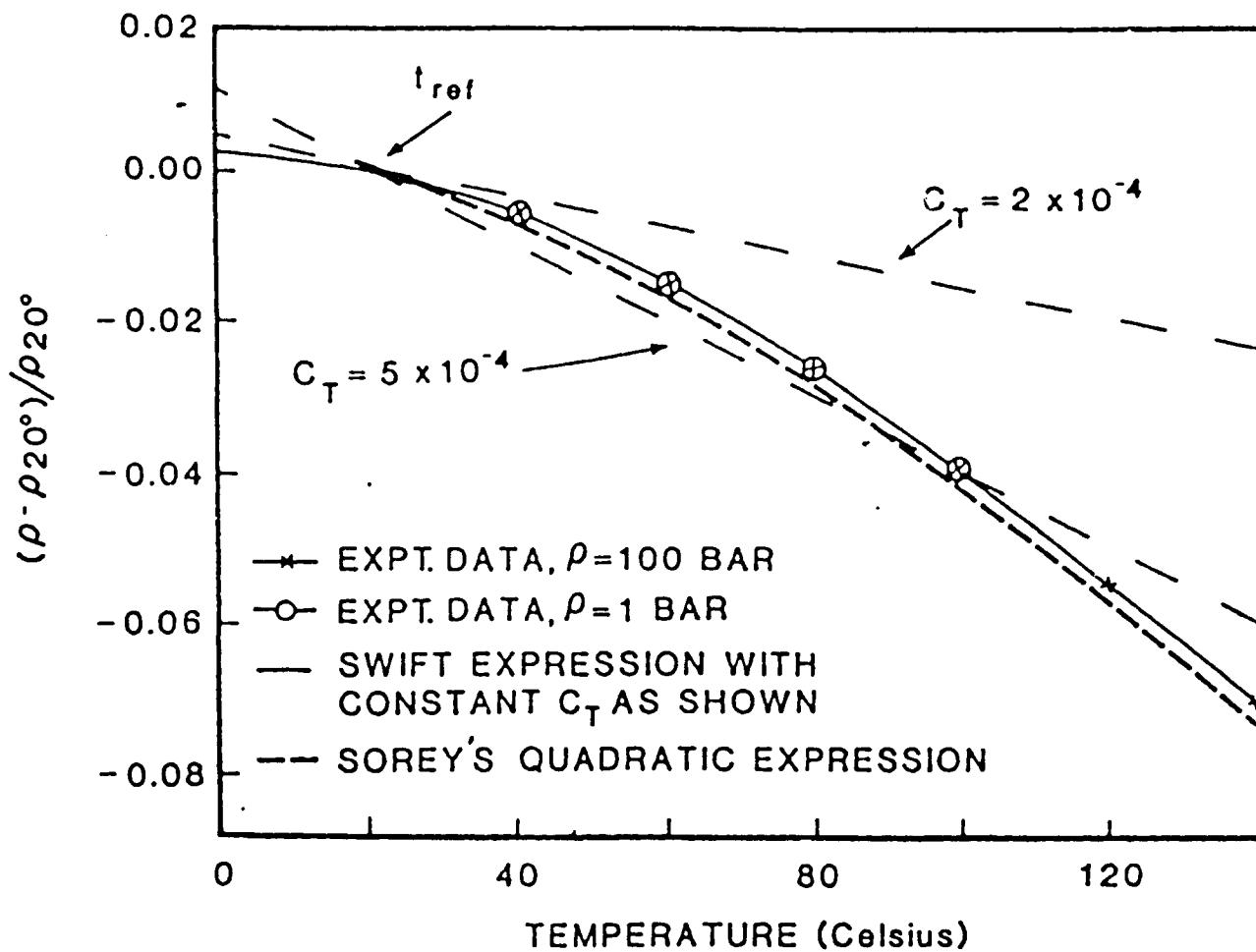


Figure 3-1. Graph of density variations as a function of temperature. The SWIFT linear model may be compared with Sorey's quadratic model and with experimental data for pur water from Kennedy and Holser (1966).

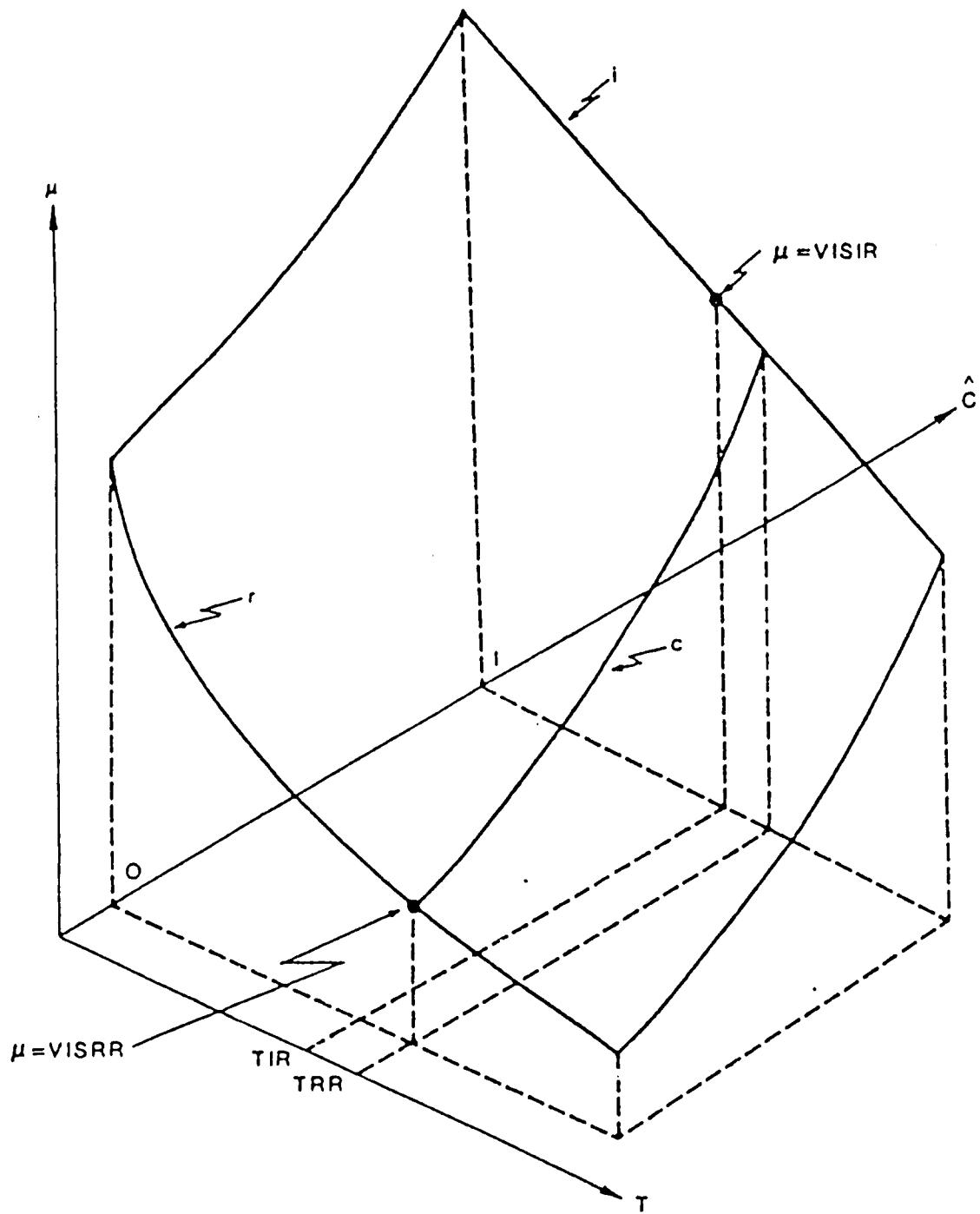


Figure 3-2. Fluid viscosity as a function of temperature and concentration.

The minimum amount of data which must be specified consists of the two points $\mu(0, \text{TRR}) = \text{VISRR}$ and $\mu(1, \text{TRR}) = \text{VISIR}$. Here, additional data from the general curve of Lewis and Squires [1934] is supplied internally by the program. Additionally, one may specify other values for $\hat{C} = 0$ and $\hat{C} = 1$, i.e., for Curves r and i in Figure 3-3. Or, in the best case, one may also supply mixture data for reference temperature $T = \text{TRR}$.

Muller, Finley and Pearson compare model calculations in two of the above cases with experimental viscosity-temperature data for pure water. Some of their results are shown graphically in Figure 3-3, where the experimental data of various researchers may be compared with results from the SWIFT model. For the curve labelled "general curve of SWIFT", only one data point is supplied. The model supplemented this single data point with the general curve of Lewis and Squires [1934] and performed a least-squares fit to obtain the parameters $\mu_R(0)$ and $B(0)$ of Eq. (3-2). Model results compare relatively poorly with the experimental data at the two extremes in temperature. Here there is a 25-percent deviation of model results from experimental data.

For the curve labelled "exact fit" in Figure 3-3, only two data points are supplied, namely viscosities at the reference temperature of 20°C and at 60°C . The model then performs an exact fit to obtain $\mu_R(0)$ and $B(0)$. The comparison with experimental data here is quite satisfactory for the temperature range $0 - 120^\circ\text{C}$. Of course, additional viscosity-temperature values could be used to improve the fit still further.

In INTERCOMP [1976], this viscosity model is compared with experimental viscosity-concentration data. Varying amounts of viscosity-temperature and viscosity-concentration (at 59°F) data are specified for the determination of the empirical functions $\mu_R(\hat{C})$ and $B(\hat{C})$. In each case, the model is then used to calculate a viscosity-concentration curve at 150°F . Results are displayed in Figure 3-4, and the observations here are quite similar to that of Muller, Finley and Pearson [1980]. In Case III, only two data points are provided, and the viscosity model uses the data of Lewis and Squires [1934]. Here, the agreement between model and experimental results is relatively poor with a maximum deviation of about 18 percent. On the other hand, in Cases I and II, where additional data is specified, calculated results are quite acceptable, showing, at most, a 5 percent deviation from the experimental data.

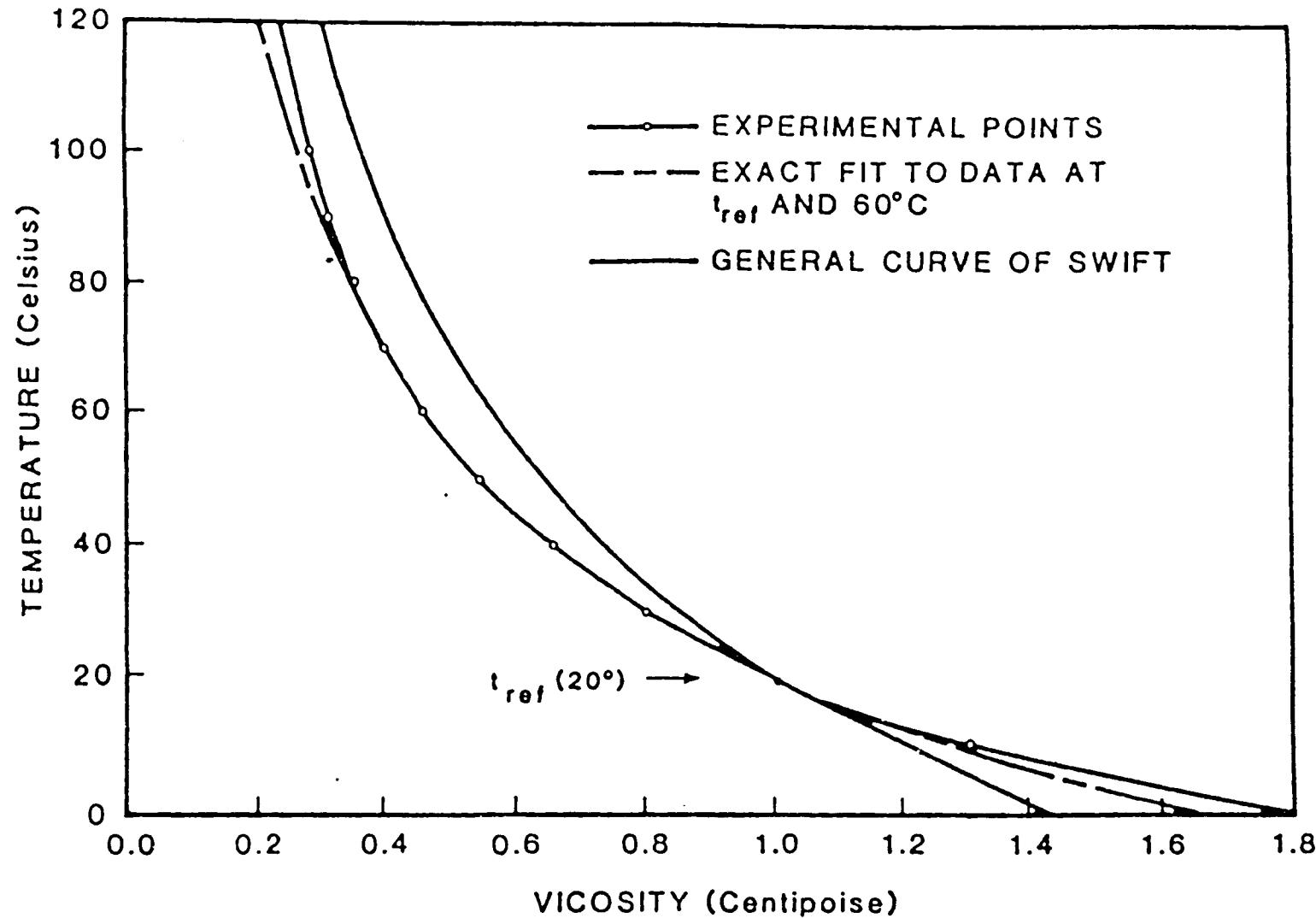


Figure 3-3. Graph comparing viscosities measured at various temperatures with those calculated with the SWIFT viscosity model.

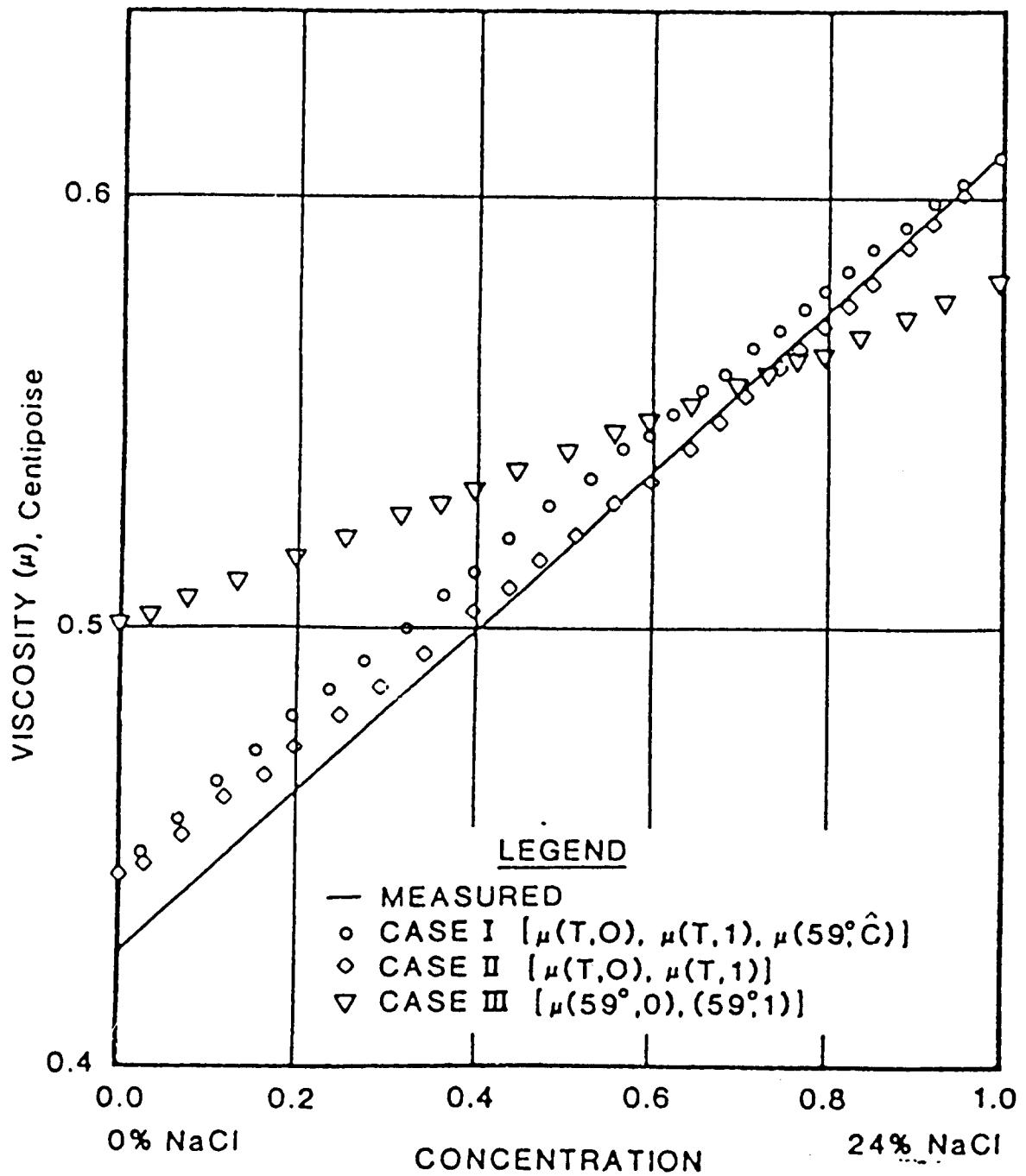


Figure 3-4. Predicted brine viscosity at 150°F with three levels of available data (T, \hat{C})

3.3 SALT DISSOLUTION

One submodel of the SWIFT model is that of salt dissolution. This mechanism appears in the fluid flow equation, Eq. (2-1), through the source term R'_s and in the brine equation, Eq. (2-3), through the source term R_s . These quantities are defined by

$$R_s = \phi \rho k_s f_s (1 - \hat{C}) \quad (3-3)$$

and by

$$R'_s = c_s R_s / (1 + c_s) \quad (3-4)$$

where coefficient c_s is defined by Eq. (2-13). It should be noted that two parameters are used to characterize the dissolution process, namely a rate constant k_s and a mass fraction f_s of solubles to total solid mass. This formulation of dissolution is similar to that of Nolen, et al. [1974] where salt-cavern formation for storage of crude oil was considered.

3.4 WASTE LEACH

Another submodel which is present is that for waste leach. The purpose of this model is to determine the source rate q_{0i} (see Eq. (2-4)) at which a radionuclide from a repository is dissolved into solution.

More specifically, this model considers each radioactive component to be in one of three distinct phases, characterized as being either

- (1) unleached from the waste matrix,
- (2) leached but undissolved, or
- (3) dissolved.

Phases (1) and (2) are coupled by the leach rate. There is, of course, considerable uncertainty in the time dependence of this rate. However, in accord with arguments given by Campbell, et al. [1978], we have chosen a constant leach rate for the implementation. Phase (2) and (3) above are coupled by the solubilities. Very simply, the source rate q_{0i} for solubilizing Phase (2) is kept sufficiently small that the solubility of any given nuclide will not be exceeded. Radioactive decay and production processes are considered throughout the analysis.

As mentioned above, there are three phases to be tracked, specifically, the unleached radionuclides within the canisters m_i , the undissolved leachate S_j , and the dissolved leachate C_j . The appropriate conservation equations may be written in the following manner. For the dissolved phase of component i :

$$\begin{aligned} -\nabla \cdot (C_i \underline{u}) - q_{oi} + \sum_j k_{ij} \lambda_j K_j \phi \rho C_j - \lambda_i K_i \phi \rho C_i \\ = \frac{\partial}{\partial t} (\phi \rho K_i C_i) \end{aligned} \quad (3-5)$$

for the undissolved, but leached, component i :

$$-R_i + q_{oi} + \sum_j k_{ij} \lambda_j S_j - \lambda_i S_i = \frac{dS_i}{dt} \quad (3-6)$$

and for the unleached component i :

$$\sum_j k_{ij} \lambda_j m_j - \lambda_i m_i = \frac{dm_i}{dt} \quad (3-7)$$

The constant fractional leach rate is taken to be $1/a$, which yields the leach rate:

$$R_i = \begin{cases} -m_i(t) \rho_W / a, & b \leq t \leq b+a \\ 0 & \text{otherwise} \end{cases} \quad (3-8)$$

It is understood that $j \neq i$ in each summation in the radioactive decay and production terms of Eqs. (3-5) - (3-7). Equations (3-5) and (3-6) are always solved numerically by the SWIFT code.

Two comments are appropriate for the waste-leach equations, Eqs. (3-5) - (3-8). First of all, for the unleached component, Eq. (3-7) either may be solved internally, and numerically, by the SWIFT code, or may be solved externally by a code such as the ORIGEN code [Bell, 1973]. In the latter case, power-law interpolation from

tabular input data is used by SWIFT. Secondly, it may be noted that Eq. (3-5) is a simplified version of Eq. (2-4), the general transport equation for a radionuclide. Dropping the source term qC_i is immaterial, if there are no withdrawal wells in the repository. Neglecting dispersion, i.e. the E term, however, deserves some explanation. Equations (3-5) - (3-8) are solved only for repository blocks and not for the entire system. The purpose is only to determine q_{0i} , and in order to make the algorithm as efficient as possible, physical dispersion is neglected. Furthermore, in order to calculate q_{0i} most easily, an explicit algorithm is used for the convective-transport term in Eq. (3-5). This results in numerical dispersion which compensates, to some extent, for the loss of the physical dispersion term. As a final word of explanation, it should be noted that the accuracy of the solution of Eq. (3-5) is important only for the case in which solubility is restrictive. Our present experience indicates that the algorithm performs quite satisfactorily even in that case in that it achieves the solubility to within a few percent.

3.5 WELLS

The term "well", as used here, denotes either a source or a sink for a system. Mathematically it is denoted by q in Eqs. (2-1) - (2-4). Physically a "well" may be used to characterize a variety of mechanisms. Originally, when the SWIFT code was strictly a waste-injection model (see INTFRCOMP, [1976] Part I, App. B), this facility was used to simulate injection and production wells. Then, when the scope of the code was enlarged to include waste isolation, application of the well submodel was likewise enlarged. Thus wells are now also used to simulate both aquifer recharge from upland areas and aquifer discharge into rivers and streams. The model option permitting switching from rate to pressure control is frequently useful for such simulations. Wells may be used strictly for observation, or they may be used strictly for injection of heat and/or radioactive components. In some applications they are used simply to establish flow boundary conditions. The effective use of wells is quite important to the application of this code.

Much of the terminology presented here derives from petroleum reservoir engineering and would appear, on the surface, to be appropriate only for injection and production wells. However, the concepts apply equally well to any type of source-sink combination. The following discussion in terms of well index, mobility, and rate

allocation attempts to illustrate the general utility even though the terminology sounds as if the use might be restricted to actual wells.

The underlying motivation for defining, in this section, the terms, well index, mobility, and rate allocation, is threefold, namely (1) to relate the pressure of source or sink at a sub-grid scale to the average grid-block pressures, (2) to distribute fluid between different permeability layers to meet a specified net source or sink rate, and (3) to define a boundary condition of constant rate (injection or production), constant pressure or a switch-over between the two. The second item is more applicable to the case of a real well, whereas the first and last items are generally applicable. The following discussion attempts to provide the necessary background for the manner in which sources and sinks are treated.

