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USER'S MANUAL FOR THE SANDIA WASTE-ISOLATION FLOW AND TRANSPORT MODEL (SWIFT/SSP) RELEASE 3.81

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ABSTRACT

This report describes a three-dimensional finite-difference model (SWIFT/SSP). The model is a specialization of a more general model (SWIFT) and is used to simulate steady-state flow and transient radionuclide transport 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/SSP simulator. Mathematical equations, submodels, application notes, and a description of the program itself are given herein.

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CHAPTER 1

INTRODUCTION

1.1 Brief Description of the SWIFT Models

There are two computer codes SWIFT (Sandia Waste Isolation, Flow and Transport Models). One of the codes, SWIFT, 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[1] miscible displacement
(4) trace-species[2] 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. The SWIFT model is described by Reeves and Cranwell [1981].

The second computer model, SWIFT/SSP (the Steady-State Pressure Model), which is the subject of this document, is a specialization of the above. The processes considered in this case are:

(1) steady-state fluid flow
(2) transient trace-species migration

Like its counterpart, this model is three-dimensional and permits a transient solution of the radionuclide equation. However, in order to achieve computer efficiency for what has been found to be a relatively large class of applications, the SWIFT-SSP version is limited to steady-state fluid flow with no heat or brine transport.

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

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1 Hereafter referred to as "brine".
2 Hereafter referred to as "radionuclides".

- 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

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 single-phase fluid flow, heat transport both through the rock and the fluid media, and fluid compositional changes for a dominant miscible component. This 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] and is available from the U.S. National Technical Information Service.

1.4 Purpose of This Document

The purpose of this document is to describe the SWIFT/SSP 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 instructions on application are reserved for a companion document by Chu, Finley and Reeves [1981]. There, seven 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/SSP computer model. The discussion begins with the basic transport equations.

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CHAPTER 2

MATHEMATICAL MODEL

2.1 Transient Fluid Flow and Radionuclide Transport

The flow and 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 [1972]; and Aziz and Settari [1979]). The resulting relations may be stated as follows for the totally transient case†:

Fluid:

$$\underset{\text{conduction}}{\nabla\cdot(\rho\underline{u})} - \underset{\text{production}}{q} + \underset{\substack{\text{salt}\\\text{dissolution}}}{R'_s} = \underset{\text{accumulation}}{\frac{\partial}{\partial t}(\phi\rho)} \qquad (2\text{-}1)$$

Radionuclide (component i):

$$\underset{\text{convection}}{-\nabla\cdot(\rho C_i\underline{u})} + \underset{\substack{\text{dispersion/}\\\text{diffusion}}}{\nabla\cdot(\rho\underline{\underline{E}}_c\cdot\nabla C_i)} - \underset{\substack{\text{injected}\\\text{component}}}{qC_i} - \underset{\substack{\text{produced}\\\text{component}}}{q_{ci}}$$

$$+ \underset{\substack{\text{waste}\\\text{leach}}}{q_{oi}} + \underset{\substack{\text{generation of}\\\text{component i by}\\\text{decay of j}}}{\sum_{j=1}^{N} k_{ij}\lambda_j K_j \phi\rho C_j} - \underset{\substack{\text{decay of}\\\text{component i}}}{\lambda_i K_i \phi\rho C_i} \qquad (2\text{-}2)$$

$$= \underset{\text{accumulation}}{\frac{\partial}{\partial t}(\phi\rho K_i C_i)}$$

Several quantities in Eqs. (2-1) and (2-2) require further definition in terms of basic parameters. The tensor in Eq. (2-2), is defined as a sum of dispersion and molecular-diffusion terms:

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† All terms are defined in the notation section.

$$\underline{\underline{E}}_c + \underline{\underline{D}} + D_m\underline{\underline{I}} \qquad (2\text{-}3)$$

where

$$D_{ij} = \alpha_T u \delta_{ij} + (\alpha_L - \alpha_T)u_i u_j/u \qquad (2\text{-}4)$$

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

$$K_i = 1 + \rho_R k_{di}(1-\phi)/\phi \qquad (2\text{-}5)$$

Equations (2-1) and (2-2) are coupled by three auxiliary relations for Darcy flux:

$$\underline{u} = -(\underline{\underline{k}}/\mu)\cdot(\nabla p - \rho \frac{g}{g_c} \nabla z) \qquad (2\text{-}6)$$

porosity:

$$\phi = \phi_o[1+c_R(p-p_o)] \qquad (2\text{-}7)$$

fluid density:

$$\rho = \rho_o [1+c_w(p-p_o) + c_s \hat{C}] \qquad (2\text{-}8)$$

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

$$c_s = (\rho_I - \rho_N)/\rho_o \qquad (2\text{-}9)$$

2.2 Steady-State Specialization of the Flow Equation

In the simulation of radionuclide transport, quite often the frame of interest may extend over many thousands of years. Typically the assumption of time-invariant flow conditions is justified in such cases due to the lack of specific precipitation data for such a long

period of time. Furthermore, the overall effect of transient rainfall boundary conditions may have a minor effect on radionuclide transport. For example, Duguid and Reeves [1976] have shown this for a combined saturated-unsaturated simulation of tritium transport over a period of only one month.