3.5.1 Well Index

The region surrounding a well is called the skin (see Figure 3-5). The ability of this region to transmit fluid may either be degraded or enhanced relative to that of the undisturbed formation, depending on well completion. This transmitting capability of the skin is characterized by the well index WI, which in general is defined by the relation

$$q = (WI/\mu) \Delta p \quad (3-9)$$

where $q = [\text{m}^3/\text{s}]$ is the flow rate and $\Delta p = [\text{Pa}]$ is the pressure drop across the skin region. For specific values of fluid properties μ_0 and ρ_0 well index may be defined in terms of head drop rather than pressure drop:

$$q = WI_0 \Delta H \quad (3-10)$$

where $WI_0 = [\text{m}^2/\text{s}]$ is defined

$$WI_0 = \rho_0 (g/g_c) WI/\mu_0 \quad (3-11)$$

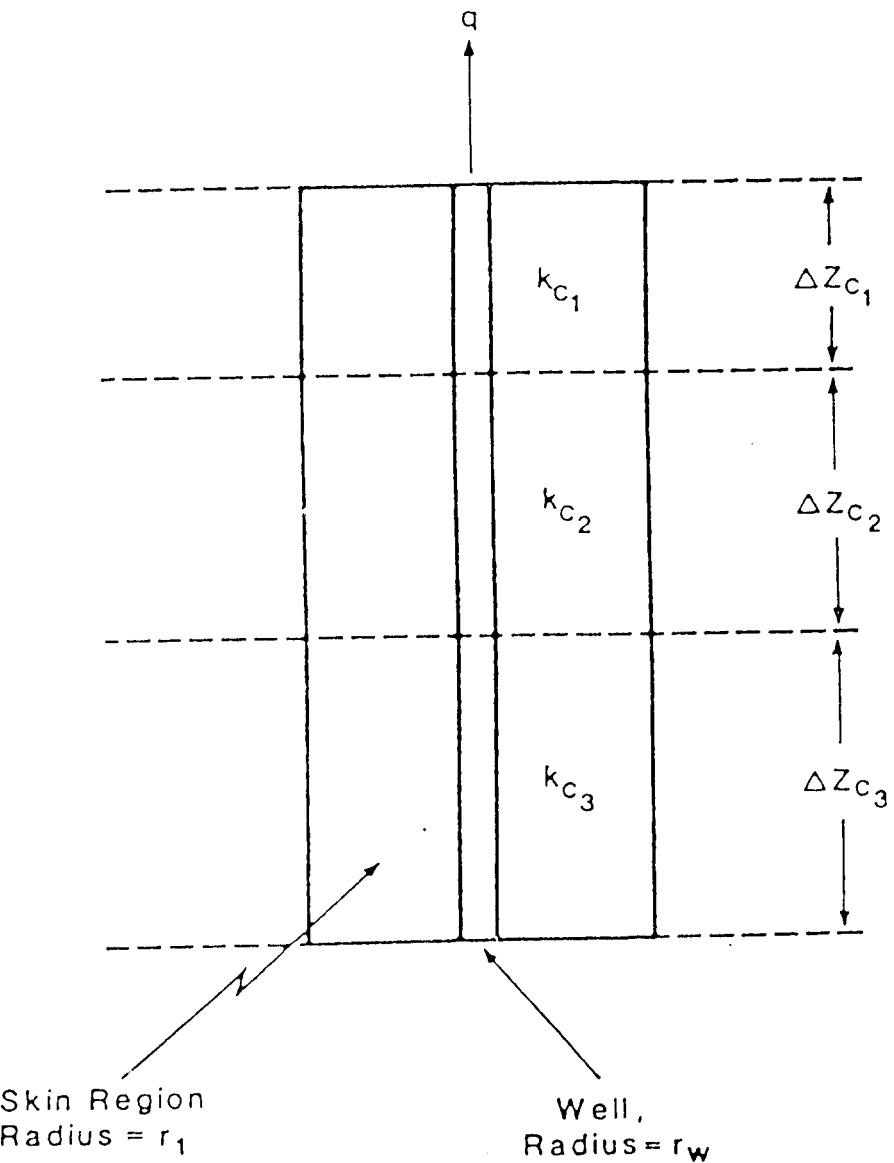


Figure 3-5. Characterization of the skin region surrounding a well.

The SWIFT code requires WI_0 as input, where ρ_0 and μ_0 are defined in terms of reference values of pressure, temperature, and concentration. For injection or production wells the well index may be estimated by a one-dimensional steady-state solution of Eq. (2-1), which yields

$$WI_0 = 2\pi K_s \sum_k \Delta z_k / \ln(r_1/r_w) \quad (3-12)$$

where K_s is the hydraulic conductivity of the skin and where index k ranges over all layers affected by the well. This equation is directly applicable for radial coordinates since radius r_1 is defined to be the first nodal point in that case. For cartesian coordinates, radius r_1 is not defined directly, but may be specified in terms of the radius

$$\bar{r} = (\Delta x \Delta y / \pi)^{1/2} \quad (3-13)$$

Schematically the assumed relation between the skin radius and this average block radius is shown in Figure 3-6. Mathematically, this relation is given by

$$\ln(r_1/r_w) = r_w - 1 + (\bar{r}/r_w)[\ln(\bar{r}/r_w) - 1] / (\bar{r} - r_w) \quad (3-14)$$

In this case the pressure drop Δp of Eq. (3-9) is the difference in pressures between the well and the grid-block pressure, which is taken to be the radially averaged pressure of the cone of influence between radii r_w and r , present at the periphery of the skin. An alternate approach to Eq. (3-14) for determining the effective radius r_1 within a cartesian system is given by Pritchett and Garg [1980].

For simulation of aquifer recharge or discharge, one might choose the skin to be identical to the block itself. In this case, well index may be related to the transmissibility, as depicted in Figure 3-7 for a block bounded on one side by a river. The well index in that case would be

$$WI_0 = K_0 \Delta y \Delta z / (\Delta x / 2) \quad (3-15)$$

where K_0 is here the block conductivity rather than the skin conductivity.

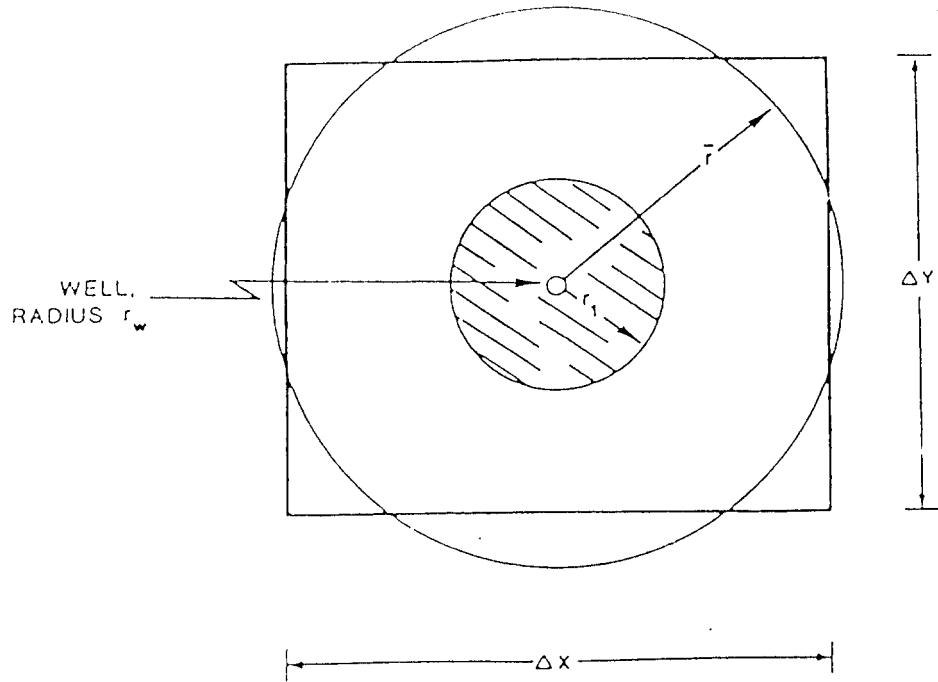


Figure 3-6. Concept of skin thickness for a cartesian grid block. Here \bar{r} is the radius of an equivalent circle and r_1 denotes the distance to the average pressure of the cone of influence between r_w and \bar{r} .

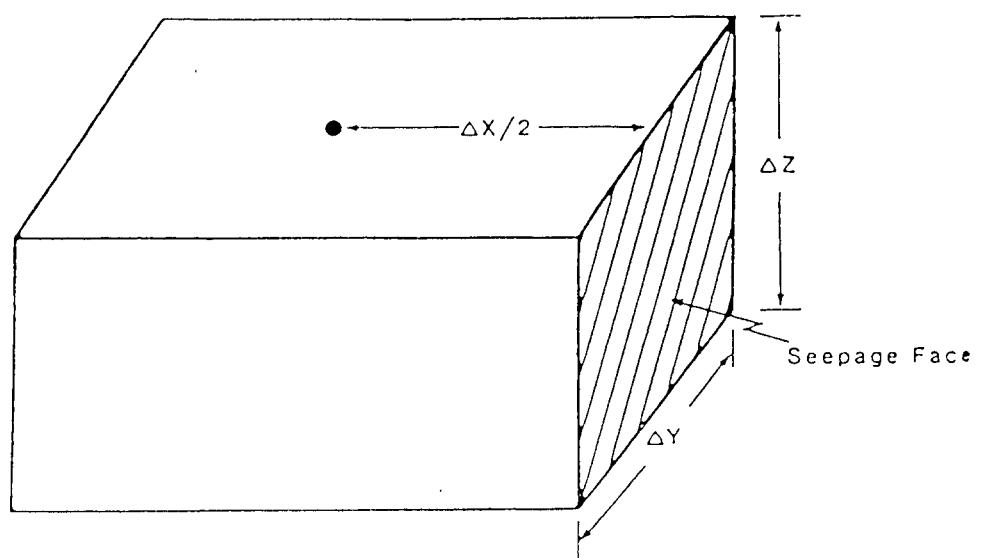


Figure 3-7. Use of a well to simulate seepage to a river.

3.5.2 Mobility

Getting back to the case of an actual well, we consider another concept which is quite similar to that of well index, namely mobility. Both terms relate to the transmission properties of the skin. For the case of a well completed into more than one layer, however, mobility is a layer-dependent term which, to some extent, partitions flow between layers. A fractional allocation factor, k_ℓ , is assigned to each layer. Typically, each factor is taken to be proportional to the thickness-permeability product for a given layer. Mobility for layer k is then defined to be

$$M_k = (k_\ell / \mu) WI \quad (3-16)$$

(For convenience, indices i and j , which locate the well itself, will be suppressed throughout the remainder of this note.)

3.5.3 Rate Allocation

There are two ways in which the partitioning of flows takes place within the code, depending on the option chosen by the user. The appropriate control parameter $IINDW1$ is specified in the input. The first option ($IINDW1 = 1$) is that of rate allocation on the basis of mobilities alone, i.e.

$$q_k = M_k q / \sum_k M_k \quad (3-17)$$

A second option ($|IINDW1| = 2$ or 3) is rate allocation on the basis of mobilities and pressure drops. Here the flow rate allocated to layer k is given by

$$q_k = - \left\{ \left[p_{bh} + (\rho g / g_c) (h_k - h_{c1}) \right] - p_k \right\} M_k \quad (3-18)$$

where the bottom-hole pressure p_{bh} is determined, in terms of the grid-block pressures, by the condition

$$q = \sum_k q_k \quad (3-19)$$

Subscript c_1 denotes the first layer in which the well is completed (see Figure 3-5). The bottom-hole pressure is defined to be the well pressure at h_{c1} , the depth of the top of this layer.

The SWIFT code applies Eq. (3-18) for the case of a rate limitation. It does so in either an explicit ($IINDW1 = 2$) or a semi-implicit ($IINDW1 = -2$) manner. In the former case, the evaluation of the right-hand side of Eq. (3-18) is lagged by one time step relative to the most current calculation. In the latter semi-implicit case, each q_k for the current time step $n+1$ is expanded about the previous time step by the relation

$$q_k^{n+1} = q_k^{it} + (dq/dp)_k \delta p_k \quad (3-20)$$

Here the derivative is taken to be

$$(dq/dp)_k = M_k \quad (3-21)$$

and term q_k^{it} is evaluated iteratively:

$$q_k^{it} = - \left\{ \left[p_{bh}^n + (\rho g / g_c) (h_k - h_{c1}) \right] - p_k^n \right\} M_k \quad (3-22)$$

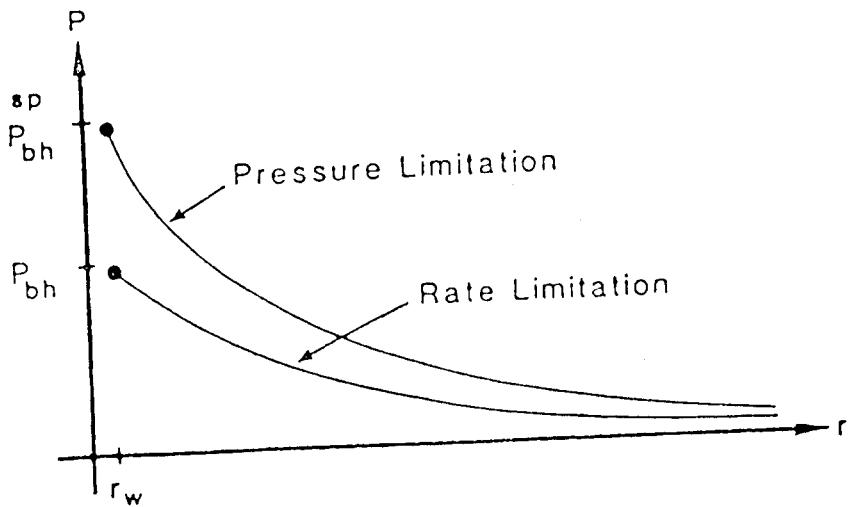
and

$$q_k^{it} = q_k^{it-1} q / \sum_k q_k^{it-1} \quad it > 1 \quad (3-23)$$

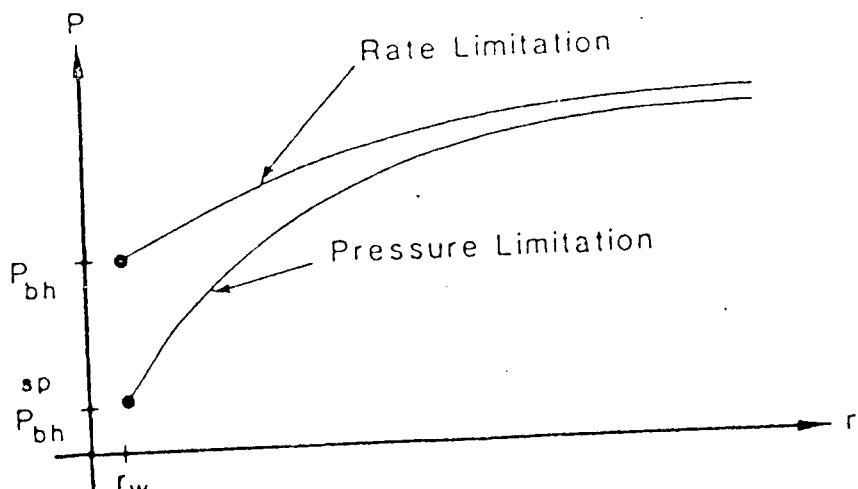
3.5.4 Variable Rate-Pressure Limitation for Transient Application

This very useful well option, ($|IINWDI| = 3$), in addition to rate allocation on the basis of mobilities and pressure drops, has another feature. It permits switching between rate and pressure limitations. Thus, for injection, both a maximum bottom-hole pressure p_{bh}^{SP} and a maximum pump rate q^{SP} may be specified so that the specified rate is maintained until the maximum pressure is attained. At that time the pressure is controlled at its maximum value, and the rate falls below the specified rate. Such cases are illustrated in Figure 3-8 for cases of both injection and production. In addition to its usefulness in simulating wells, this facility is also useful in simulating recharge, when the "bottom-hole" pressure, i.e., the surface pressure, cannot exceed atmospheric pressure. It has also been used for simulating a river by forcing a pressure limitation.

Variable rate-pressure limitation is implemented by a more flexible usage of the same equations which were used in the previous section. For example, consider the explicit ($IINDW1 = 3$) case for an injection well (see Figure 3-8a). Here Eqs. (3-18) and (3-19) are applied in the following manner, starting from a rate-controlled



(a) Injection



(b) Production

Figure 3-8. Pressure profiles illustrating the use of variable rate-pressure limitation.

situation. At each time step the following algorithm is used.

1. Pressure p_{bh} is determined from a combination of Eqs. (3-18) and (3-19) using $q = q^{SP}$.
2. If $p_{bh} < p_{bh}^{SP}$, then rate control is used, and then source terms q_k are calculated from Eq. (3-18) using p_{bh} as determined in Step 1 above. Quantities q_k are then used to solve the finite-difference equations.
3. If $p_{bh} > p_{bh}^{SP}$, the pressure control is used in that source terms q_k are calculated from Eq. (3-18) using $p_{bh} = p_{bh}^{SP}$. The total fluid injected will, in this case, be less than the specified amount, i.e., $q < q^{SP}$. These quantities q_k are then used in the finite-difference equations.
4. Pressure control, i.e., $p_{bh} = p_{bh}^{SP}$, is then maintained until the pressure gradient between the well bore and the average grid-block conditions become sufficiently great that the fluid injection rate exceeds the specified maximum, i.e., $q < q^{SP}$. At that point the code changes back to rate limitation (Step 2 above).

The corresponding algorithm for the case of a production well is easily obtained by analogy.

In contrast, the implicit (IINOW1 = -3) case is implemented by using a more flexible implementation of Eqs. (3-18) - (3-23) than for the case IINOW1 = -2. Starting from rate control, the following procedure is used for an injection well:

1. Pressure p_{bh} is determined explicitly from a combination of Eqs. (3-18) and (3-19) using $q = q^{SP}$.

2. If $p_{bh} < p_{bh}^{SP}$, then rate control is used, and source terms q_k are calculated from an iterative implementation of Eqs. (3-20) - (3-23). In this case, at each iteration, the coefficient of p_k in Eq. (3-20) is included in the diagonal of the propagation matrix, which carries the solution from one time step to the next, and q_k^{it} is included in the load vector.
3. If $p_{bh} > p_{bh}^{SP}$, then pressure control is used in that, from Eq. (3-18),
$$q_k^{it} = q_k^0 = - \left\{ \left[p_{bh}^{SP} + (\rho g / g_c) (h_k - h_{c1}) \right] - p_k^n \right\} M_k \quad (3-24)$$
4. Pressure control, i.e., $p_{bh} = p_{bh}^{SP}$, is maintained unless the fluid injection rate exceeds the specified maximum, i.e., $q > q^{SP}$. At that point the code changes back to rate limitation (Step 2 above).

The corresponding algorithm for the case of a production well is easily obtained by analogy.

3.5.5 Pressure Limitation for Steady-State Applications

In a steady-state fluid flow application, it is anticipated that the user will not need the facility for changing between rate and pressure limitations during the course of a simulation. Thus, for this model, the user may specify either flow limitation ($|IINDW| = 2$) or pressure limitation ($|IINDW1| = 3$). The flow limitation is implemented in the same manner as discussed above for the fully transient simulator, with only one exception. Time stepping there, as indicated by the superscript n in Eqs. (3-20) and (3-22), is replaced here by an iteration on the transmissibilities of the partially saturated blocks containing the free-water surface.

Furthermore, the implementation of the pressure-limitation option is quite similar to that of the rate-limitation option. In the explicit case ($|IINDW1| > 1$), Eq. (3-18) is the working equation. The only difference is the determination of the bottom-hole pressure. For a pressure limitation, this quantity is known, i.e., $p_{bh} = p_{bh}^{SP}$. However, for a rate limitation, the bottom-hole pressure is not known and must be calculated, using Eq. (3-19). In either case, the entire right-hand side of Eq. (3-18) is determined explicitly using pressure values determined by the last iterate.

For the implicit case ($|IINDW1| < -1$), the working equations become Eqs. (3-20) and (3-21). The mobility term in Eq. (3-20) is applied implicitly under both rate and pressure limitations. The difference arises again in the bottom-hole-pressure term. For the pressure limitation, the term q_k^{it} is known directly from Eq. (3-22), and no further iterations are required. For the rate limitation, however, this term is not known and must be inferred via iteration using a collection of equations, Eqs. (3-18), (3-19), and (3-22) for the first iteration and Eq. (3-23) thereafter. Hence, the application of Eqs. (3-20) and (3-21) is semi-implicit for the rate-limitation case and fully implicit for the pressure-limitation case.

In summary, then, all sources of fluid and sinks of fluid are called "wells" regardless of whether they refer to physical wells. Furthermore, all such "wells" are characterized by rate and, where appropriate, bottom-hole pressure and by position, completion layer, well indices WI_0 , layer allocation factors, k , and a specification option $|IINDW1|$. The latter determines whether rate allocation will be via mobilities alone ($|IINDW1|=1$) or via mobilities and pressure drops ($|IINDW1| = 2$ or 3). In addition, this specification option determines whether pressure control will also be applied ($|IINDW1| = 3$) and also whether the source-sink term will be applied explicitly ($|IINDW1| > 1$) or implicitly ($|IINDW1| < -1$). Finally, the meaning of the option ($|IINDW1| = 3$) is somewhat different in the two models. For the transient applications, this option means variable pressure-rate limitation. For steady-state applications, however, this option means pressure limitation only.

3.6 HEAT LOSS TO OVER AND UNDERBURDENS

Typically, the over/underburden regions will contain aquitards which effectively isolate them from the formation being calculated, which is denoted herein as the "reservoir". Nevertheless, these zones may contribute significantly to the heat transport from a heat source such as a repository. Over and underburden zones are therefore included in the SWIFT code for the purpose of simulating only the heat transport. The equation used is the following:

$$K_m \frac{\partial^2 T}{\partial z^2} = \rho_R c_{PR} \frac{\partial T}{\partial t} \quad (3-25)$$

This is a simple heat-conduction equation in which all transport and storage effects within the fluid are neglected (c.f. Eq. (2-2)). In addition, transport in the lateral x and y directions is ignored in order to limit storage requirements. (The validity of the assumption had been checked by comparison of model runs with a simple conduction-convection model by Coats, et al. [1974].

A table $T_0(z)$ of initial temperatures versus depth is required by code input. This table provides an initial condition and one boundary condition.

$$T(x, y, z, t=0) = T_0(z) \quad (3-26)$$

$$T(x, y, z=L, t) = T_0(L) \quad (3-27)$$

where L is taken to be a sufficiently large distance into the over or underburden that temperature changes there from the ambient temperature may be neglected. The other boundary condition is obtained by matching with the reservoir temperature, which, in this section, is denoted by T_R :

$$T(x, y, z=0, t) = T_R(x, y, z=0, t) \quad (3-28)$$

Here, for simplicity, the interface is taken to be the plane $z=0$.

The set of equations, Eqs. (3-25) - (3-28), is solved by a rather unique application of the finite-difference method. Dependent variable T is divided into two components, namely

$$T = T_1 + W T_2 \delta T \quad (3-29)$$

Here, temperature T_1 evolves, as a particular solution of Eq. (3-25), strictly from a redistribution of the temperature at the n -th time step. The initial boundary conditions for the step from time t_n to time t_{n+1} are, in this case, given by

$$T_1(x, y, z, t=t_n) = T(x, y, z, t=t_n) \quad (3-30)$$

and

$$T_1(x, y, z=0, t) = T(x, y, z=0, t=t_n) \quad (3-31)$$

Dimensionless temperature T_2 then evolves strictly from a change in boundary conditions appropriate for the n th time level:

$$T_2(x, y, z, t=t_n) = 0 \quad (3-32)$$

and

$$T_2(x, y, z=0, t) = 1 \quad (3-33)$$

As shown in Eq. (3-29), the dimensionless temperature is normalized by the time-weighting factor and the temperature change over Δt . The backward-in-time differencing $w = 1$ and the entire temperature change is applied. For centered-in-time differencing, $w = 1/2$ and the average temperature change is applied.

The unique feature of the superimposition specified by Eq. (3-29) is the fact that it permits implicit coupling between solution of the over/underburden transport, Eq.(3-35), and solution of the reservoir transport (Eq. (2-2)). Equation (3-29) may be differentiated and combined with appropriate factors to yield the heat loss to the over/underburden region:

$$q_L = q_{L1} + wq_{L2} \delta T \quad (3-34)$$

where q_{L1} is obtained from T_1 and q_{L2} is obtained from T_2 . Now, the transport and initial-boundary conditions which determine T_1 and T_2 are in no way dependent upon the reservoir temperature. Hence, the flow terms q_{L1} and q_{L2} may be determined prior to the reservoir solution for any time step Δt , and the implicit condition of Eq. (3-34) may be applied to the reservoir equation, Eq. (2-2), to obtain δT within the boundary blocks. Equation (3-29) may then be used to obtain the temperature within the over/underburden at time level $n+1$. Thus, the unique feature of the separation of dependent variables given in Eq. (3-29) is that it permits a fully coupled, implicit coupling of heat-transport processes within the over/underburden and reservoir zones.

3.7 RADIATION BOUNDARY CONDITION

A body at absolute temperature T surrounded by a black body at temperature T_0 will lose heat with a flux in accordance with Stefan's law:

$$F = \sigma\epsilon(T^4 - T_0^4) \quad (3-35)$$

where F is the flux, σ is the Stefan-Boltzmann constant, and ϵ is the emissivity of the surface. If the temperature difference is not too great, then Eq. (3-35) may be replaced by the expression

$$F = \beta(T - T_0) \quad (3-36)$$

where β is the coefficient of surface heat transfer.

It is because of the connection between Stefan's Law, Eq. (3-35), and Eq. (3-36) that the latter has been called the "radiation boundary condition" [Carslaw and Jaeger, 1959]. However, Eq. (3-36) is identical to Newton's Law of Cooling for forced convection. It is also appropriate for a relatively thin skin placed between the conducting media being simulated and a constant-temperature surface. Equation (3-36), which is also known as a Type 3 boundary condition, has been implemented in the SWIFT program for added flexibility in treating heat-loss processes.

CHAPTER 4 APPLICATION NOTES

The purpose of this chapter is to elucidate certain aspects of the SWIFT code which we feel will be helpful to its application. The first two topics treat numerical criteria and are extremely important for the transport simulation. The third item explains the mesh generation which may be used when radial coordinates are chosen.

4.1 NUMFRICAL CRITERIA FOR DISPERSION AND OVERSHOOT

One source of difficulty in the numerical solution of transport equations, such as Eqs. (2-2) - (2-4), is the treatment of the convection term. For conventional finite-difference and finite-element solvers, either numerical dispersion or the overshoot-undershoot phenomena may be introduced. Other methods, or variations of the above-mentioned techniques, have been introduced to help alleviate this problem. Examples are the method of characteristics [Garder, et al, 1966; Bredehoeft and Pinder, 1973], higher-order Galerkin [Price et al, 1968; Pinder, 1973] and various upstream-weighting and asymmetric weighting strategies [Nolen and Berry, 1972; Christie et al, 1976]. The Distributed-Velocity Method [Campbell, Longsine, and Reeves, 1981] holds some promise in this area also.

The SWIFT model gives the user several options. For example, he may elect to use second-order correct central-difference approximations in both time and space. These techniques have the advantage that no numerical dispersion is introduced. The disadvantage they introduce are limitations on both block size and time step. These limitations are necessary to prevent calculated concentrations from exceeding the injection or solubility levels or from being less than the initial values, i.e., overshoot-undershoot. The user also may choose to use first-order correct backward-difference approximations in both time and space. These techniques have no overshoot-undershoot, but they introduce numerical dispersion. Thus, limitations on block size and time step are again called for. The radionuclide, brine and heat-transport equations, Eq. (2-2) - (2-4), which contain convective terms, are largely responsible for the importance of numerical dispersion. The flow equation, since it does not contain a convective, i.e. first-order derivative, term, has a truncation error which is much less significant. The time-step and block-size restrictions are not overly severe for many problems. In such cases the analyst may elect to use the backward-difference schemes due to their inherent stability against overshoot.

A table is presented below which contains information on numerical dispersion and overshoot. It is based on a simple analogue of Eqs. (2-2)-(2-4) namely

$$D' \frac{\partial^2 W}{\partial x^2} - v \frac{\partial W}{\partial x} = \frac{\partial W}{\partial t} \quad (4-1)$$

where the dependent variable W may denote either temperature T , brine concentration \hat{C} , or radionuclide concentration C . Quantities v and D' denote the retarded interstitial velocity and dispersion, respectively.

In spite of the simplicity of Eq. (4-1), space- and time-step criteria derived from it have proven to be quite useful in practice. Such criteria are given in Table 4-1. Additional discussion of these relations is given in INTERCOMP [1976].

4.2 ADJUSTMENT OF THE RATE CONSTANT

Program SWIFT will adjust the rate constant if input parameter LADJ, READ R0-1, is set to one. The basis for this adjustment is another analogue equation. If one considers the static case, in which transport is negligible compared to decay, then the radionuclide decay equation, Eq. (2-4) becomes, for the parent nuclide,

$$\frac{dC}{dt} = -\lambda C \quad (4-2)$$

(The component subscript has been dropped for convenience.)

The analytic solution of Eq. (4-2) across an interval Δt is

$$C^{n+1} = C^n e^{-\lambda \Delta t} \quad (4-3)$$

which yields

$$\delta C = -C^n (1 - e^{-\lambda \Delta t}) \quad (4-4)$$

If Eq. (4-2) is solved numerically, the result is

$$\delta C = -\lambda' (w) (C^n + w \delta C) \Delta t \quad (4-5)$$

where

$$w = \begin{cases} 1/2 & \text{CIT} \\ 1 & \text{BIT} \end{cases} \quad (4-6)$$

Table 4-1 Numerical Criteria for Brine, Heat and Radionuclide Transport^{1,2}

<u>Scheme</u>	<u>Numerical Dispersion</u>	<u>Dispersion Criterion</u>	<u>Overshoot Criteria</u>
CIT-CIS	None	None	$v\Delta t/\Delta x + 2D'\Delta t/\Delta x^2 < 2$ $v\Delta x/2 < D'$ —
CIT-BIS	$v\Delta x/2$	$v\Delta x/2 \ll D'$	$\frac{v\Delta t}{2\Delta x} < 1$ —
BIT-CIS	$v^2\Delta t/2$	$v^2\Delta t/2 \ll D'$	$v\Delta x/2 < D'$ —
BIT-BIS	$v\Delta x/2 + v^2\Delta t/2$	$v\Delta x/2 + v^2\Delta t/2 \ll D'$	None

1 Here CIT means central in time, CIS means central in space, BIT refers to backward in time, and BIS refers to backward in space.

2 Definition of terms:

$$k_d = 0, \text{ brine transport}$$

$$K = \begin{cases} 1 + (1-\phi)\rho_R k_d/\phi, & \text{radionuclide or brine transport} \\ 1 + (1-\phi)\rho_R c_{PR}/\phi\rho c_{pw}, & \text{heat transport} \end{cases}$$

$$v = u/\phi K$$

$$D' = \begin{cases} (\alpha_L u + D_m)/K\phi, & \text{radionuclide or brine transport} \\ (\alpha_L u \rho c_{pw} + K_m)/K\phi\rho c_{pw}, & \text{heat transport} \end{cases}$$

To see that quantity $\lambda'(w)$, the adjusted rate constant, is indeed a function of the time-weighting constant w , we solve Eq. (4-5) for δC and substitute into Eq. (4-4). The result is

$$\lambda'_i(w) = \frac{e^{\lambda_i \Delta t} - 1}{\lambda_i \Delta t [(1-w)e^{\lambda_i \Delta t} + w]} \quad (4-7)$$

where the component subscript has been reintroduced. For the BIT algorithm $w = 1$, Eq. (4-7) reduces to Eq. (5-3) of the SWIFT document [Dillon, et al, 1978]. As described quantitatively therein, rate adjustment is appropriate for near-static cases where decay dominates transport, for the case of a parent nuclide. Furthermore, rate adjustment via Eq. (4-7) is appropriate for decay-dominant transport of a daughter nuclide providing that

$$\tau_{i-1}/\tau_i > 100 \quad (4-8)$$

Without adjustment the time step must be controlled by the criterion

$$\Delta t < \begin{cases} \tau_i/7 & \text{BIT} \\ \tau_i & \text{CIT} \end{cases} \quad (4-9)$$

where τ_i is the half life of the component. With adjustment, this criterion is removed in many cases.

4.3 MESH GENERATION FOR RADIAL COORDINATES

For a cartesian (x,y,z) coordinate system the SWIFT code requires the user to generate his own mesh by specifying all values of the increments Δx , Δy , and Δz . For radial (r,z) coordinates, however, the radial mesh may be either user-generated or automatically generated, c.f. READ R1-22 to READ R1-25. Automatic generation is based on a special steady-state solution of the flow equation which gives, for the pressure difference between two points,

$$p_2 - p_1 \sim \ln(r_2/r_1) \quad (4-10)$$

This same relation is the basis for the well index given in Eq. (3-12) of the last section.

Four parameters are used in the automatic generation, namely (1) the number of grid blocks $n = NX$, (2) the radius $r_1 = R1$ to the center of the first grid block, which is also interpreted as the outer radius of the disturbed skin zone, (3) the wellbore radius $\hat{r}_1 = RW$, and (4) the grid-block boundary $r_{n+1} = RE$.

The radial mesh, which is shown schematically in Figure 4-1, is generated by assuming equal pressure drops between adjacent mesh points for the steady-state solution of Eq. (4-10). Using the notation of Figure 4-1, this means that

$$\frac{r_{i+1}}{r_i} = A \quad (4-11)$$

and

$$\frac{\hat{r}_i}{r_i} = A^{1/2} \quad (4-12)$$

A combination of Eqs. (4-11) and (4-12) gives

$$\frac{\hat{r}_{n+1}}{r_1} = A^{n-1/2} \quad (4-13)$$

Equation (4-13) is solved by SWIFT for the common ratio A , and then Eqs. (4-11) and (4-12) are used as recursion relations to define all r_i and \hat{r}_i .

Frequently the analyst will not know the outer skin radius, r_1 , which must be input to the code. In such an event, it is suggested that Eq. (4-13) be extended by taking

$$\frac{r_1}{\hat{r}_1} = A^{1/2} \quad (4-14)$$

and

$$\frac{\hat{r}_{n+1}}{r_1} = A^n \quad (4-15)$$

Equation (4-15) may be solved for A . This parameter may then be used in Eq. (4-14) to calculate the skin radius r_1 from the wellbore radius \hat{r}_1 .

4.4 NUMERICAL CRITERIA FOR SECULAR EQUILIBRIUM

In considering the transport of chains of radionuclides, cases involving secular equilibrium are encountered. For such situations, the numerical criteria of Sections 4.1 and 4.2 above frequently may be relaxed. However, before examining the criteria, it is appropriate to give a definition for secular equilibrium.

Considering, for simplicity, the case of parent and daughter nuclei, the former follows a simple exponential decay law

$$N_1 = N_{10} e^{-\lambda t} \quad (4-16)$$

for the case of static flow. Here, for convenience, the concentration notation C has been changed to number-of-nuclei notation N, with subscripts added to denote nuclide identity and initial values. For the daughter component

$$\frac{dN_2}{dt} = \lambda_1 N_1 - \lambda_2 N_2 \quad (4-17)$$

which yields the solution

$$N_2 = \lambda_1 N_{10} (e^{-\lambda_1 t} - e^{-\lambda_2 t}) / (\lambda_2 - \lambda_1) \quad (4-18)$$

If the half life of the parent is much greater than that of the daughter, i.e., if

$$\tau_i \gg \tau_{i+1} \quad (4-19)$$

or, for the decay constants,

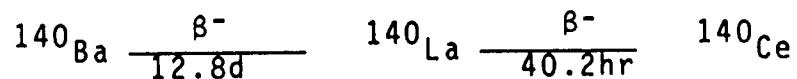
$$\lambda_i \ll \lambda_{i+1} \quad (4-20)$$

then secular equilibrium occurs. This means, for the case of parent and daughter, that

$$\lambda_1 N_1 = \lambda_2 N_2 \quad (4-21)$$

a relation easily derived from Eqs. (4-16) and (4-18).

Figure 4-2 provides an example of secular equilibrium for the decay chain



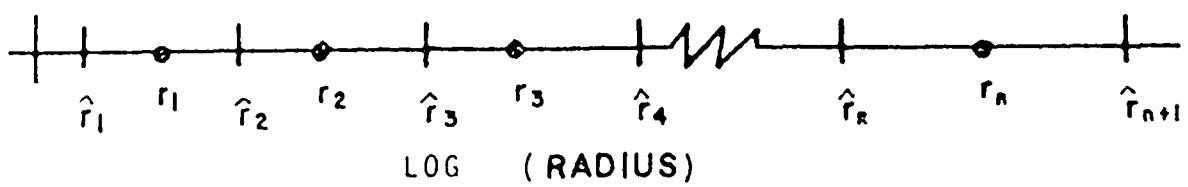


Figure 4-1 Schematic of radial mesh including grid-block centers, r_i , and grid-block boundaries, \hat{r}_i .

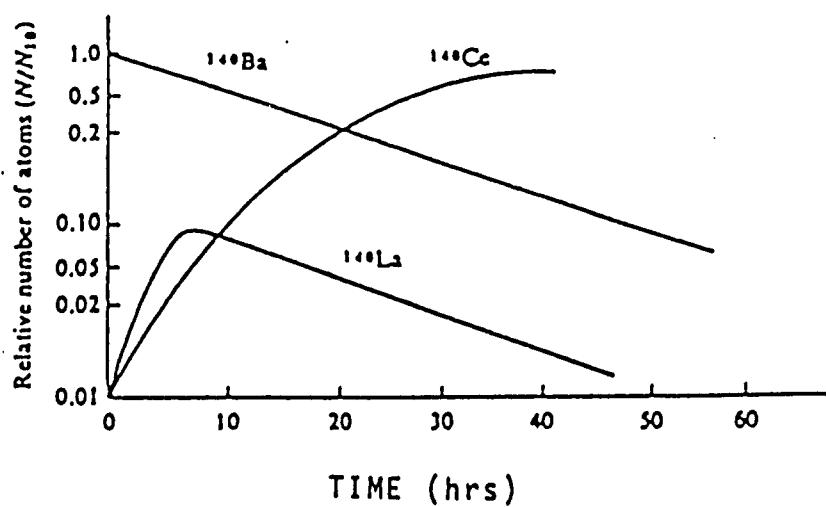


Figure 4-2 Decay of Radioactive ^{140}Ba . After approximately 15 hours the ^{140}Ba and ^{140}La will be in secular equilibrium.

Since the half life of ^{140}Ba is approximately seven times greater than that of ^{140}La , the condition for secular equilibrium is considered to be satisfied, and secular equilibrium occurs, in this case, after only 15 hours have elapsed from the initial, nonequilibrium condition.

For a long chain, such as that of ^{232}Th , where all elements of the chain (except for the final stable daughter product) are in secular equilibrium, each radionuclide builds up to equilibrium with its parent. When this occurs, a generalized form of Equation (4-21) is valid, namely

$$\lambda_1 N_1 = \lambda_2 N_2 = \lambda_3 N_3 = \dots \quad (4-22)$$

This means simply that under conditions of secular equilibrium, the activities of all components are equal.

A more complete discussion of various types of equilibria is given in Evans [1955]. However, the point to be made here is that secular equilibrium under nonstatic conditions is significant insofar as the numerical criteria are concerned, for the following reason. It has been found by experimental numerical methods that the criteria for the daughter components may frequently be ignored in such a case. For example, in the case of the actinide chain



time steps would have to be controlled via the relatively short 1600y half life of ^{226}Ra were it not for its secular equilibrium with ^{238}U . This means that only the time step of the latter, as determined from Table 4-1, need be enforced. Since the criteria for chains in secular equilibrium have not been derived theoretically, one must proceed with some caution, however, making appropriate numerical checks. Nevertheless, the relaxation of numerical criteria resulting from secular equilibrium is a necessary consideration for applications in which computer efficiency is important.

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CHAPTER 5 PROGRAM DESCRIPTION

5.1 PROGRAM STRUCTURE

This particular version of the SWIFT program has been developed to implement the formalism described in previous chapters. It consists of a main routine, three integration subroutines, and about 50 supporting subroutines. In this chapter five items are presented. First, the structure of routine MAIN is shown in Figure 5-1. As may be inferred from this figure, the basic organization of MAIN is focused upon the three integration subroutines ITER, ITERS and ITERC. Generally speaking, subroutines READ1 through PRINT2 perform the functions of input, initialization, parameter definition, and output in support of either ITER or ITERS, which integrate the flow, brine and heat equations, or ITERC, which integrates the radio-nuclide equations.

The second, third and fourth items presented show the structure of the three integration subroutines. Routine ITER is shown diagrammatically in Figure 5-2; ITERS in Figure 5-3; and ITERC in Figure 5-4. As shown, these routines are quite similar. All contain matrix set-up followed by matrix solution. The solution, in each case, may be performed in one of three different ways depending upon user preference. The user options are two-line successive overrelaxation (L2SOR) and Gaussian elimination (GAUS3D or GAUS1D) with the latter algorithm streamlined within a special subroutine for one-dimensional applications.

The major difference between the three integrators is the complexity of the setup process, with ITER, the coupled-equation transient simulator, understandably the most complex and with ITERC, the transient radionuclide simulator, the least complex. Comparing ITER (Figure 5-2) with ITERS (Figure 5-3), the major difference is SCOEF. This routine sets up time-derivative coefficients in the former which are, of course, absent from the later since ITERS is a steady-state integrator. In addition, the COEFF routines are called a second time in ITERS in order to calculate converged values of Darcy velocities and selected flow variables and to print them out if so desired. Comparing ITERS and ITERC, the major difference is the absence of the COEFF subroutines in ITERC. This is due to the fact that flow and transport transmissibilities need not be determined in ITERC, having been determined already in ITERS or in ITER. Furthermore, mass balances are computed directly in ITERC, whereas in ITERS, as in ITER, such computations are deferred to PRINT2.

The final item presented in this chapter is Table 5-1. There the functions of the major subroutines are given very briefly. For more detailed information on the numerical algorithms the reader is referred to INTERCOMP [1976], Part I, Appendix A.

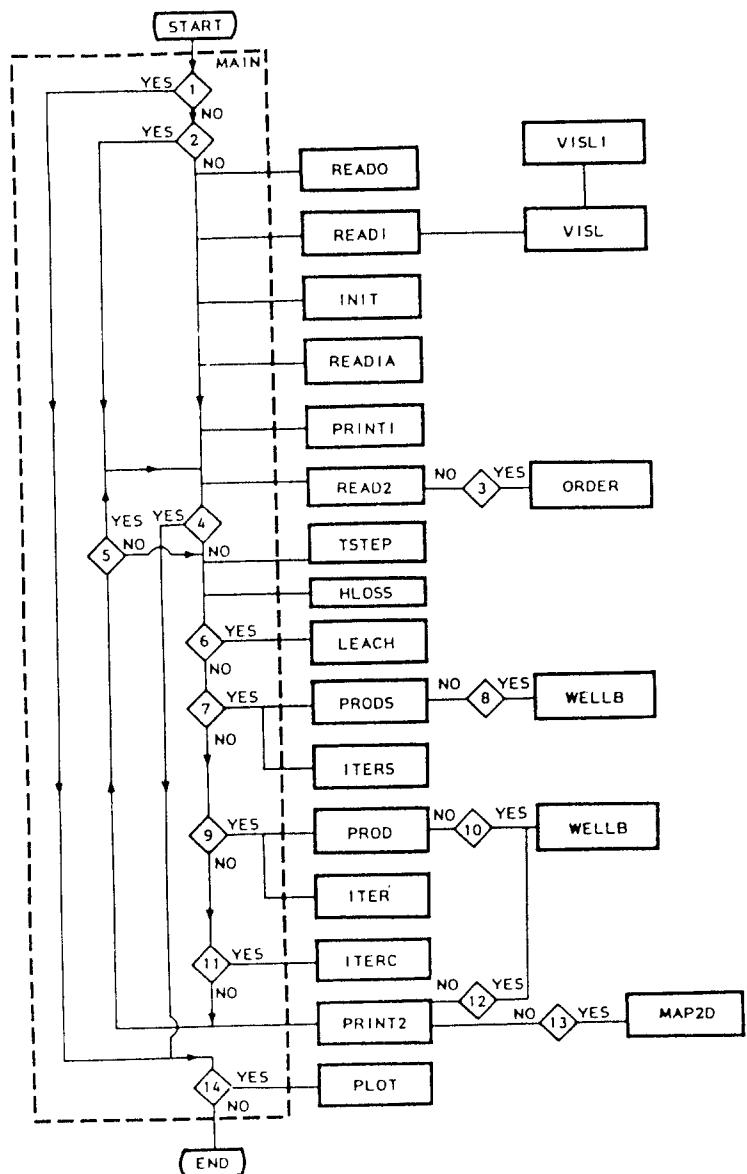


Figure 5-1. Structure of SWIFT model.

Conditions for Figure 5-1 are as follows:

- (1) Are plots desired for a previous run?
- (2) Is this a restart run?
- (3) Is reduced bandwidth direct method of solution used? (Multi-dimensional problems only)
- (4) Is run to be terminated at this time step?
- (5) Are the recurrent data read at this time step?
- (6) Is the waste-leach submodel employed?
- (7) Is the steady-state pressure solution sought?
- (8) Are steady-state wellbore calculations to be performed?
- (9) Is the transient pressure solution sought?
- (10) Are the transient wellbore calculations to be performed?
- (11) Are the radionuclide transport equations to be solved?
- (12) In the transient wellbore calculations are the well rates calculated semi-implicitly?
- (13) Are any two-dimensional contours maps desired?
- (14) Are any plots desired for this run?

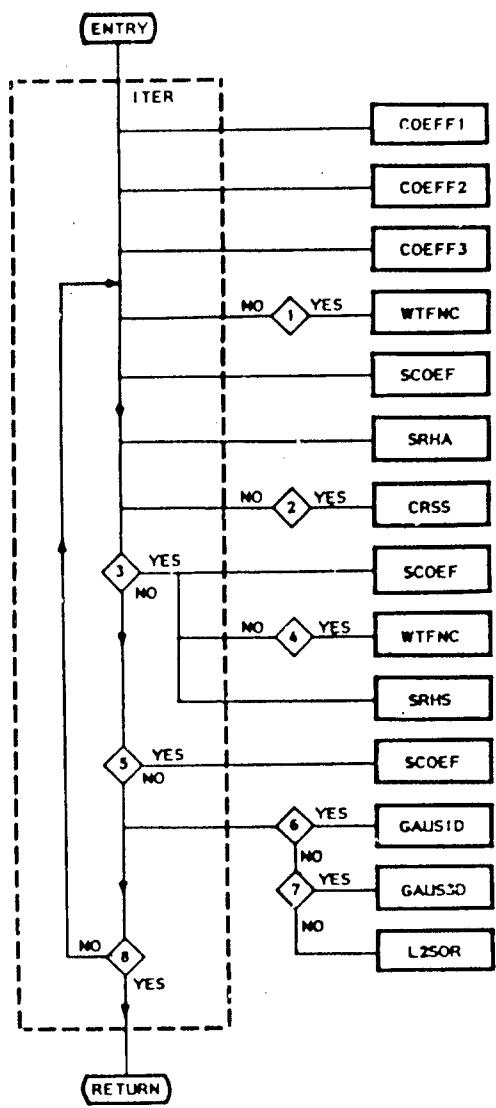


Figure 5-2. Breakdown of transient coupled solution algorithm.

Conditions for Figure 5-2 are as follows:

- (1) Is this the first iteration?
- (2) Are the cross-derivative dispersion terms to be included?
- (3) Is the temperature equation to be solved?
- (4) Is this the first iteration?
- (5) Is the brine concentration equation to be solved?
- (6) Is the problem one-dimensional?
- (7) Is a direct solution desired?
- (8) Has convergency been achieved?

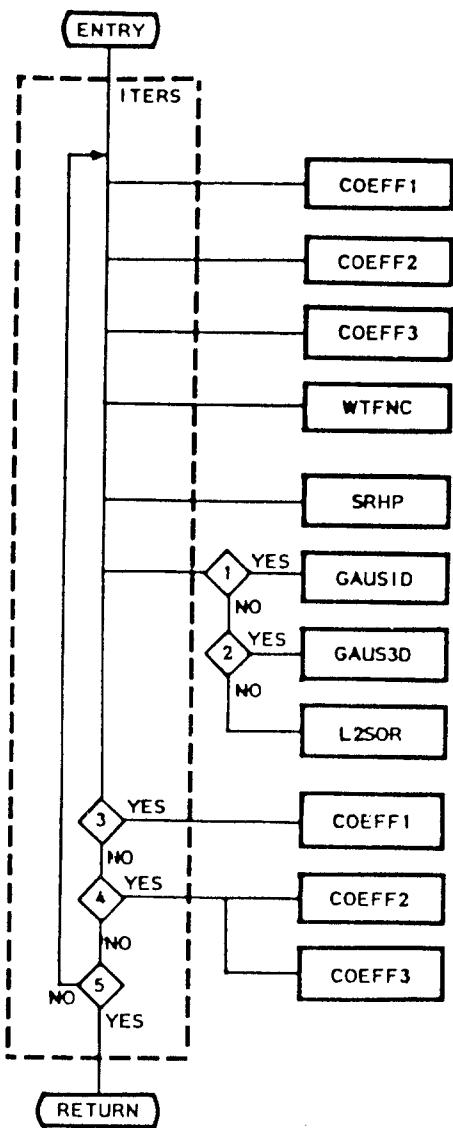


Figure 5-3. Breakdown of steady-state coupled solution algorithm.

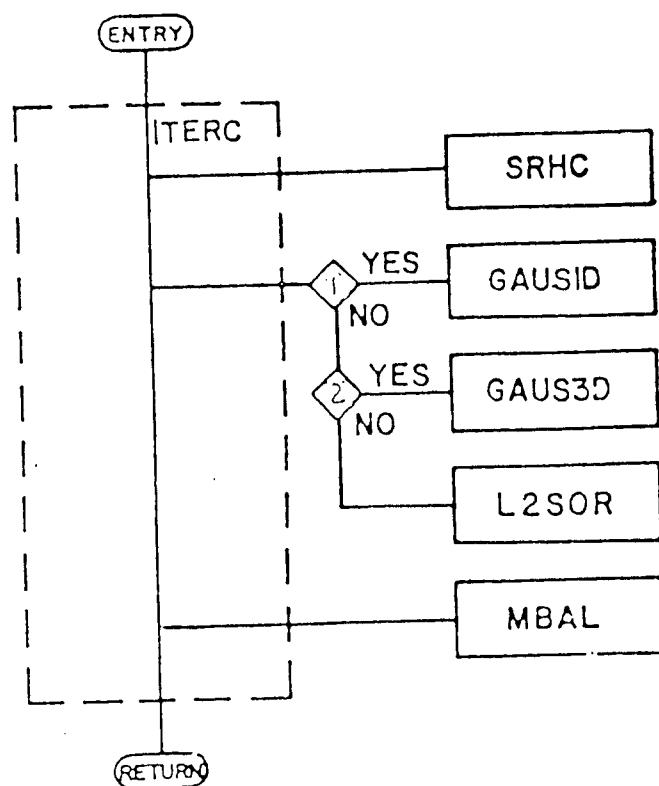


Figure 5-4. Breakdown of radionuclide-transport solution algorithm.

Conditions for Figure 5-4 are as follows:

- (1) Is the problem one-dimensional?
- (2) Is a direct solution desired?

Table 5-1. Subroutine Functions

<u>Subroutine</u>	<u>Function</u>
COEFF1	Determination and output of flow transmissibilities and Darcy velocities.
COEFF2	Computation of implicit block-to-block convection terms.
COEFF3	Determination of dispersion, heat and brine transmissibilities, explicit block-to-block dispersion terms and explicit salt-dissolution quantities.
GAUS1D	Gaussian elimination for a 1-D system.
GAUS3D	Gaussian elimination for 2-D and 3-D systems.
INIT	Initialization of pressures and concentrations.
ITER	Solution of transient flow, heat and brine equations by setting matrix coefficients and invoking matrix solution.
ITERC	Solution of transient-state radionuclide chains by setting matrix coefficients and invoking matrix solution.
ITERS	Solution of steady-state flow and brine equations by setting matrix coefficients and invoking matrix solution.
LEACH	Calculation of radionuclide sources from a repository based on initial inventory, leach rate, decay, and solubility.
L2SOR	Solution of matrix equations by the method of Two-Line-Successive Overrelaxation.
MAIN	Dynamic allocation of storage and supervisory control of entire calculation.
MAP2D	Printing of 2-D contour plots of either pressure or concentration.
MBAL	Computation of radionuclide material balance based on the initial material in place and input/output flows.
ORDER	Optimal nodal numbering for direct Gaussian solution of the matrix equations.

Table 5-1. Subroutine Functions, Continued

<u>Subroutine</u>	<u>Function</u>
PRINT2	Output of fluid-flow results: well summary, material-balance summary, and profiles of pressure, temperature, brine concentrations and radionuclide concentrations.
PRINT1	Echo of time-invariant input variables pertaining to geometrical, hydrological and geochemical characterization of the system.
PRODS	Set up of both implicit and explicit well terms.
READ0	Radionuclide-chain input including distribution coefficients.
READ1	Input of geometrical, hydrological and dispersion data. Calculation of constant portion of transmissibilities.
READ1A	Reading of rock-type modifications and repository information including solubilities.
READ2	Time-variant input for fluid-heat, brine and radionuclide calculations including solution control, wells, and output control.
SCOEF	Sets up matrix coefficients and load-vector terms arising from both time derivatives and salt dissolution for use in ITER.
SRHC	Determination of load-vector terms for the radionuclide-transport equations.
SRHP	Determination of load-vector terms for the pressure and brine equations.
VISL	Evaluation of viscosity as a function of temperature and brine concentration.
VISL1	Set up of viscosity-model parameters.
WELLB	Implements the well-bore model to obtain subsurface conditions from surface conditions.
WTFNC	Computation of upstream weighting parameters.

5.2 SAMPLE PROBLEMS

As mentioned in the introduction, eleven sample problems have been developed and published in a companion document by Finley and Reeves [1981]. The discussion therein includes the physical setting along with a description of input and output. The English Engineering system of units is used therein. In order to complement that work and, at the same time, make this document complete, a listing of input and output for those same eleven problems has been attached to this document. Here, however, the SI system of units has been adopted.

5.3 PROGRAM LISTING

Also attached to this document is a microfiche listing of the SWIFT source code.

CHAPTER 6 DATA INPUT GUIDE

The purpose of this chapter is to assist in the utilization of the SWIFT code. Three items are given here. First, the data input forms are described. Secondly, the use of these forms to obtain maps from restart records is discussed. Finally, the auxiliary data files are identified.

Utilization of the data input forms is further facilitated by three appendices which give definitions of errors, definitions of program variables, and a variable index.

6.1 DATA INPUT FORMS

The data input cards are divided into several groups. The groups are defined by the subroutines which read the cards. The "M" cards are read from the main program and the general setup of the problem is defined by these cards. The "R0" cards are read from subroutine READ0. This subroutine inputs information appropriate for the radioactive components. The "R1" cards are read from subroutine READ1. These cards provide the detailed information on the problem geometry, physical characteristics and boundary conditions. The "R1A" cards are read from the READ1A subroutine. Here four different types of data are specified: 1) rock-type modifications, 2) rock-type dependent salt-dissolution constants, 3) waste-storage information, and 4) solubilities to be applied within the repository. Subroutine INIT reads the "I" cards. The "I" cards provide the initial conditions for the simulation.

All of the above cards are read only once during a simulation. The "R2" cards are called the recurrent data because they typically are read several times during a simulation. Subroutine READ2 reads these data. The "R2" cards control the time steps and the time-dependent parameters such as leach-rate, well injection rates and radioisotope source rates.

The last group of cards to be read are the "P" cards. The specifications for plotting the calculated and observed data are entered here.

6.1.1 The "M" and RO" Cards

The "M" cards are read from the main program. The information provided by these cards sets up a general framework which the analysis will build on. The framework includes items such as:

Which equations will be solved,
The type of wellbore calculations to be used,
Setting printing and plotting controls,
Grid size,
Type of aquifer representation,
The method of numerical solution to be used.

The "RO" cards input information pertaining to the radioactive components. This information defines each isotope in terms of its parents; branching ratios for each parent, mass of the isotope, half life and distribution coefficient for each rock type.

Read M-1 (20A4/20A4) Title.

LIST: TITLE

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

READ M-2 (7I5) Option Parameters.

LIST: NCALL, RSTRT, ISURF, IIPRT, NPLP, NPLT, NPLC, IUNIT

NCALL Control parameter for solving the basic partial differential equations. To solve all three equations, enter zero.

NCALL	Pressure	Temperature	Inert Comp	Radioactive Comp
0	X	X	X	*
-2	X	X		*
1	X			*
2	X		X	*
3				*
4	SS			*
5	SS		SS	*

X - Equation solved

* - Equation solved only if radioactive source is present

SS - Steady-state pressure equation

RSTART -1 - Total core storage required will be printed and program execution will stop.
 0 - A normal run starting from initial conditions.
 >0 - The number of the time step at which calculations are to resume for a restart run. A restart record from a previous simulation run corresponding to the specified time step must exist on the restart tape mounted on Tape Unit Number 4.

ISURF Control parameter for wellbore calculations.
 0 - This means only rates or aquifer formation level pressures will be specified.
 1 - Surface values will be specified. The wellbore model will calculate changes from the surface to the aquifer level.

IIPRT Transmissibility printing key. The value entered here is not used. This version of the model has been modified to read IIPRT in READ R2-13 which activates printing of several intermediate parameters on a one time step basis.

NPLP Control parameter for plotting pressures in the wells.

1 - Bottom-hole and surface pressures are plotted if wellbore calculations are performed. Only the bottom-hole pressures are plotted if no wellbore calculations are performed. For an observation well 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 R2-17 and proceed to Read P-1.

NPLT Control parameter for plotting temperatures in the well.

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 bottomhole 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 R-17 and proceed to READ P-1.

NPLC Control parameter for plotting concentration in the well.

1 - The concentration in the well is plotted for observation and production wells only.

0 - No concentration plots are desired.

-1 - Concentration plots are desired for a previous run. Skip READ M-3 through R2-17 and proceed to READ P-1.

IUNIT Unit specification control.

0 - English Engineering System

1 - SI system

NOTE: Proceed to READ P-1 if any of NPL's are negative.

NOTE: Skip to READ M-4 if this is a restart run, i.e., RSTRT > 0.

READ M-3 (15I5) Core Allocation and Control.

LIST: NX, NY, NZ, HTG, NCP, NRT, KOUT, PRT, NSMAX, NABLMX,
METHOD, NAAR, NTIME, NCOMP, NREPB

ERROR MESSAGE:

(Number 1) NX is less than or equal to one or
NY is less than one or
NZ is less than one.
The minimum dimensions on the grid block system are
2x1x1. The maximum size is limited only by the
available computer storage.

(Number 7) HTG is not within the permissible range.
HTG is less than 1 or greater than 3.

(Number 8) The entered value for KOUT is not permissible. KOUT
is not equal to 0, 1 or 3.

(Number 9) PRT exceeds permissible range of -1 to +2.

NX Number of grid cells in the x direction (greater
than or equal to 2).

NY Number of grid cells in the y direction (greater
than or equal to 1).

NZ Number of grid cells in the z direction (greater
than or equal to 1).

HTG Control parameter for input of reservoir descrip-
tion data.

1 - Homogeneous aquifer, cartesian geometry.

2 - Heterogeneous aquifer, aquifer data entered
on regional basis, cartesian geometry.

3 - Radial geometry. The aquifer may be heter-
ogeneous in the vertical direction.

NCP Number of radioactive/trace components in the
system.

NRT Number of rock types.

NOTE: Distribution coefficients, dispersivities, thermal conductivities and salt-dissolution coefficients are all functions of rock or strata type. Rock types of all blocks are initialized to IRT = 1. Changes of rock type to other values are entered in the R1A-1 cards.

KOUT Output control.

- 0 - All initialization output activated.
- 1 - All initialization output except initial arrays (concentrations, pressures, etc.) are activated.
- 3 - No initialization output is activated. A value of 3 for KOUT can be used to omit printing of most initialization data.

PRT Output array orientation control.

- 1 - Print output arrays as areal layers (x-y). Block numbers in the x direction increase from left to right and decrease down the computer page in the y direction.
- +1 - Printout is similar to above except that J-block numbers increase down the computer page.
- 2 - Print output arrays as vertical sections (x-z).

NSMAX Maximum number of radioactive/trace component sources that will be used during the run.

NABLMX Maximum number of aquifer influence function blocks. This data is used for dimensioning the aquifer influence function arrays. This number is equal to the number of peripheral blocks, if aquifer influence functions are to be used.

METHOD The matrix solution technique for which core is to be allocated.

0, +1 - Storage is allocated for direct solution.

+2 - Storage is allocated for the L2SOR method.

NOTE: Parameters METHOD and NAAR are coupled in that if NAAR is nonzero, then NAAR words of core are allocated for matrix solution. If, however, NAAR is zero, then core is allocated either for the L2SOR method or for the direct method, depending on the value of METHOD. In the case of allocation for the direct solution via METHOD, an approximate algorithm is used.

NOTE: Parameter METHOD may be changed in READ R2-2 to effect the actual solution technique. Thus, for example, core may be allocated for the direct method, and L2SOR may actually be used. However, the converse is not true. Since the direct technique requires more core than does L2SOR, core may not be allocated for L2SOR followed by solution with the direct method.

NOTE: In the case of direct-solution allocation, the approximate algorithm is not always correct. Therefore, one should compare the approximate allocation with the required allocation, both of which are printed. If the latter is larger, resulting in job termination, then NAAR must be specified.

NAAR Storage allocation for the working array A in the direct solution routine.

0 - Length of A array will be calculated internally using an approximate formula.

>0 - Storage allocation for A array. If direct solution is intended, then this number must be equal to or greater than the minimum length required, which is printed by the program.

NTIME Number of times for which concentrations of unleached radioactive components within the repository area are to be input. If NTIME is greater than one, then power-law interpolation is to be used. If NTIME equals one, then only initial concentrations are input and the time-dependent concentrations within the repository are calculated.

NCOMP Number of components for which descriptive information is to be read in the R1A cards. Note that $NCOMP \geq NCP$ must be the case.

NREPB Number of repository blocks.

NOTE: Data group R0 should be entered only if $RSTART \leq 0$ and $NCP > 0$. Otherwise skip READ R0-1 and READ R0-2.

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

NOTE: Enter NCP (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)

ERROR MESSAGE:

(Number 51) I is equal to zero or greater than NCP (entered in READ M-3) or NP(1) is negative.

(Number 52) DEC is negative for at least one of the components.

(Number 53) For one or more of the components, KP is less than 1 or greater than NCP (entered in READ M-3) or AP is negative.

MASS Mass number of the isotope.

DI Identification for radioactive component I.

I Component number.

NP Number of parent components for I.

LADJ Lambda (rate constant) adjustment index.

1 - Modify rate constant of the isotope I.

0 - Do not modify rate constant.

DEC Half life of component I in years. For stable components, enter zero.

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

NOTE: Skip this list if NP(I) equals zero (see LIST 1).

KP Parent component number.

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

READ R0-2 (7E10.0) Rock-Dependent Distribution Coefficients.

LIST: DIS(I), I=1, NCP for each rock type.

ERROR MESSAGE:

(Number 54) At least one of DIS is negative.

DIS Adsorption distribution coefficient in ft³/lb (m³/kg). Enter one value for each component for a total of NCP (see READ M-3) values for each rock type. Start new rock type values on a separate card.

NOTE: If RSTART < 0 (READ M-2), this is the end of your data set.

NOTE: If RSTART = 0, (READ M-2), skip to READ R1-1.

READ M-4 (I10) Restart Control Integer.

LIST: ILAST

ILAST Length of the variable blank common. It is printed out at the beginning of each run. See your initial run for this number.

READ M-5 (F10.0) Restart Time.

LIST: TMCHG

TMCHG Time in days (seconds) at which the next set of recurrent data is to be read. If TMCHG is less than or equal to the time corresponding to RSTART (READ M-2), a set of recurrent data will be read immediately to resume the previous simulation.

NOTE: Proceed to READ R2-1 for a restart run, i.e. RSTART > 0.

6.1.2 The "R1" Cards

The data supplied by the R1 cards define the physical parameters of the system being simulated; the reference temperature, pressure and elevation for calculating pressures; the detailed geometry of the system and the boundary conditions for the system being simulated. The general procedure for defining spatially dependent parameters is to specify large homogeneous regions followed by modification cards to insert inhomogeneities.

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

LIST: CW, CR, CTW, CPW, CPR

CW Compressibility of the aquifer fluid, (psi)₋₁
 ((Pa)⁻¹).

CR Compressibility of pore structure, (psi)₋₁
 ((Pa)⁻¹).

CTW Coefficient of thermal expansion of the aquifer
 fluid, ($^{\circ}$ F)₋₁ (($^{\circ}$ C)⁻¹).

CPW The fluid heat capacity, Btu/lb- $^{\circ}$ F (J/kg- $^{\circ}$ C).

CPR The rock heat capacity per unit volume of solid,
 Btu/ft³- $^{\circ}$ F (J/m³- $^{\circ}$ C).

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

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

UKTX Thermal conductivity of the fluid saturated
 porous medium in the x direction, Btu/ft-day- $^{\circ}$ F
 (J/m-sec- $^{\circ}$ C) (see CONV).

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-day- $^{\circ}$ F (J/m-sec- $^{\circ}$ C). If entered as zero,
 thermal conductivities should be read in
 Btu/ft-day- $^{\circ}$ F (J/m-sec- $^{\circ}$ C).

ALPHL Longitudinal dispersivity factor, ft (m).

ALPHT Transverse dispersivity factor, ft (m).

DMEFF Molecular diffusivity in the porous medium,
 includes porosity and tortuosity effects (porosi-
 ty x fluid molecular diffusivity/tortuosity),
 ft²/day (m²/sec).

READ R1-2.5 (LIST 1: (3E10.0); LIST 2: (7E10.0)) Rock-Dependent Physical Properties.

NOTE: Skip this read if NRT = 1, and proceed to R1-3.

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

UTCX Thermal conductivity of media in x-direction for rock type I, Btu/ft-day-°F (J/m-sec-°C).

UTCY Thermal conductivity in y-direction.

UTCZ Thermal conductivity in z-direction.

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

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

ALPHAT Transverse dispersivity factor (m).

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

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

LIST: BROCK, PBWR, TBWR, BWRN, BWRI

ERROR MESSAGE:

(Number 5) Either one or both the fluid densities (BWRN and BWRI) is zero or negative

BROCK Actual rock density (solid particle) 1b/ft³ (kg/m³).

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

TBWR Reference temperature at which the densities are to be entered, °F (°C).

BWRN The density of the natural aquifer fluid (concentration=0) at PBWR and TBWR, 1b/ft³ (kg/m³).

BWRI The density of the contaminated fluid (concentration=1) at PBWR and TBWR, 1b/ft³ (kg/m³).

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

READ R1-4 (15) Wellbore Data.

LIST: NOUT

NOUT	Output control parameter for wellbore calculations.
0	- No output is activated
1	- Iteration summary (number of outer iterations, 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 subroutine WELLB is called.
3	- The pressure and temperature in the well are printed over each increment (see DELPW in READ R1-5).

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

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 wellbores proceed in increments. The length increment corresponding to DELPW is calculated, and the temperature change over each increment is simulated.
TDIS	Thermal diffusivity of the rock surrounding the wellbores, ft ² /day (m ² /sec).

NOTE: With the exception of one control parameter pertaining to the initial temperature distribution, the input data in READ R1-6 through READ R1-8 pertains to the viscosity function $\mu(\hat{C}, T)$. The first card contains control parameters which limit input from those following. A detailed discussion of the options available for the specification of this function appears in Section 3.2. Thus, only a summary is given here. The minimum viscosity data consists of the two points $VISRR = \mu(\hat{C} = 0, T = TRR)$ and $VISIR = \mu(\hat{C} = 1, T = TIR)$ (READ R1-7). The remainder of the function will then be 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 Section 3.2, 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 $\hat{C} = 0$ may be included by using arrays TR(I) and VISR(I) (READ R1-9) with control parameter NTVR. Temperature data for $\hat{C} = 1$ 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 $\hat{C} = 0$ (or $\hat{C} = 1$), it is necessary to specify the same value for two different temperatures. For example, a constant function $\mu(\hat{C} = 0, T) = 1$ cp is determined by specifying NTVR = 1 and VISRR = VISR = 1.0 with TRR \neq TR.

READ R1-6 (415) Viscosity and Temperature Controls.

NOTE: The number of entries called for below (except for NDT) refers to the viscosity values to be entered in addition to the reference viscosities.

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 $\hat{C} = 0$ and $\hat{C} = 1$. If only the two 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 $\hat{C} = 0$.

NTVI Number of entries in the temperature-viscosity table for $\hat{C} = 1$.

NDT Number of entries in the depth versus temperature table.

READ R1-7 (4E10.0) Viscosity Data.

LIST: TRR, VISRR, TIR, VISIR

TRR Reference temperature for the resident viscosity fluid, $^{\circ}\text{F}$ ($^{\circ}\text{C}$).

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

TIR Reference temperature for the contaminated fluid viscosity, $^{\circ}\text{F}$ ($^{\circ}\text{C}$).

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

READ R1-8 (7F10.0) Viscosity Data.

NOTE: If NCV = 0, omit READ R1-8.

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

ERROR MESSAGE:

(Number 6) One or more of the viscosity values is entered as zero or negative.

SC Concentration, mass fraction.

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

READ R1-9 (7F10.0) Viscosity Data.

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

ERROR MESSAGE:

(Number 6) One or more of the viscosity values is entered as zero or negative.

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

TR Temperature, °C.

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

READ R1-10 (7F10.0) Viscosity Data.

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

ERROR MESSAGE:

(Number 6): One or more of the viscosity values is entered as zero or negative.

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

TI Temperature, °C

VISI Viscosity of the saturated brine at the temperature TI, cp (Pa-sec). Do not enter the reference viscosity at TIR (READ R1-7).

READ R1-11 (2F10.0) Initial Temperatures.

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

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

ZT Depth, ft (m).

TD Temperature, °F (°C).

NOTE: As described in Section 3.6, heat transport between the reservoir and the overburden and/or underburden may be 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). 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 overburden/underburden region and to define the heat-transport parameters.

READ R1-12 (2I5) Overburden and Underburden Parameters.

NOTE: If NZ = 1, the underburden heat loss is assumed to be equal to the overburden heat loss.

LIST: NZOB, NZUB

ERROR MESSAGE:

(Number 10) Either NZOB is greater than 2 and KOB is negative or NZUB is greater than 2 and KUB is negative.

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

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

READ R1-13 (4E10.0) Overburden-Underburden Parameters.

NOTE: Skip this READ if both NZOB = 0 and NZUB = 0.

LIST: KOB, CPOB, KUB, CPUB

ERROR MESSAGE:

(Number 10) Either NZOB is greater than 2 and KOB is negative or NZUB is greater than 2 and KUB is negative.

KOB, KUB Vertical thermal conductivities of the overburden and the underburden blocks, respectively, Btu/ft-day-°F (J/m-sec-°C).

CPOB, CPUB Overburden and underburden heat capacities per unit volume, Btu/ft³-°F (J/m³-°C).

READ R1-14 (7E10.0) Overburden-Underburden Parameters.

NOTE: Skip this READ if NZOB = 0.

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 aquifer. The overburden block numbers increase moving away from the aquifer.

READ R1-15 (7E10.0) Overburden-Underburden Parameters.

NOTE: Skip this READ if NZUB = 0.

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

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

READ R1-16 (4E10.0) Reference Temperature, Initial Pressures, and Datum Location.

LIST: T0, PINIT, HINIT, HDATUM

T0 A reference temperature for both conductivities and densities, °F (°C).

NOTE: Permeabilities are determined assuming that the input conductivities are referenced to temperature T0. Also, densities are related internally to this temperature in that only changes from the density at T0 are calculated.

PINIT Initial pressure at the depth HINIT, psi (Pa).

HINIT An arbitrary depth for setting up initial conditions measured relative to the reference plane, ft (m). HINIT can be any depth within the aquifer. HINIT is used only to set up initial pressures in the aquifer.

NOTE: Quantities HINIT, HDATUM, DEPTH (READ R1-20) and UH (READ R1-21) are all referenced to the same reference plane.

HDATUM A datum depth measured relative to the reference plane, ft (m).

NOTE: Quantity HDATUM is for printing the dynamic pressures ($p - \rho gh$). The depth h is measured from the datum HDATUM. The fluid density used for computing dynamic pressures is the resident fluid density at T0 and PINIT. This value is not used internally except for the pressure-at-datum calculation.

READ R1-17 (LIST DIRECTED)[†] Grid-Block Definition.

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

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

ERROR MESSAGE:

(Number 11) One or more grid block sizes (DELX, DELY, DELZ) are zero or negative.

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

READ R1-18 (LIST DIRECTED)[†] Grid-Block Definition.

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

ERROR MESSAGE:

(Number 11) One or more grid block sizes (DELX, DELY, DELZ) are zero or negative.

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

READ R1-19 (LIST DIRECTED)[†] Grid-Block Definition.

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

ERROR MESSAGE:

(Number 11) One or more grid block sizes (DELX, DELY, DELZ) are zero or negative.

DELZ Thickness of each vertical layer, ft (m).

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

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

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

ERROR MESSAGE:

(Number 12) One or more of KX, KY and KZ is negative or PHI is less than 0.001 or greater than 1.0 or SINX or SINY is less than -1 or greater than +1.

[†]LIST DIRECTED READ:

Input data consists of a string of values separated by one or more blanks, a comma or 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

Marginal identifiers are illegal for records using a list directed format.

KX Hydraulic conductivity in x direction, ft/day
 (m/sec).
 KY Hydraulic conductivity in y direction, ft/day
 (m/sec).
 KZ Hydraulic conductivity in z direction, ft/day
 (m/sec).
 PHI Porosity (fraction).
 SINX Sine of the reservoir dip angle along the x-axis
 (positive down).
 SINY Sine of the reservoir dip angle along the y-axis
 (positive down).
 DEPTH Depth to top center of grid block (1,1,1,)
 measured from the reference plane.

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

NOTE: These data are read only if HTG = 2. Enter as many sets of data as required. Follow the data with a blank card.

LIST 1: I1, I2, J1, J2, K1, K2.
 LIST 2: KX, KY, KZ, PHI, UH, UTH, UCPR.

ERROR MESSAGE:

(Number 13) I is greater than NX or
 J is less than 1 or greater than NY or
 K is less than 1 or greater than NZ or
 KX or KY or KZ is negative or
 PHI is less than 0.001 or greater than 1.0.

I1, I2 Lower and upper limits inclusive, on the I-coordinate of the region to be described.
 J1, J2 Similar definition for the J-coordinate.
 K1, K2 Similar definition for the K-coordinate.
 KX x direction hydraulic conductivity for flow,
 ft/day (m/sec).
 KY y direction conductivity for flow, ft/day (m/sec).
 KZ z direction conductivity for flow, ft/day (m/sec).
 PHI Porosity, fraction.

UH Depth in ft (m) measured positive downward from reference place to top of the cell. If entered 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 in READ R1-19, UTH may be entered as zero.

UCPR Heat capacity of the rock per unit volume, Btu/ft³-°F (J/m³-°C). If the rock heat capacity is equal to CPR (READ R1-1), UCPR may be entered as zero.

NOTE: Skip to READ R1-26 if HTG is not equal to 3.

READ R1-22 (4E10.0) Radial Aquifer Data.

NOTE: The following three records are read for a radial geometry with only one well. The well is located at the center of the grid-block system. The user has the option of dividing the grid blocks on an equal $\Delta \log(r)$ basis, (i.e., r_i/r_{i-1} is constant) or entering the radius of each grid-block center. For the former option automatic mesh generation is available as described in Section 4.3.

LIST: RWW, R1, RE, DEPTH

ERROR MESSAGE:

(Number 14) The first grid block (R1) is less than or equal to the well radius (RWW), or R1 is greater than or equal to the aquifer boundary radius (RE).

RWW Well radius, ft (m).

R1 The center of the first grid block for dividing grid blocks on an equal $\Delta \log(r)$ basis.

RE External radius of the aquifer, ft (m).

DEPTH Depth from a reference plane to the top of the aquifer, ft (m).

READ R1-23 (5E10.0) Radial Aquifer Data.

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

ERROR MESSAGE:

(Number 15) The layer thickness (DELZ) is less than or equal to zero or KYY or KZZ is negative or porosity (POROS) is less than 0.001 or greater than 1.0.

DELZ Layer thickness in the vertical direction, ft (m).
KYY Horizontal hydraulic conductivity, ft/day (m/sec).
KZZ Vertical hydraulic conductivity, ft/day (m/sec).
POROS Porosity, fraction.
CPR1 Rock heat capacity, Btu/ft³·°F (J/m³·°C). If
 the rock heat capacity in the layer is equal to CPR
 (READ R1-1), CPR1 may be entered as zero.

NOTE: One card should be entered for each vertical layer.

READ R1-26 (LIST 1: 6I5; LIST 2: 6E10.0) Reservoir Description
Modifications.

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

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

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

ERROR MESSAGE:

(Number 17) One or more of I1, I2, J1, J2, K1, K2 are out of
 permissible ranges 1-NX, 1-NY, and 1-NZ,
 respectively, or
 I1 is greater than I2 or
 J1 is greater than J2 or
 K1 is greater than K2.

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

J1, J2 (Similar definition for J-coordinate).

K1, K2 (Similar definition for K-coordinate).

NOTE: The x transmissibility (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 (I, J, K) refers to the transmissibility at the boundary separating grid-blocks (I, J-1, K) and (I, J, K).

FTX	If <u>positive</u> or zero, this is the factor by which the x direction transmissibilities within the defined region are to be multiplied. If <u>negative</u> , 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 the pore volume.
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.
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.

NOTE: In regions in which more than one modification has been made to a parameter subject to additive modifications, the order of the modifications has no effect and the final net adjustment is simply the algebraic sum of all the additive factors or 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 multiplicative factors (FTX, FTY, FTZ, FPV) read the corresponding factor as 1 0, not zero. Zero additive factors (HADD AND THADD) result in no changes to the depth and thickness values.

NOTE: If no aquifer influence functions are used (no flow across aquifer boundaries), insert a blank card and proceed to READ I-1. If a natural migration velocity is desired in the aquifer, a steady-state aquifer option must be used.

READ R1-27 (215) Aquifer Influence Functions.

NOTE: Aquifer influence blocks are defined as those cells in the model that communicate directly with an aquifer that is not itself modeled as part of the calculation grid, but whose effects are introduced through the aquifer terms read here. This feature can be used to introduce water influx (or efflux) from an edge without the expense that would be required to model the aquifer as part of the grid system.

LIST: IAQ, PRTAB

ERROR MESSAGE:

(Number 18)

IAQ is greater than 4, or one or more of I1, I2, J1, J2, K1, K2, are out of permissible ranges 1-NX, 1-NY, and 1-NZ, respectively; or I1 is greater than I2 or J1 is greater than J2 or K1 is greater than K2.

IAQ Control parameter for selecting the type of aquifer block representation.

0 - No aquifer influence blocks are to be used. Skip to READ R1-1.

1 - A pot-aquifer representation will be used.

2 - A steady-state aquifer representation will be used.

3 - Use the Carter-Tracy Representation.

4 - Constant pressure and brine component concentration boundary conditions will be used at blocks specified in READ R1-28. Boundary conditions for heat transport may be either constant temperature or radiative.

PRTAB Print control key for the aquifer influx coefficient.

0 - No printing of aquifer influx coefficients will be activated.

1 - The locations and values of the aquifer influx coefficients will be printed.

READ R1-28 (LIST 1: 615; LIST 2: 4E10.0) Aquifer Influence Functions.

NOTE: If IAQ is 3 (READ R1-27), skip this READ and proceed to READ R1-29.

NOTE: Follow the last VAB card of this data group by a blank card

NOTE: The read group consists of two cards or any number of sets of two cards, 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 to be assigned to the overlapped subregion. If these data are read, i.e., IAQ ≠ 3, then skip READS R1-29 through R1-32 and proceed to READ R1-33.

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

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

ERROR MESSAGE:

(Number 18) IAQ is greater than 4, or one or more of I1, I2, J1, J2, K1, K2, are out of permissible ranges 1-NX, 1-NY, and 1-NZ, respectively; or I1 is greater than I2 or J1 is greater than J2 or K1 is greater than K2.

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

J1, J2 (Similar definition for J-coordinate).

K1, K2 (Similar definition for K-coordinate).

KAQ Control variable for heat-transport equation only for IAQ = 4.

-1 - Type 3 radiation condition only. T1 is not used. T2 and T3 are used.

0 - Type 1 temperature condition only. T1 is used. T2 and T3 are not used.

1 - Type 1 temperature condition and Type 3 radiation condition. T1, T2, and T3 are all used.

For IAQ = 1 or 2 (READ R1-27)

VAB Aquifer influence coefficient for each block within the region defined by I1, I2, etc. The units of VAB are ft³/psi (m³/Pa) for a pot-aquifer representation and ft³/psi-day (m³/Pa-sec) for a steady-state representation.

P1, T1, C1, T2, T3 Not used.

For IAQ = 4 (READ R1-27)

VAB Boundary block type.
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,C1 Constant values of pressure in psi (Pa), temperature in °F (°C) and concentration (fraction) at the block boundary specified according to VAB and KAQ.

T2 Temperature of surrounding media, °F (°C).

T3 Coefficient of surface heat transfer Btu/day-ft-°F (W/m-°C).

NOTE: If IAQ is not equal to 3, omit these 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) Aquifer-Influence Functions.

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 in 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.
2 - The VAB will be calculated by the program and assigned to each grid block in the last areal plane, K=NZ only.

NPT Number of points in the influence function versus dimensionless time table ($P(t_D)$ versus t_D). If NPT is zero, the program will select the Hurst-Van Everdingen infinite aquifer solution internally.

PRTIF Print control key for the influence function table.

0 - Suppress printing

1 - Print the table of $P(t_D)$ versus t_D .

READ R1-30 (LIST 1: 6I5 LIST 2: E10.0) Carter-Tracy Functions.

NOTE: Enter this data only if NCALC is zero. Otherwise, skip to READ R1-31.

NOTE: Follow the last VAB card of this data group by a blank card.

NOTE: This READ group consists of two cards or any number of sets of two cards, 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 to be assigned to the overlapped subregion.

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

LIST 2: VAB

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

J1, J2 (Similar definition for J-coordinate).

K1, K2 (Similar definition for K-coordinate).

VAB Aquifer influence coefficient for each block within the defined region. The aquifer-influence coefficient VAB for the Carter-Tracy method is actually the fraction of the total aquifer-reservoir boundary that is represented by the length of any given grid block. 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 Functions.

LIST: KH, PHIH, RAQ, THETAQ

KH Conductivity-thickness for aquifer, ft^2/day (m^2/sec). 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. To retain the validity of usage of circular reservoir influence functions, the grid system should be chosen as accurately as possible.

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 360°.

READ R1-32 (2F10.0) Carter-Tracy Functions.

NOTE: This data is entered if NPT is not equal to zero. If NPT is zero, the program will select the aquifer influence functions for an infinite aquifer and the influence-function data need not be entered. If NPT equals zero, omit this READ and proceed to READ R1-33.

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

TD Dimensionless time, $kt/\mu\phi cTr^2$.

PTD Terminal rate case influence function as given by Van Everdingen and Hurst.

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

NOTE: These data allow the user to modify the aquifer influx coefficient VAB by the relation $VAB(I,J,K) = VAB(I,J,K) \times FAB$. 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 set to zero or a small number to reduce the VAB along the boundary. Follow these data with one blank card. If no modifications are desired, one blank card is still required.

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

LIST 2: FAB

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

J1, J2 (Similar definition for the J-coordinate).

K1, K2 (Similar definition for the K-coordinate).

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

6.1.3 The "I" Cards

These data are read for initializing concentrations and natural flow in the aquifer. If the initial concentrations are zero everywhere in the aquifer and there is no natural flow, insert a blank card and proceed to READ R2-1.

READ I-1 (315) Initial Velocity and Concentrations.

NOTE: These data are read for initializing concentrations and natural flow in the aquifer. If the initial concentrations are zero everywhere in the aquifer and there is no natural flow, insert a blank card and proceed to READ R2-1.

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 aquifer fluid is static initially.

1 - The resident fluid velocity will be entered in READ I-3.

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.

READ I-2 (6I5, F10.0) Initial Brine Concentrations.

NOTE: Skip this READ if ICOMP is zero.

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

ERROR MESSAGE:

(Number 21)

One or more of I1, I2, J1, J2, K1, K2 are out of permissible ranges 1-NX, 1-NY, and 1-NZ, respectively; or
I1 is greater than I2 or
J1 is greater than J2 or
K1 is greater than K2 or
CINIT is negative.

I1, I2

Lower and upper limits, inclusive on the I-coordinate of the region having a nonzero initial brine concentration.

J1, J2

(Similar definition for the J-coordinate).

K1, K2

(Similar definition for the K-coordinate).

CINIT

Initial brine concentration in each of the blocks within the defined region, dimensionless.

NOTE: Read as many of these cards as necessary to describe the concentrations everywhere in the aquifer. Only nonzero concentrations need be specified. Follow the last card with a blank card.

READ I-3 (F10.0) Initial-Velocity Condition.

NOTE: If INAT = 0, skip this record.

LIST: VEL

VEL

Initial velocity of the resident aquifer fluid in the x direction, ft/day (m/sec). The 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 the boundaries during the run.

READ I-4 (6I5, F10.0) Initial Radionuclide Concentrations.

NOTE: If IRD = 0, skip this READ.

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

ERROR MESSAGE:

(Number 22)

One or more of I1, I2, J1, J2, K1, K2 are out of permissible ranges 1-NX, 1-NY, and 1-NZ, respectively; or
I1 is greater than I2 or
J1 is greater than J2 or
K1 is greater than K2 or
CINIT is negative.

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

J1, J2 (Similar definition for the J-coordinate).

K1, K2 (Similar definition for the K-coordinate).

CINIT Initial radionuclide concentration for the component being entered.

NOTE: Read as many of these cards as necessary to describe the nonzero radionuclide component concentrations, following the last card with a blank card. A total of NCP such sets of data are required, one for each radionuclide component.

6.1.4 The "R1A" Cards

Here four different types of data are specified: 1) rock-type modifications, 2) rock-type dependent salt-dissolution constants, 3) waste-storage information and 4) solubilities to be applied within the repository. Thermal conductivities of the media, distribution coefficients and salt-dissolution coefficients all vary with the rock-type of the geologic media. Initially, all grid blocks are assumed to be of Type 1. The R1A cards provide regional modification of this initial specification.

READ R1A-1 (715) Modification of Rock Types.

NOTE: If NRT = 1, skip this READ. Otherwise enter the desired number of changes, terminating with a blank card.

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

I1A, I1B Upper and lower limits inclusive on the I-coordinate of region of modified rock type.

J1A, J1B (Similar definition for the J-coordinate).

K1A, K1B (Similar definition for the K-coordinate).

IRT Rock type.

READ R1A-2 (7F10.0) Salt-Dissolution Coefficients.

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

ERROR MESSAGE:

(Number 56) One or more values of ACS is negative.

ACS Product of the rate of salt dissolution and the mass fractions of solubles to total dry mass, (day)⁻¹ ((sec)⁻¹).

NOTE: The remainder of the R1A cards pertain only to waste leach from a nuclear waste repository. Thus, the user must skip to READ R2-1 if one or more of the following conditions is true:
(1) NCP = 0, (2) NCOMP = 0, (3) NTIME = 0, or (4) NREPB = 0.

READ R1A-3 (15) Waste Type.

LIST: ILEVEL

ILEVEL If ILEVEL = 1, then canistered storage is to be used in which canister radii and separations are defined. If ILEVEL = 0, then uncanistered storage is to be used in which only the waste-volume density is specified.

READ R1A-4 (4F10.0) Storage Specifications.

LIST: SDRIFT, SCNSTR, DCNSTR, HCNSTR

ERROR MESSAGE:

(Number 57) One or more of SDRIFT, SCNSTR, DCNSTR, or HCNSTR are negative.

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 DCNSTR is the diameter of each canister, ft (m). For uncanistered wastes DCNSTR is the volumetric waste density (volume of wastes/bulk volume).

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

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

READ R1A-5 (3F10.0) Unit Conversions.

LIST: CONVL, CONVC, CONVT

CONVL For canistered wastes CONVL multiplies SDRIFT, SCNSTR, DCNSTR, and HCNSTR to convert them to ft (m). For uncanistered wastes CONVL multiplies only DCNSTR to convert it to ft³ (m³) of wastes per bulk ft³ (m³).

CONVC This parameter multiplies the waste concentrations (RIA-8) to convert them to 1b/ft³ (Kg/m³) of wastes.

CONVT This parameter multiplies the specified interpolation times (RIA-7) to convert them to days (seconds).

READ RIA-6 (6I5) Location of Repository.

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

ERROR MESSAGE:

(Number 22) One or more of I1, I2, J1, J2, K1, K2 are out of permissible ranges 1-NX, 1-NY, and 1-NZ, respectively; or
I1 is greater than I2 or
J1 is greater than J2 or
K1 is greater than K2 or
CINIT is negative.

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

J1A, J1B (Similar definition for the J-coordinate).

K1A, K1B (Similar definition for the K-coordinate).

READ RIA-7 (7F10.0) Interpolation Times.

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

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

ERROR MESSAGE:

(Number 59) One or more of the interpolation times, CTIME, is negative.

CTIME Interpolation times, day (sec).

NOTE: Arbitrary units may be used here and then converted via READ RIA-5 if desired.

NOTE: The user should enter NCOMP groups of cards as specified in READ RIA-8. However, the information will be used only in those cases where CNAME matches DI, as specified in READ R0-1.

READ R1A-8 (2A4, 2X, 6F10.0/(7F10.0)) Interpolation of Repository 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 fractions. If interpolation is not used, then CNDUM(1) is the initial concentration.

READ R1A-9 (7F10.0) Solubility Limits.

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

ERROR MESSAGE:

(Number 61) One or more of the solubilities is negative.

CS Solubility limits expressed as mass fractions.

6.1.5 The "R2" Cards (Recurrent Data)

The data defined in the previous section is required to describe the aquifer and fluid properties and to establish initial conditions. The data discussed in this section, however, is time dependent. It is read before the first time step and at subsequent time steps when changes are desired in the time-step data, the wells, the source data, the wellbore data, the solution method, or the mapping specifications. Note that any of the data entered up to this point cannot be changed. The overburden and underburden blocks specifications or aquifer influence functions cannot be changed in any manner once they have been specified at the beginning.

READ R2-1 (9I5) Control Parameters.

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

INDQ Control parameter for reading well rates.

0 - Do not read well rates.

1 - Read well rates on one card (READ R2-5).

2 - Read one card for each well rate (READ R2-6).

IWELL Control parameter for reading well definition data.

0 - Do not read well data.

1 - Read new or altered well data.

IMETH Control parameter for reading method of solution.

0 - Do not read method of solution.

1 - Read new or altered method of solution.

ITHRU Run termination control.

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., 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.

0 - Do not read trace components source data.

1 - Read new or altered source-rate data defined by block number.

2 - Read time parameters for waste-leach submodel.

IPROD Control parameter for reading wellbore data.

0 - Do not read wellhead data.

1 - Read new or altered wellhead data.

IOPT Control parameter for reading iteration data for the wellbore solution.

0 - Do not read wellbore iteration data. If it is a new run, and wellbore calculations are desired, then default values of the iteration parameters will be used for wellbore calculations.

1 - Read new or altered wellbore iteration data.

INDT Control parameter for reading reservoir solution iteration data for the reservoir solution.

0 - Do not read iteration data. If entering data before the first time step, default values of the iteration parameters will be used.

1 - Read new or altered iteration data.

ICLL 0 - Do not read change in equation solution control, NCALL

1 - Read new equation solution control, NCALL.

READ R2-2 (I5, F10.0) Differencing and Solution Techniques.

NOTE: This data is entered if IMETH is not equal to zero. If it is a new run and IMETH is equal to zero, the program selects METHOD=1 and WTFAC=1.0 (direct solution with backward space and time approximations).

LIST: METHOD, WTFAC

ERROR MESSAGE:

(Number 40) METHOD is less than -2 or greater than +2 or WTFAC is greater than 1.0.

METHOD Method of solution. (If zero is entered, the program selects METHOD = 1.) 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.

2 - Two line successive-overrelaxation (L2SOR) solution with a backward finite-difference approximation in time. Use only if NY is greater than one.

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

-2 - Two-line successive overrelaxation solution with a centered finite-difference approximation in time. Use only if NY is greater than one.

WTFAC Weight factor for finite-difference approximation in space.

1.0 - Backward difference.

0.5 - Central difference.

NOTE: If $WTFAC \leq 0$ is entered, the program selects $WTFAC = 1.0$.

READ R2-3 (I5, 4F10.0) Wellbore Data.

NOTE: This data is entered if IOPT is greater than zero. If default values are desired, insert a blank card and proceed to READ R2-4. The default values of the parameters are discussed below.

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 wellhead pressure is calculated iteratively to obtain the bottom-hole pressure necessary to inject the specified rate. If entered as zero or a negative number, the program selects the default value of 20.

TOLX The tolerance on the fractional change in pressure over an iteration. If entered as zero or a negative number, the default value of 0.001 is selected.

TOLDP The tolerance, on pressure, psi (Pa). The default value is 7000.

DAMPX Damping factor in estimating the next value of the pressure (surface for an injection well and 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.

NOTE: If INDQ is equal to zero, skip READ R2-4 through READ R2-6 and proceed to READ R2-7.

READ R2-4 (I5) Well Specifications.

LIST: NWT

ERROR MESSAGE:

(Number 25) Total number of wells (NWT) is less than 1 or exceeds dimension limit NWMAX.

NWT Total number of wells.

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

NOTE: Enter this data only if INDQ is equal to one.

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

Q Production rate, ft³/day (m³/sec). If it is 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.

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

NOTE: Enter this data only if INDQ is equal to two. Read as many cards as necessary to describe all the modified injection and production well rates. Follow the last card with a blank card.

LIST: I, QWELL

ERROR MESSAGE:

(Number 26) Well number I is less than 1 or greater than NWT.

I Well number.

QWELL Production rate, ft³/day (m³/sec). Enter negative values for injection rates. Enter only the well rates which are to be changed from an earlier recurrent data set.

READ R2-7 (LIST 1: (615); LIST 2: (4E10.0); LIST 3: (8E10.0); LIST 4: (7E10.0)) Well Specifications.

NOTE: This data is entered for IWELL equal to one. Read one set of data for each well and follow the last card with a blank card.

LIST 1: I, IIW, IJW, IIC1, IIC2, IINDW1

ERROR MESSAGE:

(Number 27) Well location IIIW, IJW, is outside aquifer, i.e., IIW is less than 1 or greater than NX or IJW is less than 1 or greater than NY

(Number 28)	The well perforations are outside the aquifer, i.e., IIC1 or IIC2 is out of the range of 1-NZ or IIC1 is greater than IIC2 or the top block of the completion interval (K-IIC1) is a zero pore volume block.
(Number 30)	The entered value of IINDWI is not permissible. The permissible values are +1, <u>+2</u> , and <u>-3</u> .
(Number 32)	A well index of zero is permissible only if IINDWI is equal to one. This error occurs if IINDWI is not equal to one and WI is zero or negative.
(Number 33)	IINDW is <u>+3</u> and BHP is 0. The specified value of the bottom-hole pressure is a limiting value of the well pressure if IINDW is <u>+3</u> .
(Number 35)	All completion layers of a well are in zero pore volume blocks.
(Number 37)	One or more of KHL values are negative.
(Number 38)	All KHL values are zero for some wells. At least one KHL value must be non-zero.
(Number 39)	A well number I is negative or exceeds NWT.
I	Well number.
IIW	I-coordinate of grid cell containing the well.
IJW	J-coordinate of grid cell containing the well.
IIC1	Uppermost layer in which the well is completed.
IIC2	Lowermost layer in which the well is completed.
IINDWI	Well specification option.
	1 - Layer allocation via mobilities alone. Rate control only.
	<u>+2</u> - Layer allocation via mobility and pressure drop between wellbore and grid block. Rate control only.
	<u>+3</u> - Layer allocation via mobility and pressure drop between wellbore and grid block. Variable rate-pressure control.

2,3 - The rate is expressed explicitly.

-2,-3 - The rate is expressed in the semi-implicit manner:

$$q^{n+1} = q^n + \frac{dq}{dp} (p^{n+1} - p^n)$$

LIST 2: WI, BHP, TINJ, CINJ

WI Well index, ft^2/day (m^2/sec).

BHP Bottom-hole pressure, psi (Pa). This must be specified only if $\text{IINDW1} = \pm 3$.

TINJ Temperature of the injection fluid, $^{\circ}\text{F}$ ($^{\circ}\text{C}$). If surface conditions are being specified, it is the temperature at the surface.

CINJ Brine concentration in the injection fluid, dimensionless.

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

NOTE: Skip this list if $\text{ISURF} = 0$.

X Pipe (wellbore) length to top of perforations, ft (m).

DW Inside wellbore (pipe) diameter, ft (m).

ED Pipe roughness (inside) ft (m). Enter zero if it is a smooth pipe.

OD Outside wellbore (casing) diameter, ft (m).

TTOPW Rock temperature surrounding the wellbore at the surface, $^{\circ}\text{F}$ ($^{\circ}\text{C}$).

TBOTW Rock temperature surrounding the wellbore at the bottom-hole, $^{\circ}\text{F}$ ($^{\circ}\text{C}$).

UCOEF Overall heat transfer coefficient between the inner surface of the pipe and outer surface of the casing, $\text{Btu}/\text{ft}^2 \cdot ^{\circ}\text{F-day}$ ($\text{W}/\text{m}^2 \cdot ^{\circ}\text{C}$).

THETA Angle of the wellbore with the vertical plane, degrees.

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

NOTE: Skip this READ if the well is completed in only one layer, i.e., IIC1=IIC2.

KHL(K) Layer allocation factors for well I.

NOTE: These factors should be proportional to the total productivity of individual layers, taking into account layer kh (permeability x thickness). Only the relative values of these factors are important since these factors are renormalized to a unit sum. In terms of the normalized allocation-factor values, the absolute productivity (injectivity) of layer K is computed as WI x KHL(K).

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

NOTE: Skip this READ if IPROD is zero.

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

THP Tubing hole or the surface pressure for each well, psi (Pa).

NOTE: If ISURF is one, THP must be specified for the wells with well option IIDW1 = +3. A production (or injection) rate is calculated from THP, and the lower of the calculated and specified rate is used for allocation between layers.

NOTE: If IRSS=0, skip READ R2-9 and R2-10.

READ R2-9 (I5) Source Data.

LIST: NSS

NSS Number of radioactive source (sinks) blocks.

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

NOTE: Skip this READ if IRSS ≠ 1,

LIST 1: I, IIS, IJS, IKS

ERROR MESSAGE:

(Number 50) NSS is greater than NSMAX (entered in READ M-3) or
I is greater than NSS or
IIS is greater than NX or
IJS is less than 1 or greater than NY or
IKS is less than 1 or greater than NZ.

I Source Number

IIS I location of the source block.

IJS J location of the source block

IKS K location of the source block.

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

QWW Fluid discharge rate lb/day (kg/sec). A negative rate implies a source and a positive a sink.

QHH Heat discharge rate, Btu/day (J/sec).

QCC Discharge rates of radioactive components, lb/day (kg/sec).

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

READ R2-10.5 (2E10.0) Source Data.

NOTE: Skip this READ if IRSS ≠ 2.

LIST: ALCH, BLCH

ALCH Leach time for radioactive waste within repository boundaries, day (sec).

BLCH Lag time for initiation of leaching of waste from repository. Time from start of simulation to the beginning of leaching, day (sec).

READ R2-11 (3I5) Iteration Specifications.

NOTE: This data is entered if INDT is not zero. If default values are desired, enter INDT as zero and skip this READ.

LIST: MINITN, MAXITN, IMPG

ERROR MESSAGE:

(Number 41) Minimum number of outer iterations (MINITN) is less than 1 or MINITN is greater than maximum number of outer iterations (MAXITN)

(Number 42) Method of solution is L2SOR (METHOD=+2) and IMPG is less than or equal to zero.

MINITN Minimum number of outer iterations in the subroutine ITER. The default value is one.

MAXITN Maximum number of outer iterations in the subroutine ITER. The default value is 5.

IMPG Number of time steps after which the optimum parameters for the inner iterations are recalculated for the two-line successive overrelaxation method. This data need be entered only if METHOD is equal to +2. The default value for IMPG is 5.

READ R2-11.5 (I5) Solution Control.

NOTE: Skip this READ if ICLL is zero.

LIST: NCALL

NCALL Same definition as for READ M-2.

READ R2-12 (8E10.0) Time Stepping Information.

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

ERROR MESSAGE:

(Number 43) The time at which next set of recurrent data are to be entered (TCHG) is less than or equal to current TIME.

(Number 44) DT is zero for the first transient time step. Automatic time step control may not be initiated until at least the second time step.

(Number 45) DTMAX is less than DTMIN.

TCHG Time at which next set of recurrent data will be read, day (sec). The restart records can be written at TCHG only. Also, the mapping subroutine can be activated at TCHG only.

DT Time step specification, day (sec). 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. DT must not be zero for the first time step of a run starting from zero time, unless the steady-state option (NCALL=4) is used.

DCMX Maximum trace component concentration change desired per time step. The default value is 0.95.

DSMX Maximum brine concentration change desired per time step. The default value is 0.25.

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

DTPMX Maximum temperature change desired per time step, °F (°C). The default value is 10°F (5°C).

DTMAX Maximum time step allowed, day (sec). The default value is 30 days (2.6×10^6 sec).

DTMIN Minimum time step required, day (sec). The default value is 1.0 day (8.64×10^4 sec).

NOTE: The last six parameters are used only if the automatic time-step feature is selected, i.e. DT = 0. If this feature is selected, the program will automatically increase or decrease the time step size every time step to seek a value such that the maximum changes in the concentration, pressure and temperature are less than or equal to the specified values.

READ R2-13 (1115) Output Control.

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

ERROR MESSAGE: The value entered for MAP is not permissible. All
(Number 46) three digits must be either 0 or 1.

I01 Control parameter for frequency of the time step summary output. The time step summary gives cumulative field injections and productions, material and heat balances, average aquifer pressure, cumulative heat loss to the overburden and the underburden, cumulative water, brine and heat influxes across the peripheral boundaries, and the maximum pressure, concentration and temperature changes in any block during the time step.

I02 Control parameter for frequency of the well summary output. This summary gives water, heat and brine fluid production and injection rates, cumulative production and injection, wellhead and bottom-hole pressures, wellhead and bottom-hole temperatures and the grid block pressure in which the well is located. This summary also gives the total production and injection rates and cumulative production and injection.

I03 Control parameter for listings of the grid block values of concentration, temperature and pressure.

I04 Control parameter for injection/production rate in each layer for each well.

I05 Control parameter for listings of the grid block values of radionuclide concentrations.

I06 Control parameter for listing of aquifer influence functions.

The following values apply to all five 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 through to the step ending at TCHG.
- 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 listings of the grid block values of the dependent variables. The listings are printed according to the frequency specified (I03). This parameter gives one the option for not printing the tables not desired. This parameter requires a three digit specification and the first digit refers to pressure, the second to temperature and the third to concentration:

- 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 absolute 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.

- 0 - No restart record will be written.
- 1 - Restart record will be written on Tape 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 radial system and for x-y coordinates (areal maps) and x-z coordinates (for NY = 1 only) in a cartesian system. This parameter requires a four digit specification, the first digit referring to parent radionuclide concentrations, the second to pressures, the third to temperatures, and the fourth to brine concentrations:

- 0 - The variable will not be mapped.
- 1 - The variable will be mapped at TCHG.

For example, if contour maps are desired for pressure and temperature only, enter MAP = 0110.

MDAT Control parameter for entering the mapping specifications:

- 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.

IIPRT Intermediate print control. Activated only for first time step in recurrent data set.

- 0 - none of the following output will be activated.
- 1 - Darcy velocities will be printed.
- 2 - Flow, thermal dispersion and mass dispersion transmissibilities will be printed in addition to the velocities.
- 3 - Fluid density, viscosity, enthalpy and net dispersivities will be printed in addition to the quantities listed above.

READ R2-14 (I5, 2F10.0) Map Data.

NOTE: Enter this data only if contour maps are desired (MAP is not equal to 000), and if MDAT is equal to one.

LIST: NORIEN, XLGTH, YLGTH

NORIEN Map orientation factor.

- 0 - The map is oriented with x (refers to r for radial geometry) increasing from left to right and y (z for radial geometry or for cartesian geometry with NY = 1) increasing up the computer page, i.e. the x = 0, y = 0 point is the lower left-hand corner.
- 1 - The map is oriented with x increasing from left to right and y increasing down the computer page. The origin is the upper left-hand corner.

XLGTH The length, in inches, on the computer output which is desired in the x (or r) direction.

YLGTH The length, in inches, on the computer output which is desired in the y (or z for radial geometry) direction.

READ R2-15 (6I5, 2F10.0) Map Data.

NOTE: Enter this data only if pressure contour maps are desired, and if MDAT equals one. These entries refer to pressure mapping only.

LIST: IP1, IP2, JP1, JP2, KP1, KP2, AMAXP, AMINP

ERROR MESSAGE:

(Number 47) IP2 is greater than NX or
KP2 is greater than NZ or
HTG is not equal to 3 and JP2 is greater than NY.

IP1, IP2 Lower and upper limits, inclusive, on the I-coordinate of the region to be mapped.

JP1, JP2 (Similar definition for J-coordinate).

KP1, KP2 (Similar definition for K-coordinate).

NOTE: For a cartesian system with NY > 1 (KP2-KP1+1) areal maps will be processed. For a cartesian system with NY = 1 one map will be processed.

AMAXP, AMINP The maximum and minimum value of the pressure (psi or Pa) used to obtain 20 contour intervals. If the pressure in any grid block is higher than AMAXP, it will be indicated as AMAXP, and similarly a pressure lower than AMINP is printed as AMINP. If AMAXP is entered as zero or a negative value, the program will search for a maximum and use the value as AMAXP. If AMINP is entered as a large negative number (<-99.0), the program will search for a minimum and use that value as AMINP.

READ R2-16 (6I5, 2F10.0) Map Data.

NOTE: This READ refers to temperature contour maps. Enter this data only if temperature maps are desired, and if MDAT equals one.

LIST: IT1, IT2, JT1, JT2, KT1, KT2, AMAXT, AMINT

ERROR MESSAGE: IT2 is greater than NX or
KT2 is greater than NZ or
HTG is not equal to 3 and JT2 is greater than NY.

NOTE: The user is referred to READ R2-15 for definition of these parameters. This card refers to temperature mapping only as opposed to pressure mapping for R2-15.

READ R2-17 (6I5, 2F10.0) Map Data.

NOTE: This READ refers to brine concentration contour maps. Enter this data only if concentration maps are desired, and if MDAT equals one.

LIST: IK1, IK2, JK1, JK2, KK1, KK2, AMAXK, AMINK

ERROR MESSAGE:

(Number 49) IK2 is greater than NX or
KK2 is greater than NZ or
HTG is not equal to 3 and JK2 is greater than NY.

NOTE: See READ R2-15 for definition of these parameters. This card refers to concentration mapping only as opposed to pressure mapping for READ R2-15.

READ R2-18 (6I5, 2F10.0) Map Data.

NOTE: This READ refers to parent radionuclide concentration contour maps. Enter this data only if concentration maps are desired, and if MDAT equals one.

LIST: JT1, JT2, JT1, JT2, KT1, KT2, AMAXT, AMINT

NOTE: See READ R2-15 for definition of the parameters. Either radionuclide concentration or temperature (but not both) may be mapped at the same TCHG.

NOTE: The data entered up to this point are sufficient to execute the program until time equals TCHG. The recurrent data may be read again at that point to continue a run. To terminate the simulation phase of a run, enter ITHRU = 1 (READ R2-1 after R2-17). If any plots are desired (if NPLP or NPLT or NPLC equals one), enter the plotting data (READ P-2 through P-4) as well. If no plots are desired, ITHRU = 1 will terminate the execution.

6.1.6. The "P" Cards (Plotting Data)⁺

The specifications for the plots and observed data are entered here. Plots may be obtained even if no observed data are available. Enter no plotting data if no plots are desired. Plots can be obtained for the values of the dependent variables of the well (at the wellhead and at the bottom-hole). The quantities plotted depend upon the type of the well. The quantities plotted for different wells are as follows:

<u>TYPE OF WELL</u>	<u>Quantities Plotted</u>
Observation well	Bottom-hole pressure, temperature and concentration

⁺ The term "plot," as used herein, refers to a two-dimensional plot of pressure, temperature, or brine concentrating at either the wellhead or bottom-hole versus time including both experimental and calculated data. In contrast, the term "map," as used in previous sections, refers to contour plots of pressure, temperature or concentration for two spatial dimensions including calculated data only.

Injection well-bottom-hole conditions specified (ISURF=0)	Bottom-hole pressure
Injection well-surface conditions specified (ISURF=1)	Bottom-hole pressure and temperature, surface pressure
Production well-bottom-hole conditions specified	Bottom-hole pressure, temperature and concentration
Production well-surface conditions specified	Bottom-hole pressure, temperature and concentration, surface pressure and temperature

 NOTE: 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 the 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, follow the last set with a blank card.

READ P-1 (I5) Plotting Data.

NOTE: Enter this data only if NPLP or NPLT or NPLC equals -1, i.e. the plots are desired for a previous run.

LIST: NWT

 NWT Total number of wells.

READ P-2 (I5, 5X, 10A4) Plotting Data.

LIST: KW, ID

 KW The well number.

 ID A title for the plots for well number KW.

READ P-3 (7F10.0) Plotting Data.

NOTE: These variables define the ranges of the coordinate axes for plots.

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

TMN	Lower limit on time, days (seconds).
TMX	Upper limit on time, days (seconds).
DT	Time step for each row, days (seconds). For example, if TMN = 5, TMX = 15 and DT = 0.5, the time coordinate axis will be 20 rows long.
PWMN, PSMN, TWMN, TSMN CMN	Lower limits on bottom-hole pressure, psi (Pa); surface 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); and brine concentration, dimensionless, respectively.

READ P-4 (6F10.0) Plotting Data.

NOTE: Read as many cards as the observed data points (one card for each value of time at which the observed values are available). Follow the last card with a negative number in the first field specification (F10.0).

LIST TOX, POW, POS, TOW, TOS, COS

TOX	Observation time, days (seconds).
POW	Bottom-hole pressure, psi (Pa).
POS	Surface pressure, psi (Pa).
TOW	Bottom-hole temperature, °F (°C).
TOS	Surface temperature. °F (°C).
COS	Brine concentration, dimensionless.

NOTE: The calculated data are read from Tape 12. If plots for a previous run are desired, Tape 12 should be attached. If less than NWT sets of the plotting data are entered, follow the last card with a blank card. This is the end of the data set.

6.2 MAPS FROM RESTART RECORDS

Restart records may be edited to obtain maps for the dependent variables. The following set of data cards are required to obtain maps for a previous run.

READ M-1 Two title cards.

READ M-2 Control parameters. RSTRT must be greater than zero.

READ M-4 Length of the variable blank common.

READ M-5 Enter any negative value for TM.HG.

READ M-6 (I5)

LIST: IMPT

IMPT The time step number at which the maps are desired. A restart record must exist corresponding to this time step.

READ M-7 (I5)

LIST: MAP

MAP Requires a three-digit specification as in READ R2-13, except that it should be negative.

READ R2-15 to R2-17 Map Specifications

NOTE: Insert as many sets of mapping data (M-6, M-7, R2-15 to R2-17) as you desire. Follow the last set with a blank card.

6.3 AUXILIARY DISC FILES

The program uses disc files for data input and output, for restart records and for plotting data.

Two restart files are used for program continuation from a previous run. Restart records are always written on Unit 8 and read from Unit 4.

Plotting data at the end of each time step are written on Unit 12. If plots are desired at the end of the run, Unit 12 is rewound, plotting data is read in and plots printed. Unit 12 may be saved for subsequent plotting.

On Control Data machines, no control cards are required to access or store these files unless a restart record or a plot file for subsequent plotting is desired. The FORTRAN unit numbers used internally and their functions are described in Table 6-1.

Table 6-1. Auxiliary Disc Files

<u>Unit No.</u>	<u>Function</u>
4	For a continuation run, restart record is <u>read</u> from this unit.
5	Card reader
6	Line printer
8	Restart records are <u>written</u> on this unit.
12	Plotting data are written on this unit.

NOTATION

Roman

a	total leach time
B	viscosity parameter
b	time of initiation of leach process
C	concentration of the radioactive/trace component
\hat{C}	concentration of the inert contaminant
c_p	specific heat
c_R	compressibility of rock (formation)
c_T	coefficient of thermal expansion
c_w	compressibility of the fluid
c_s	coefficient for increase in fluid density with increasing brine content
D	initial volumetric density of wastes
$\underline{\underline{D}}$	dispersion tensor
D_m	molecular diffusion
$\underline{\underline{E}}$	dispersivity tensor (hydrodynamic + molecular)
g	acceleration due to gravity
g_c	units conversion factor equal to 32 ft/sec^2 for the English System and equal to unity for the SI system
h	depth
H	fluid enthalpy
$\underline{\underline{I}}$	unit tensor
$\underline{\underline{k}}$	permeability tensor

k_{di} equilibrium adsorption distribution constant
 k_x fractional allocation factor
 K equilibrium retardation factor
 K_m molecular heat conductivity of fluid and rock
 K_o hydraulic conductivity
 K_s hydraulic conductivity of the skin region surrounding a well
 m mass density
 M mobility
 N number of nuclei
 p pressure
 q rate of fluid withdrawal
 q_c rate of brine withdrawal
 q_{ci} rate of radionuclide withdrawal
 q_H rate of energy withdrawal
 r radius
 r_w radius of well bore
 r_1 radius of well skin
 \bar{r} equivalent grid-block radius
 \hat{r} grid-block edge (radial coordinates)
 R_s brine source rate due to salt dissolution
 R'_s fluid source rate due to salt dissolution
 S concentration of undissolved leachate

t time
T temperature
U specific internal energy
u Darcy velocity vector
u magnitude of u
v interstitial velocity
w weighting factor for numerical time integration
WI well index
z depth below a reference plane

Greek Letters

α dispersivity
 δ Kronecker delta
 ΔH change in total head
 Δx spatial increment in x
 Δy spatial increment in y
 Δz spatial increment in z
 Δt increment in time
 λ decay coefficient
 ϕ porosity
 ϕ_0 porosity at the reference pressure
 ρ fluid density
 ρ_0 fluid density at the reference temperature and pressure
and at zero brine concentration

ρ_1 fluid density at the reference temperature and pressure
and at unit brine concentration
 ρ_R formation density
 μ viscosity
 μ_R viscosity parameter
 τ radioactive half-life

Subscripts

i component index
H heat (energy)
R rock (formation)
w water (fluid)
s salt (brine)

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APPENDIX A ERROR DEFINITIONS

The program checks the input data for a number of possible errors to protect the user from running an entire problem with an error. A detected error will prevent execution, but the program will continue to read and check remaining data completely through the last recurrent data set.

If the number of elements in a fixed-dimension array exceeds the dimensions, the array must be redimensioned. This requires recompiling the program.

The errors detected in the data input are printed in a box and if an error has occurred, its number will appear in the box. Positions with zeros do not have errors. Error numbers 1 through 61 represent the following errors:

- (1) This error refers to READ M-3.
NX is less than or equal to one or
NY is less than one or
NZ is less than one.
The minimum dimensions on the grid block system are 2x1x1. The maximum size is limited only by the available computer storage.
- (3) This error refers to READ R1-1.
One or more of CW, CR, CPW and CPR is negative.
Physically, compressibilities and heat capacities are always equal to or greater than zero.
- (4) This error refers to READ R1-2.
One or more of UKTX, UKTY, UKTZ, ALPHL, ALPHT and DMEFF is negative.
- (5) This error refers to READ R1-3.
Either one or both the fluid densities (BWRN and BWRI is zero or negative.
- (6) This error refers to READ R1-7 through R1-10.
One or more of the viscosity values is entered as zero or negative.

Error numbers 7 through 9 refer to READ M-3.

- (7) HTG is not within the permissible range.
HTG is less than 1 or greater than 3.
- (8) The entered value for KOUT is not permissible. KOUT is not equal to 0, 1 or 3.

- (9) PRT exceeds permissible range of -1 to +2.
- (10) This error refers to READ R1-12 and R1-13. Either NZOB is greater than 2 and KOB is negative or NZUB is greater than 2 and KUB is negative.
- (11) This error refers to READ R1-17 through R1-19. One or more of grid block sizes (DELX, DELY, DELX) are zero or negative.
- (12) This error refers to aquifer properties for a homogeneous aquifer (READ R1-20). One or more of KX, KY and KZ is negative or PHI is less than 0.001 or greater than 1.0 or SINX or SINY is less than -1 or greater than +1.
- (13) This error refers to heterogeneous aquifer data, READ R1-21.
I is greater than NX or
J is less than 1 or greater than NY or
K is less than 1 or greater than NZ or
KX or KY or KZ is negative or
PHI is less than 0.001 or greater than 1.0.
- (14) This error refers to READ R1-22.
The first grid block center (R1) is less than or equal to the well radius (RWW), or R1 is greater than or equal to the aquifer boundary radius (RE).
- (15) This error refers to READ R1-23.
The layer thickness (DELZ) is less than or equal to zero or
KYY or KZZ is negative or
porosity (POROS) is less than 0.001 or greater than 1.0.
- (16) This error refers to READ R1-25. One or more of the RR's is greater than RE.
- (17) This error refers to aquifer description modifications, READ R1-26.
One or more of I1, I2, J1, J2, K1, K2 are out of permissible ranges 1-NX, 1-NY, and 1-NZ respectively, or
I1 is greater than I2 or
J1 is greater than J2 or
K1 is greater than K2.
- (18) This error refers to READ R1-27 and R1-28.
IAQ is greater than 4 or
one or more of I1, K2, J1, J2, K1, K2 are out of permissible ranges 1-NX, 1-NY, and 1-NZ respectively or
I1 is greater than I2 or
J1 is greater than J2 or
K1 is greater than K2.

- (19) The number of aquifer influence blocks (NABL) are greater than NABLMX specified in READ M-3.
- (21) This error refers to READ I-2.
One or more of I1, I2, J1, J2, K1, K2 are out of permissible ranges 1-NX, 1-NY, and 1-NZ respectively, or
 - I1 is greater than I2 or
 - J1 is greater than J2 or
 - K1 is greater than K2 or
 - CINIT is negative.
- (22) This error refers to READ I-4.
The description is the same as error 21 for radioactive/trace components.
- (23) Some grid block which has a nonzero pore volume also has a zero sum of transmissibilities over its surface.
- (24) Some grid block pore volume is negative.
- (25) This error refers to READ R2-4.
Total number of wells (NWT) is less than 1 or exceeds dimension limit NWMAX.
- (26) This error refers to READ R2-6.
Well number I is less than 1 or greater than NWT.

Error numbers 27 through 39 refer to READ R2-7.

- (27) Well locatin IIW, IJW is outside aquifer, i.e.
IIW is less than 1 or greater than NX or
IJW is less than 1 or greater than NY.
- (28) The well perforations are outside the aquifer, i.e.
IIC1 or IIC2 is out of the range of 1-NZ or
IIC1 is greater than IIC2 or
the top block of the completion interval (K=IIC1) is a zero pore volume block.
- (30) The entered value of IINDW1 is not permissible. The permissible values are +1, +2 and +3.
- (32) A well index of zero is permissible only if IINDW1 is equal to one. This error occurs if IINDW1 is not equal to one and WI is zero or negative.
- (33) IINDW1 is +3 and BHP is 0. The specified value of the bottom-hole pressure is a limiting value of the well pressure if IINDW1 is +3.

- (35) All completion layers of a well are in zero pore volume blocks.
- (37) One or more of KHL values are negative.
- (38) All KHL values are zero for some well. At least one KHL value must be non-zero.
- (39) A well number I is negative or exceeds NWT.
- (40) This error refers to READ R2-2. METHOD is less than -2 or greater than +2 or WTFAC is greater than 1.0.

Error numbers 41 and 42 refer to READ R2-11.

- (41) Minimum number of outer iterations (MINITN) is less than 1 or MINITN is greater than maximum number of outer iterations (MAXITN).
- (42) Method of solution is L2SOR (METHOD=+2) and IMPG is less than or equal to zero.

Error numbers 43 through 46 refer to READ R2-12 and R2-13.

- (43) The time at which next set of recurrent data are to be entered (TCHG) is less than or equal to current TIME.
- (44) DT is zero for the first transient time step. Automatic time step control may not be initiated until at least the second time step.
- (45) DTMAX is less than DTMIN.
- (46) The value entered for MAP is not permissible. All three digits must be either 0 or 1.

Error numbers 47, 48 and 49 refer to READ R2-15, R2-16 and R2-17, respectively.

- (47) IP2 is greater than NX or KP2 is greater than NZ or HTG is not equal to 3 and JP2 is greater than NY.
- (48) IT2 is greater than NX or KT2 is greater than NZ or HTG is not equal to 3 and JT2 is greater than NY.

(49) IK2 is greater than NX or
KK2 is greater than NZ or
HTG is not equal to 3 and JKZ is greater than NY.

(50) This error refers to READ R2-10.
NSS is greater than NSMAX (entered in READ M-3) or
I is greater than NSS or
IIS is greater than NX or
IJS is less than 1 or greater than NY or
IKS is less than 1 or greater than NZ.

Error numbers 51 through 54 refer to READ group R0.

(51) This error refers to READ R0-1, LIST 1.
I is equal to zero or greater than NCP (entered in READ M-3) or
NP(I) is negative.

(52) This error also refers to READ R0-1, LIST 1.
DEC is negative for at least one of the components.

(53) This error refers to READ R0-1, LIST 2.
For one or more of the components,
KP is less than 1 or greater than NCP (entered in READ M-3) or AP is negative.

(54) This error refers to READ R0-2.
At least one of DIS is negative.

Error numbers 55 through 61 refer to READ Group R1A.

(55) This error refers to rock type specification READ R1A-1.
One or more of I1A, I1B, J1A, J1B, K1A, K1B are out of
permissible ranges 1-NX, 1-NY, and 1-NZ respectively,
or
I1A is greater than I1B or
J1A is greater than J1B or
K1A is greater than K1B.

(56) This error refers to salt dissolution rate-fraction
product, R1A-2.
One or more values of ACS is negative.

(57) This error refers to the repository specifications,
R1A-4.
One or more of SDRIFT, SCNSTR, DCNSTR, or HCNSTR are
negative.

(58) This error refers to repository boundary location, R1A-6. One or more of I1A, I1B, J1A, J1B, K1A, K1B are out of permissible ranges 1-NX, 1-NY, and 1-NZ respectively, or
I1A is greater than I1B or
J1A is greater than J1B or
K1A is greater than K1B.

(59) This error refers to the interpolation times, R1A-7. One or more of the interpolation times, CTIME, is negative.

(60) This error refers to the repository specifications, R1A-4. For high-level storage, SDRIFT or SCNSTR exceed the greater of DELX or DELY, or HCNSTR exceeds THH.

(61) This refers to the radionuclide solubilities, R1A-9. One or more of the solubilities is negative.

APPENDIX B
DEFINITION OF PROGRAM VARIABLES

ACS(NRT)	Product of the rate of salt dissolution and the mass fractions of solubles to total dry mass, day ⁻¹ (sec ⁻¹)
ALCH	Leach time for radioactive waste within repository boundaries, day (sec)
ALPHAL(NRT)	For a rock type, the longitudinal dispersivity factor, ft (m)
ALPHAT(NRT)	For a rock type, the transverse dispersivity factor, ft (m)
ALPHL	Longitudinal dispersivity factor, ft (m)
ALPHT	Transverse dispersivity factor, ft (m)
AMAXK	The maximum value of the concentration to be plotted, dimensionless
AMAXP	The maximum value of the pressure to be plotted, psi (Pa)
AMAXT	The maximum value of the temperature in °F (°C) to be plotted or the maximum parent radionuclide concentration (dimensionless)
AMINK	The minimum value of the concentration to be plotted, dimensionless
AMINP	The minimum value of the pressure to be plotted, psi (Pa)
AMINT	The minimum value of the temperature in °F (°C) to be plotted or the maximum parent radionuclide concentration to be plotted, dimensionless
AP(NP)	Fraction of parent component KP that decays to the component I
BHP	Bottom-hole pressure for a well, psi (Pa)
BLCH	Lag time for initiation of leaching of waste from repository, day (sec)
BROCK	Actual rock density (solid particle), 1b/ft ³ (kg/m ³)

BWRI	The density of the contaminated fluid (concentration = 1) at PBWR and TBWR, 1b/ft ³ (kg/m ³)
BWRN	The density of the natural aquifer fluid (concentration = 0) at PBWR and TBWR, 1b/ft ³ (kg/m ³)
CINIT	Initial concentration (brine or radionuclide) of each of the blocks within a defined region, dimensionless
CINJ	Contaminant concentration in the injection fluid, dimensionless
CMN	Lower limit on the range of the coordinate axis for plotting the well brine concentration, dimensionless
CMX	Upper limit on the range of the coordinate axis for plotting the well brine concentration, dimensionless
CNAME(2)	Identification of radioactive component .
CNDUM (NTIME)	Pertains to the interpolation of concentrations. If interpolation is to be used, then CNDUM represents the concentrations at the interpolation times. If interpolation is not used, then CNDUM(1) is the initial concentration, dimensionless.
CONV	Conversion factor for the thermal conductivities to obtain units of Btu/ft-day-°F (J/m-sec-°C)
CONVC	This parameter multiplies the waste concentrations to convert them to 1b/ft ³ (kg/m ³)
CONVL	For canistered wastes CONVL multiplies 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	This parameter multiplies the specified interpolation times (R1A-7) to convert them to day (sec)
COS	Observed concentration in a well to be plotted, dimensionless
CPOB	Overburden heat capacity per unit volume, Btu/ft ³ -°F (J/m ³ -°C)
CPR	Heat capacity of the rock per unit volume of solid, Btu/ft ³ -°F (J/m ³ -°C)
CPR1(NZ)	The rock heat capacity of a layer, Btu/ft ³ -°F (J/m ³ -°C)

CPUB	Underburden heat capacity per unit volume, Btu/ft ³ -°F (J/m ³ -°C)
CPW	The heat capacity of the aquifer fluid, Btu/lb-°F (J/kg-°C)
CR	Compressibility of pore structure, (psi) ⁻¹ , (Pa) ⁻¹)
CS(NCP)	Solubility limits expressed as mass fractions, dimensionless
CTIME(NTIME)	Interpolation times, day (sec)
CTW	Coefficient of thermal expansion of the aquifer fluid, (°F) ⁻¹ ((°C) ⁻¹)
CW	Compressibility of the aquifer fluid, (psi) ⁻¹ (Pa) ⁻¹)
C1	Constant value of brine concentration at the block-boundary specified according to VAB, dimensionless
DAMPX	Damping factor in estimating the next value of the pressure in well calculations (surface pressure for an injection well and bottom-hole pressure for a production well), dimensionless
DCMX	Maximum trace component concentration change desired per time step, dimensionless
DCNSTR	For canistered wastes, DCNSTR is the diameter of each canister in ft (m). For uncanistered wastes, DCNSTR is the volumetric waste density (volume of waste/bulk volume)
DEC(NCP)	Component half life in years
DELPW	Incremental value of pressure over which wellbore calculations are to be performed, psi (Pa)
DELX(NX)	Length of each row of blocks in the X direction, ft (m)
DELY(NY)	Length of each row of blocks in the Y direction, ft (m)
DELZ(NZ)	Thickness of each vertical layer, ft (m)
DEPTH	Depth to top of grid-block (1,1,1), ft (m)
DI(2,NCP)	Identification for radioactive component I, alphanumeric
DIS(NCP)	Adsorption distribution coefficient, ft ³ /lb (m ³ /kg)

DMEFF	Molecular diffusivity in the porous medium, includes porosity and tortuosity effects (porosity x fluid molecular diffusivity x tortuosity), ft ² /day (m ² /sec)
DPMX	Maximum (over grid) pressure change desired per time step, psi (Pa)
DSMX	Maximum (over grid) concentration change desired per time step, dimensionless
DT	Time step specification for the run and the smallest time interval used in creating the coordinate axis for plotting, day (sec)
DTMAX	For automatic time stepping, the maximum allowed size of the time step, day (sec)
DTMIN	The minimum required size of the time step for automatic time stepping, day (sec)
DTPMX	Maximum (over grid) temperature change desired per time step, °F (°C)
DW	Inside wellbore (pipe) diameter, ft (m)
DZOB	Thickness of each overburden block, ft (m)
DZUB	Thickness of each underburden block, ft (m)
ED	Pipe roughness (inside), ft (m)
EPS	The tolerance on calculating temperature from given values of enthalpy and pressure, °F (°C)
FAB	Factor by which the aquifer influence coefficient (VAB) will be modified, dimensionless
FPV	If positive or zero, this is the factor by which the pore volumes within a defined region are to be multiplied. If negative, the absolute value will be used for pore volume within a defined region, replacing the values read earlier or determined from the porosity data, dimensionless.
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, replacing the values read earlier or determined from the permeability data, dimensionless.

FTY	"Same wording as FTX but substitute y for x"
FTZ	"Same wording as FTX but substitute z for x"
HADD	This is an increment that will add to the depths within a specified region, ft (m)
HCNSTR	Canister height, ft (m)
HDATUM	A datum depth measured relative to the reference plane, ft (m) for printing the dynamic pressures
HINIT	An arbitrary depth for setting up initial conditions, ft (m)
HTG	Control parameter for input of reservoir description data
I	Used to indicate either radioactive component number, well number or radioactive component source number
IAQ	Control parameter for selecting the type of aquifer block representation
ICLL	Control parameter for changing the equation solution control
ICOMP	Control parameter for initializing brine concentrations
ID	A title for the plots for a specified well, alphanumeric
IIC1	Uppermost layer in which a well is completed
IIC2	Lowermost layer in which a well is completed
IINDW1	Well specifications option
IIPRT	In the R1 data, this parameter should be ignored. In the R2 data, this variable is the intermediate parameters printing index
IIS	The x-direction (or I) location of a source block for fluid, heat or radionuclides
IIW	The x-direction (or I) coordinate of a grid cell containing a well
IJS	The y-direction (or J) location of a source block for fluid, heat or radionuclides

IJW	The y-direction (or J) coordinate of a grid cell containing a well
IKS	The z-direction (or K) location of a source block for fluid, heat or radionuclides
IK1	For concentration mapping, this is the lower z-direction limit of mapping
IK2	For concentration mapping, this is the upper z-direction limit of mapping
ILAST	Length of the variable blank common, words
ILEVEL	An indicator for specifying either canistered waste storage (ILEVEL = 1) or uncanistered waste storage (ILEVEL = 0).
IMETH	A control parameter for reading method of solution (i.e., 0 = do not read method of solution and 1 = read 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
INAT	Control parameter for entering initial fluid velocity (i.e., 0 = the aquifer fluid is initially static and 1 = the resident fluid velocity will be entered in READ I-3)
INDQ	Control parameter for reading well rates (i.e., 0 = do not read well rates, 1 = read well rates on one card and 2 = read one card for each well rate)
INDT	Control parameter for reading reservoir solution iteration data (i.e., 0 = do not read iteration data and 1 = read iteration data)
IOPT	Control parameter for reading well-bore iteration data (i.e., 0 = do not read the data and 1 = read the data)
I01	Control parameter for frequency of the time-step summary output
I02	Control parameter for frequency of the well-summary output
I03	Control parameter for listings of the grid-block values of concentration, temperature and pressure
I04	Control parameter for injection/production rate in each layer for each well
I05	Control parameter for listings of the grid-block values of trace-component concentrations

I06	Control parameter for listing of aquifer-influence functions
I08	Control parameter for listings of the grid-block values of the dependent variables (pressure, temperature and concentration)
IPROD	Control parameter for reading well-bore data (i.e., 0 = do not read the data and 1 = read the data)
IP1	The lower limit on the x-direction (or I) coordinate of a region for pressure mapping
IP2	The upper limit on the x-direction (or I) coordinate of a region for pressure mapping
IRD	A control parameter for initializing radioactive trace components concentration, i.e. 0 = initial concentrations are zero and 1 = non-zero concentrations will be entered in READ I-4
IRSS	Control parameter for reading radioactive components source data (i.e., 0 = do not read the data, 1 = read the data and 2 = leach model will be activated)
IRT	Rock-type indicator
ISURF	Control parameter for wellbore calculations
ITHRU	Run termination control (i.e. 0 = continue and 1 = terminate)
IT1	The lower limit on the x-direction (or I) coordinate of a region for temperature mapping
IT2	The upper limit on the x-direction (or I) coordinate of a region for temperature mapping
IUNIT	Units control parameter specifying either English Engineering System (IUNIT = 0) or SI system (IUNIT = 1)
IWELL	Control parameter for reading well definition data (i.e. 0 = do not read well data and 1 = read well data)
I1	This variable is used several times to specify the lower limit on the x-direction coordinate for defining a region.
I1A	Same as I1
I1B	Same as I2
I2	This variable is used several times to specify the upper limit on the x-direction coordinate for defining a region.

JK1	The lower limit, inclusive, on the y-direction (or J) coordinate of a region to be mapped for concentrations
JK2	The upper limit, inclusive, on the y-direction (or J) coordinate of a region to be mapped for concentrations
JP1	The lower limit, inclusive, on the y-direction (or J) coordinate of a region to be mapped for pressures
JP2	The upper limit, inclusive, in the y-direction (or J) coordinate of a region to be mapped for pressures
JT1	The lower limit, inclusive, on the y-direction (or J) coordinate of a region to be mapped for temperatures
JT2	The upper limit, inclusive, on the y-direction (or J) coordinate of a region to be mapped for temperatures
J1	This variable is used several times to specify the lower limit on the y-direction (or J) coordinate for defining a region.
J1A	Same as J1
J1B	Same as J2
J2	This variable is used several times to specify the upper limit on the y-direction coordinate for defining a region.
KAQ	Control variables for setting boundary conditions on the heat flow equation (i.e. -1 = radiation condition only, 0 = temperature condition only, 1 = temperature and radiation conditions)
KH	The conductivity-thickness for the aquifer, ft ² /day (m ² /sec)
KHL	Layer allocation factors for a well, dimensionless
KK1	The lower limit, inclusive, on the z-direction (or K) coordinate of a region to be mapped for concentrations
KK2	The upper limit, inclusive, on the z-direction (or K) coordinate of region to be mapped for concentrations
KOB	Vertical thermal conductivities of the overburden Btu/ft-day-°F (J/m-sec-°C).

KOUT	Output control parameter (i.e., 0 = all program output activated, 1 = all program activated except initial arrays and 3 = no program output is activated)
KP(NP)	Parent component number
KP1	The lower limit, inclusive, on the z-direction (or K) coordinate of a region to be mapped for pressures
KP2	The upper limit, inclusive, on the z-direction (or K) coordinate of a region to be mapped for pressures
KT1	The lower limit, inclusive, on the z-direction (or K) coordinate of a region to be mapped for temperatures
KT2	The upper limit, inclusive, on the z-direction (or K) coordinate of a region to be mapped for temperatures
KUB	Vertical thermal conductivities of the underburden, Btu/ft-day-°F (J/m-sec-°C)
KW	The well number used for identifying a well to be plotted
KX	Hydraulic conductivity for flow in the x-direction, ft/day (m/sec)
KY	Hydraulic conductivity for flow in the y-direction, ft/day (m/sec)
KYY(NZ)	Horizontal hydraulic conductivity, ft/day (m/sec)
KZ	Hydraulic conductivity for flow in the z-direction, ft/day (m/sec)
KZZ(NZ)	Vertical hydraulic conductivity, ft/day (m/sec)
K1	This variable is used several times to specify the lower limit on the z-direction (or K) coordinate for defining a region.
K1A	Same as K1
K1B	Same as K2
K2	This variable is used several times to specify the upper limit on the z-direction (or K) coordinate for defining a region.
LADJ(NCP)	Lambda (rate constant) adjustment index (i.e., 0 = do not modify the rate constant and 1 = modify the rate constant)

MAP	Control parameter for printing contour maps at time TCHG
MASS(NCP)	Mass number of a radioactive component
MAXITN	Maximum number of outer iterations in subroutine ITER
MDAT	Control parameter for entering the mapping specifications (0 = no mapping specifications to be read and 1 = read mapping specifications)
METHOD	The method-of-solution indicator
MINITN	Minimum number of outer iterations in the subroutine ITER
NAAR	Storage allocation for working array A in the direct-solution routine, words
NABLMX	Maximum number of aquifer-influence-function blocks
NCALC	Control parameter for selecting how the Carter-Tracy aquifer coefficients are to be assigned
NCALL	Control parameter for solving the basic partial differential equations
NCOMP	Number of components for which descriptive information is to be read in the R1A cards
NCP	Number of radioactive/trace components in the system
NCV	The number of entries in the concentration-viscosity table
NDT	The number of entries in the depth-versus-temperature table
NITQ	The maximum number of outer iterations in the wellbore calculations
NORIEN	The control parameter for map orientation
NOUT	Output control parameter for wellbore calculations
NP(NCP)	Number of parent components for a radioisotope
NPLC	Control parameter for plotting concentrations in the wells
NPLP	Control parameter for plotting pressures in the wells
NPLT	Control parameter for plotting temperatures in the wells

NPT	Number of points in the influence-function-versus-dimensionless-time table
NREPB	Number of repository blocks
NRT	Number of rock types. Distribution coefficients, thermal conductivities, dispersivities and salt-dissolution coefficients are input as functions of rock type.
NSMAX	Maximum number of radioactive/trace components that will be used during the run
NSS	Number of radioactive component sources/sinks
NTIME	Number of times for which concentrations of unleached radioactive components within the repository are to be input
NTVI	Number of entries in the temperature-viscosity table for the contaminated fluid
NTVR	Number of entries in the temperature-viscosity table for the resident aquifer fluid
NWT	Total number of wells
NX	The number of grid blocks in the x-direction
NY	The number of grid blocks in the y-direction
NZ	The number of grid blocks in the z-direction
NZOB	Number of overburden blocks
NZUB	Number of underburden blocks
OD	Outside wellbore (casing) diameter, ft (m)
PBASE	Atmospheric or reference pressure at the well heads, psi (Pa)
PBWR	Reference pressure at which the fluid densities are to be entered, psi (Pa)
PHI	Porosity, dimensionless
PHIH	Porosity-thickness for an aquifer, ft (m)
PINIT	Initial pressure at the depth HINIT, psi (Pa)

POROS (NZ)	Porosity, dimensionless
POS	Surface pressure for plotting observed data points, psi (Pa)
POW	Bottom-hole pressure for plotting observed data points, psi (Pa)
PRT	Output-array-orientation control
PRTAB	Print control key for the aquifer-influence coefficient (0 = no printing, 1 = print)
PRTIF	Print control key for the influence-function table (0 = suppress printing, 1 = print)
PSMN	The lower limit on the range of the coordinate axis for plotting the well surface pressure, psi (Pa)
PSMX	The upper limit on the range of the coordinate axis for plotting the well surface pressure, psi (Pa)
PTD(NPT)	Terminal-rate-case influence function, dimensionless
PWMN	The lower limit on the range of the coordinate axis for plotting the well bottom-hole pressure, psi (Pa)
PWMX	The upper limit on the range of the coordinate axis for plotting the well bottom-hole pressure, psi (Pa)
P1	The constant value of pressure, at the block boundary specified according to VAB, psi (Pa)
Q(NWT)	Well production rate, ft ³ /day (m ³ /day)
QCC(NSS,NCP)	The radioactive-component discharge rate, lb/day (kg/sec)
QHH(NSS)	The heat discharge rate, Btu/day (J/sec)
QWELL	The well production rate, ft ³ /day (m ³ /sec)
QWW(NSS)	The fluid discharge rate, lb/day (kg/sec)
RAQ	Equivalent aquifer radius, ft (m)
RE	External radius of the aquifer for radial coordinates, ft (m)
RR(NX)	Radius of grid-block center, ft (m)

RER(5)	Radii of the boundaries between different regions, ft (m)
RSTRT	Code restart-control parameter
RSTWR	Restart record control parameter (0 = no restart record, 1 = write restart record)
RWW	Well radius, ft (m)
R1	For radial coordinates, the first grid block center, ft (m)
SC(NCV)	Concentration to be used in defining the concentration-versus-viscosity functions, dimensionless
SCNSTR	Center-to-center waste-canister separation within each row, ft (m)
SDRIFT	Separation of rows of waste canisters, 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
TBWR	Reference temperature at which the densities BWRN and BWRI are to be entered, °F (°C)
TBOTW	The rock temperature surrounding the wellbore at the bottom hole, °F (°C)
TCHG	Time at which the next set of recurrent data will be read, day (sec)
TD(NDT)	The temperatures in the depth-versus-temperature table, °F (°C)
TD(NPT)	Dimensionless time
TDIS	Thermal diffusivity of the rock surrounding the wellbore, ft ² /hr (m ² /sec)
THADD	This is an increment that will add to the thickness values within a defined region, ft (m)
THETA	Angle of the wellbore with the vertical plane, degrees
THETAQ	Angle of influence for Carter-Tracy functions, degrees
THP(NWT)	Tubing hole or the surface pressure for each well, psi (Pa)

TI(NTVI) Temperatures for the temperature-versus-viscosity table,
 °F (°C)

 TINJ Temperature of the injection fluid of a well, °F (°C)

 TIR Reference temperature for the contaminated fluid viscosity,
 °F (°C)

 TITLE(40) Title for the run, alphanumeric

 TMCHG Time at which the next set of recurrent data is to be read,
 day (sec)

 TMN Lower limit on the time axis for plotting, day (sec)

 TMX Upper limit on the time axis for plotting, day (sec)

 TO A standard temperature for calculating fluid density,
 °F (°C)

 TOLDP The tolerance on pressure calculations, psi (Pa)

 TOLX The tolerance on the fractional change in pressure over an
 iteration, fraction

 TOS Surface temperature for plotting observed data, °F (°C)

 TOW Bottom hole temperature for plotting observed data, °F (°C)

 TOX Observation time of data to be plotted, day (sec)

 TR(NTVR) Temperatures for the temperature-versus-viscosity table of
 the resident fluid, °F (°C)

 TRR Reference temperature for the resident viscosity fluid,
 °F (°C)

 TSMN The lower limit on the coordinate for plotting surface
 temperatures, °F (°C)

 TSMX The upper limit on the coordinate for plotting surface
 temperatures, °F (°C)

 TTOPW Rock temperature surrounding the wellbore at the surface,
 °F (°C)

 TWMN The lower limit on the coordinate for plotting the bottom-
 hole temperatures, °F (°C)

 TWMX The upper limit on the coordinate for plotting the bottom-
 hole temperatures, °F (°C)

T1	Constant value of temperature at the block boundary, specified according to KAQ, °F (°C)
T2	Temperature of surrounding media, specified according to KAQ, °F (°C)
T3	Coefficient of surface heat transfer, specified according to KAQ, Btu/day-ft-°F (W/m ² -°C)
UCOEF	For wells, the overall heat transfer coefficient between the inner surface of the pipe and the outer surface of the casting, Btu/ft ² -°F-hr (W/m ² -°C)
UCRP	Modified heat capacity of the rock per unit volume, Btu/ft ³ -°F (J/m ³ -°C)
UH	Modified depth (measured positively downward from the reference plane to the top of a grid block), ft (m)
UKTX	Thermal conductivity of the fluid saturated porous medium in the x-direction, Btu/ft-°F-day (J/m-sec-°C)
UKTY	Thermal conductivity of the fluid saturated porous medium in the y-direction, Btu/ft-°F-day (J/m-sec-°C)
UKTZ	Thermal conductivity of the fluid saturated porous medium in the z-direction, Btu/ft-°F-day (J/m-sec-°C)
UTCX(NRT)	For a rock type, the thermal conductivity of the media in the x-direction, Btu/ft-°F-day (J/m-°C-sec)
UTCY(NRT)	For a rock type, the thermal conductivity of the media in the y-direction, Btu/ft-°F-day (J/m-°C-sec)
UTCZ(NRT)	For a rock type, the thermal conductivity of the media in the z-direction, Btu/ft-°F-day (J/m-°C-sec)
UTH	Modified grid-block thickness in the vertical direction, ft (m)
VAB	Specifies either the aquifer-influence coefficient for each block within a defined region (IAQ = 1,2, or 3) or the boundary block type (IAQ = 4). Dimensions depend on the option chosen.
VCC(NCV)	Viscosity of a fluid mixture at a specified (SC) concentration and temperature (TRR), cp (Pa-sec)

VEL	Initial velocity of the resident aquifer fluid in the x-direction, ft/day (m/sec)
VISI(NTVI)	Viscosity of the contaminated fluid at a specified temperature (TI), cp (Pa-sec)
VISIR	Reference viscosity of the contaminated fluid at the reference temperature (TIR), cp (Pa-sec)
VISR(NTVR)	Viscosity of the aquifer resident fluid at a specified temperature (TR), cp (Pa-sec)
VISRR	The reference viscosity of the aquifer resident fluid at the reference temperature (TRR), cp (Pa-sec)
WI	Well index, ft ² /day, (m ² /sec)
WTFAC	Weight factor for finite-difference approximation in space
X	Pipe (wellbore) length to the top of the perforations, ft (m)
XLGTH	The length on the computer-output maps which is desired in the x (or r) direction, inches
YLGTH	The length on the computer-output map which is desired in the y (or z for radial geometry or for cartesian geometry with NY = 1) direction, inches
ZT(NDT)	Depth for the depth-versus-temperature table, ft (m)

APPENDIX C
VARIABLE INDEX

	<u>READ CARD(S)</u>	<u>FORMAT</u>	<u>COLUMNS</u>	<u>DIMENSIONS</u>
ACS(NRT)	R1A-2	F10.0	1-70	day ⁻¹ (sec ⁻¹)
ALCH	R2-10.5	E10.0	1-10	day(sec)
ALPHAL(NRT)	R1-2.5(List 2)	E10.0	1-70	ft(m)
ALPHAT(NRT)	R1-2.5(List 2)	E10.0	1-70	ft(m)
ALPHL	R1-2	E10.0	41-50	ft(m)
ALPHT	R1-2	E10.0	51-60	ft(m)
AMAXK	R2-17	F10.0	31-40	*
AMAXP	R2-15	F10.0	31-40	psi(Pa)
AMAXT	R2-16	F10.0	31-40	°F(°C)
	R2-18	F10.0	31-40	*
AMINK	R2-17	F10.0	41-50	*
AMINP	R2-15	F10.0	41-50	psi(Pa)
AMINT	R2-16	F10.0	41-50	°F(°C)
	R2-18	F10.0	41-50	*
AP(NP)	R0-1(Card 2)	E10.0	11-20, 31-40...	*
BHP	R2-7(List 2)	E10.0	11-20	psi(Pa)
BLCH	R2-10.5	E10.0	11-20	day(sec)
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	F10.0	31-40	*
CINJ	R2-7(List 2)	E10.0	31-40	*
CMN	P-3(Card 2)	F10.0	41-50	*
CMX	P-3(Card 2)	F10.0	51-60	*
CNAME(2)	R1A-8	2A4	1-8	**
CNDUM(NTIME)	R1A-8	F10.0	11-70	*
CONV	R1-2	E10.0	31-40	+
CONVC	R1A-5	F10.0	11-20	+
CONVL	R1A-5	F10.0	1-10	+
CONVT	R1A-5	F10.0	21-30	+
COS	P-4	F10.0	51-60	*
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)
CPR1(NZ)	R1-23	E10.0	41-50	Btu/ft ³ -°F(J/m ³ -°C)

* Dimensionless

** Alphanumeric

+ Depends on Input

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)
CS(NCP)	R1A-9	F10.0	1-70	*
CTIME(NTIME)	R1A-7	F10.0	1-70	day(sec)
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	 F10.0	 26-35	 *
DCMX	R2-1	E10.0	21-30	*
DCNSTR	R1A-4	F10.0	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	7E10.0	1-70	ft(m)
DELY(NY)	R1-18	7E10.0	1-70	ft(m)
DELZ(NZ)	R1-19	7E10.0	1-70	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	7E10.0	1-70	ft ³ /lb m ³ /kg
DMEFF	R1-2	E10.0	61-70	ft ² /day(m ² /sec)
DPMX	R2-12	E10.0	41-50	psi(Pa)
DSMX	R2-12	E10.0	31-40	*
DT	R2-12	E10.0	11-20	day(sec)
	P-3(Card 1)	F10.0	21-30	day(sec)
DTMAX	R2-12	E10.0	61-70	day(sec)
DTMIN	R2-12	E10.0	71-80	day(sec)
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)
DZUB(NZUB)	R1-15	7E10.0	1-70	ft(m)
 ED	 R2-7(List 3)	 E10.0	 21-30	 ft(m)
EPS	R2-3	F10.0	36-45	°F(°C)
 FAB	 R1-33(List 2)	 E10.0	 1-10	 *
FPV	R1-26(List 2)	E10.0	31-40	*
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	*

* Dimensionless
** Alphanumeric

HADD	R1-26(List 2)	E10.0	41-50	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	I5	16-20	++
 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	++
ICLL	R2-1	I5	41-45	++
ICOMP	I-1	I5	1-5	++
ID	P-2	10A4	11-50	**
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	M-2	I5	16-20	++
	R2-13	I5	51-55	++
IIS	R2-10(List 1)	I5	6-10	++
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	++
IK1	R2-17	I5	1-5	++
IK2	R2-17	I5	6-10	++
ILAST	M-4	I10	1-10	++
ILEVEL	R1A-3	I5	1-5	++
IMETH	R2-1	I5	11-15	++
IMPG	R2-11	I5	11-15	++
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	R2-1	I5	6-10	++
IO3	R2-13	I5	11-15	++
IO4	R2-13	I5	16-20	++
IO5	R2-13	I5	21-25	++
IO6	R2-13	I5	26-30	++
IO8	R2-13	I5	31-35	
IPROD	R2-1	I5	26-30	++
IP1	R2-15	I5	1-5	++
IP2	R2-15	I5	6-10	++

** Alphanumeric

++ Indicates a program flag, switch, option indicator or other indicator for which dimensions do not apply

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	++
IT1	R2-16	I5	1-5	++
	R2-18	I5	1-5	++
IT2	R2-16	I5	6-10	++
	R2-18	I5	6-10	++
IUNIT	M-2	I5	36-40	++
IWELL	R2-1	I5	6-10	++
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	++
I1A	R1A-1	I5	1-5	++
	R1A-6	I5	1-5	++
I1B	R1A-1	I5	6-10	++
	R1A-6	I5	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	++

JK1	R2-17	I5	11-15	++
JK2	R2-17	I5	16-20	++
JP1	R2-15	I5	11-15	++
JP2	R2-15	I5	16-20	++
JT1	R2-16	I5	11-15	++
	R2-18	I5	11-15	++
JT2	R2-16	I5	16-20	++
	R2-18	I5	16-20	++
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	++
J1A	R1A-1	I5	11-15	++
	R1A-6	I5	11-15	++
J1B	R1A-1	I5	16-20	++
	R1A-6	I5	16-20	++

++ Indicates a program flag, switch, option indicator or other indicator for which dimensions do not apply

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	++
	I-2	I5	16-20	++
KAQ	R1-28(List 1)	I5	31-35	++
KH	R1-31	E10.0	1-10	$ft^2/day(m^2/sec)$
KHL(IIC2)	R2-7(List 4)	E10.0	1-80	*
KK1	R2-17	I5	21-25	++
KK2	R2-17	I5	26-30	++
KOB	R1-13	E10.0	1-10	$Btu/ft-day-^{\circ}F(J/m-sec-^{\circ}C)$
KOUT	M-3	I5	31-35	++
KP(NP)	R0-1(list 2)	I5	1-5, 21-25...	++
KP1	R2-15	I5	21-25	++
KP2	R2-15	I5	26-30	++
KT1	R2-16	I5	21-25	++
	R2-16	I5	21-25	++
KT2	R2-16	I5	26-30	++
	R2-16	I5	26-30	++
KUB	R1-13	E10.0	21-30	$Btu/ft-day-^{\circ}F(J/m-sec-^{\circ}C)$
KW	P-2	I5	1-5,6-10	++
KX	R1-20	E10.0	1-10	$ft/day(m/sec)$
	R1-21(List 2)	E10.0	1-10	$ft/day(m/sec)$
KY	R1-20	E10.0	11-20	$ft/day(m/sec)$
	R1-21(List 2)	E10.0	21-30	$ft/day(m/sec)$
KYY(NZ)	R1-23	E10.0	11-20	$ft/day(m/sec)$
KZ	R1-20	E10.0	21-30	$ft/day(m/sec)$
	R1-21(List 2)	E10.0	21-30	$ft/day(m/sec)$
KZZ(NZ)	R1-23	E10.0	21-30	$ft/day(m/sec)$
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	++
K1A	R1A-1	I5	21-25	++
	R1A-6	I5	21-25	++
K1B	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	++

* Dimensionless

++ Indicates a program flag, switch, option indicator or other indicator for which dimensions do not apply

LADJ(NCP)	RO-1(List 1)	I5	26-30	++
MAP	R2-13	I5	41-45	++
MASS(NCP)	RO-1(List 1)	I3	1-3	++
MAXITN	R2-11	I5	6-10	++
MDAT	R2-13	I5	46-50	++
METHOD	M-3	I5	51-55	++
	R2-2	I5	1-5	++
MINITN	R2-11	I5	1-5	++
NAAR	M-3	I5	56-60	++
NABLMX	M-3	I5	46-50	++
NCALC	R1-29	I5	1-5	++
NCALL	M-2	I5	1-5	++
	R2-11.5	I5	1-5	++
NCOMP	M-3	I5	66-70	++
NCP	M-3	I5	21-25	++
NCV	R1-6	I5	1-5	++
NDT	R1-6	I5	16-20	++
NITQ	R2-3	I5	1-5	++
NORIEN	R2-14	I5	1-5	++
NOUT	R1-4	I5	1-5	++
NP(NCP)	RO-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	++
NREPB	M-3	I5	71-75	++
NRT	M-3	I5	26-30	++
NSMAX	M-3	I5	41-45	++
NSS	R2-9	I5	1-5	++
NTIME	M-3	I5	61-65	++
NTVI	R1-6	I5	11-15	++
NTVR	R1-6	I5	6-10	++
NWT	R2-4	I5	1-5	++
	P-1	I5	1-5	++
NX	M-3	I5	1-5	++
NY	M-3	I5	6-10	++
NZ	M-3	I5	11-15	++
NZOB	R1-12	I5	1-5	++
NZUB	R1-12	I5	6-10	++

++ Indicates a program flag, switch, option indicator or other indicator for which dimensions do not apply

OD	R2-7(List 3)	E10.0	31-40	ft(m)
PBASE	R1-5	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	*
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	F10.0	21-30	psi(Pa)
POW	P-4	F10.0	11-20	psi(Pa)
PRT	M-3	I5	36-40	++
PRTAB	R1-27	I5	6-10	++
PRTIF	R1-29	I5	11-15	++
PSMN	P-3(Card 1)	F10.0	51-60	psi(Pa)
PSMX	P-3(Card 1)	F10.0	61-70	psi(Pa)
PTD(NPT)	R1-32	F10.0	11-20, 31-40...	*
PWMN	P-3(Card 1)	F10.0	31-40	psi(Pa)
PWMX	P-3(Card 2)	F10.0	41-50	psi(Pa)
P1	R1-28(List 2)	E10.0	11-20	psi(Pa)
Q(NWT)	R2-5	E10.0	1-70	ft ³ /day(m ³ /day)
QCC(NSS,NCP)	R2-10(List 2)	E10.0	21-80	lb/day(kg/sec)
QHH(NSS)	R2-10(List 2)	E10.0	11-20	Btu/day(J/sec)
QWELL	R2-6	E10.0	6-16	ft ³ /day(m ³ /sec)
QWW(NSS)	R2-10(List 2)	E10.0	1-10	lb/day(kg/sec)
RAQ	R1-31	E10.0	21-30	ft(m)
RE	R1-22	E10.0	21-30	ft(m)
RR(NX)	R1-25	E10.0	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)
RI	R1-22	E10.0	11-20	ft(m)
SC(NCV)	R1-8	F10.0	1-20, 21-30...	*
SCNSTR	R1A-4	F10.0	11-20	ft(m)

* Dimensionless

++ Indicates a program flag, switch, option indicator or other indicator for which dimensions do not apply

SDRIFT	R1A-4	F10.0	1-10	ft(m)
SINX	R1-20	E10.0	41-50	*
SINY	R1-20	E10.0	51-60	*
TBWR	R1-3	E10.0	21-30	°F(°C)
TBOTW	R2-7(List 3)	E10.0	51-60	°F(°C)
TCHG	R2-12	E10.0	1-10	day(sec)
TD(NDT)	R1-11	F10.0	11-20, 31-40...	°F(°C)
TD(NPT)	R1-32	F10.0	1-10, 21-30...	*
TDIS	R1-5	E10.0	21-30	ft ² /hr(m ² /sec)
THADD	R1-26(List 2)	E10.0	51-60	ft(m)
THETA	R2-7(List 3)	E10.0	71-80	*
THETAQ	R1-31	E10.0	31-40	*
THP(NWT)	R2-8	E10.0	1-70	psi
TI((NTVI)	R1-10	F10.0	1-20, 21-30...	°F(°C)
TINJ	R2-7(List 2)	E10.0	21-30	°F(°C)
TIR	R1-7	E10.0	21-30	°F(°C)
TITLE	M-1	20A4/20A4 1-80		*
TMCHG	M-5	F10.0	1-10	day(sec)
TMN	P-3(Card 1)	F10.0	1-10	day(sec)
TMX	P-3(Card 1)	F10.0	11-20	day(sec)
TO	R1-16	E10.0	1-10	°F(°C)
TOLDP	R2-3	F10.0	16-25	psi(Pa)
TOLX	R2-3	F10.0	6-15	*
TOS	P-4	F10.0	41-50	°F(°C)
TOW	P-4	F10.0	31-40	°F(°C)
TOX	P-4	F10.0	1-10	day(sec)
TR(NTVR)	R1-9	F10.0	1-10, 21-30...	°F(°C)
TRR	R1-7	E10.0	1-10	°F(°C)
TSMN	P-3(Card 2)	F10.0	21-30	°F(°C)
TSMX	P-3(Card 2)	F10.0	31-40	°F(°C)
TTOPW	R2-7(List 3)	E10.0	41-50	ft(m)
TWMN	P-3(Card 2)	F10.0	1-10	°F(°C)
TWMX	P-3(Card 2)	F10.0	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/day-ft-°F(W/m-°C)
UCOEF	R2-7(List 3)	E10.0	61-70	Btu/ft ³ -°F-hr(W/m-°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-day(W/m-°C)
UKTY	R1-2	E10.0	11-20	Btu/ft-°F-day(W/m-°C)
UKTZ	R1-2	E10.0	21-30	Btu/ft-°F-day(W/m-°C)

* Dimensionless

UTCX(NRT)	R1-2.5(List 1)	F10.0	1-10	Btu/ft-°F-day(W/m-°C)
UTCY(NRT)	R1-2.5(List 1)	F10.0	11-20	Btu/ft-°F-day(W/m-°C)
UTCZ(NRT)	R1-2.5(List 1)	F10.0	21-30	Btu/ft-°F-day(W/m-°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	F10.0	11-20, 31-40...
VEL	I-3	F10.0	1-10	ft/day
VISI(NTVI)	R1-10	F10.0	11-20, 31-40...	cp(Pa-sec)
VISIR	R1-7	E10.0	31-40	cp(Pa-sec)
VISR(NTVR)	R1-9	F10.0	11-20, 31-40...	cp(Pa-sec)
VISRR	R1-7	E10.0	11-20	cp(Pa-sec)
WI	R2-7(List 2)	E10.0	1-10	ft ² /day(m ² /sec)
WTFAC	R2-2	F10.0	6-15	*
X	R2-7(List 1)	E10.0	1-10	ft(m)
XLGTH	R2-14	F10.0	6-15	in
YLGTH	R2-14	F10.0	16-25	in
ZT(NDT)	R1-11	F10.0	1-10, 21-30...	ft(m)

- * Dimensionless
- + Depends on the input

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APPENDIX D

ENGLISH AND SI UNITS

<u>Variable</u>	<u>English</u>	<u>SI</u>
Area	ft ²	m ²
Compressibility	1/psi	1/Pa
Component mass flow rate	lb/day	kg/sec
Component transmissibility	lb/day	kg/sec
Concentration	fraction	fraction
Darcy velocity	ft/day	m/sec
Density	lb/ft ³	kg/m ³
Diffusivity	ft ² /day	m ² /sec
Dispersivity	ft	m
Distribution coefficient	ft ³ /lb	m ³ /kg
Enthalpy	Btu	J
Fluid flow transmissibility	lb/day	kg/sec
Fluid heat capacity	Btu/lb-°F	J/kg-°C
Fluid mass flow rate	lb/day	kg/sec
Half-life	yr	yr
Heat flow rate	Btu/day	J/sec
Hydraulic conductivity	ft/day	m/sec
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/day	1/sec
Temperature	°F	°C
Thermal conductivity	Btu/ft-day-°F	J/m-sec-°C
Thermal expansion	1/°F	1/°C
Thermal transmissibility	Btu/day-°F	J/sec-°C
Time	day	sec
Viscosity	cp	Pa-sec
Volume	ft ³	m ³
Waste concentration	lb/ft ³	kg/m ³
Well flow rate	ft ³ /day	m ³ /sec
Well index	ft ² /day	m ² /sec

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APPENDIX E

CONVERSION OF ENGLISH TO METRIC UNITS
FOR SWIFT MODEL

MULTIPLY	BY	TO OBTAIN
1/PSI	1.4504E-4	1/PA
1/DEG.F	1.800	1/DEG.C
BTU/LBM-DEG.F	4185.0	J/KG-DEG.C
BTU/CU.FT-DEG.F	67037.	J/CU.M.-DEG.C
BTU/FT-DAY-DEG.F	.07208	J/M-SEC-DEG.C
FEET	.3048	M
SQ.FT/DAY	1.0753E-6	SQ.M/SEC
LBM/CU.FT	16.018	KG/CU.M.
PSI	6894.6	PA
DEG.F	.5556-17.78	DEG.C
CP	.001	PA-SEC
BTU/LBM	2325.0	J/KG
FT/DAY	3.5278E-6	M/SEC
LBM	.45359	KG
CU.FT.	.028317	CU.M.
BTU	1054.6	J
CU.FT/DAY	3.2774E-7	CU.M/SEC
DAY	86,400	SEC
LB/DAY	5.2498E-6	KG/SEC

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