In addition, it is appropriate, for some applications, to assume time-invariant distributions of temperature and brine concentrations. For example, a geothermal gradient and a relatively simple stratigraphy will permit a hand calculation of such distributions. In such cases, the steady-state flow equation may be solved in combination with the transient radionuclide equations.

To take advantage of the inherent savings in core storage for such problems, the simulator described herein, i.e., the SWIFT/SSP code, has been developed. The result is an increase in the maximum permissible number of grid blocks by about 25 percent and a very substantial decrease in the computer time required to simulate the flow (as compared to a transient simulation of flow).

The flow equation used in the SWIFT/SSP model is a specialization of Eq. (2-1). It is:

Fluid (steady state)

$$\underset{\text{conduction}}{\nabla\cdot(\rho\underline{u})} - \underset{\text{production}}{q} = 0 \qquad (2\text{-}10)$$

In addition to the usual setting of the accumulation term to zero, the salt dissolution R_S' of Eq. (2-1) has also been dropped since brine transport is not considered in the SWIFT/SSP model.

However, the possible presence of brine is included through the variable-density formulation of Eqs. (2-8) and (2-9). As shown there, the presence of a steady-state brine distribution may be accounted for through a spatially variable fluid density, ρ, which is dependent on brine concentration. Internally, the value of viscosity is set to

$$\mu = 1 \text{ cp} = 10^{-3} \text{ Pa-sec} \qquad (2\text{-}11)$$

However, spatial variations in viscosity due to a steady-state brine distribution may easily be included by simply adjusting the input values of the permeability tensor $\underline{\underline{k}}$.

2.3 Solution Techniques

The equations for steady-state fluid flow, Eq. (2-10), and transient radionuclide transport, Eq. (2-2) are solved by the SWIFT/SSP simulator. Together, they form a set of coupled parabolic equations. These equations are relatively weakly coupled due to the assumption of trace concentrations of radionuclides. Thus, Darcy velocity, porosity, fluid density and viscosity are determined independently of radionuclide concentrations. Thus, 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] with but two exceptions. First, the finite-difference equations for the steady-state solution in SWIFT/SSP are written in terms of p rather than δp. Such a change permits calculation of steady-state pressure without any intermediate steps. Secondly, the formal gaussian elimination between the discretized equations for flow, heat, and brine transport is unnecessary here since the latter two processes are not considered.

One of the attractive features of the solution procedure 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 [1974] 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. This feature and most of the others discussed in this section are present in both the SWIFT and the SWIFT/SSP versions.

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CHAPTER 3

SUBMODELS

The SWIFT models contain several submodels which have been implemented in order to broaden their ranges of applicability. With the density model, pressure- and brine-dependent effects upon density may be included. Through use of the well model, both pressure- and rate-dependent sources of fluid may be treated. Finally, with the waste-leach model, the release of radionuclides from a depository may be simulated for both leach- and solubility-limited cases.

3.1 Fluid Density

One of the unique features of the SWIFT/SSP model is that it permits variable densities. The submodel for density is given in Eq. (2-8) and assumes an isothermal system. It is[+]:

$$\rho = \rho_o[1 + c_w(p-p_o) + c_s\hat{C}] \qquad (3\text{-}1)$$

This relation has been investigated recently by Muller, Finley and Pearson [1981]. They conclude that the use of constant values for c_w and c_s is quite adequate for most simulations. They argue that since the variation of c_w is only 0.5 percent for a pressure change of 100 bars, the use of a constant value of c_w is appropriate for most hydrological simulations. As for the brine coefficient c_s, they note that the experimentally observed variation of density with concentration is slightly nonlinear 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 many simulations. The reference INTERCOMP [1976] examines parameters c_w and c_s as coupled functions of both brine concentration and temperature and makes similar observations.

3.2 Wells

The term "well", as used here, denotes either a source or a sink for a system. Mathematically it is denoted by q in Eq. (2-1). Physically, a well may be used to characterize a variety of mechanisms. Originally, when the SWIFT code was strictly a waste-injection model (see INTERCOMP [1976], Part I, App. B), this facility was used to

[+] All terms are defined in the notation section.

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. Wells may be used strictly for observation, or they may be used strictly for injection of radioactive components. In some applications they are used 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 is derived 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 source or sink pressure 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 a constant rate (injection or production), or a constant pressure. 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.

Well Index. The region surrounding a well is called the skin (see Figure 3-1). 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

$$q = (WI/\mu)\ \Delta p \qquad (3\text{-}2)$$

where q = [ft^3/day] or [m^3/sec] is the flow rate and Δp = [psi] or [Pa] is the pressure drop across the skin region. For specific

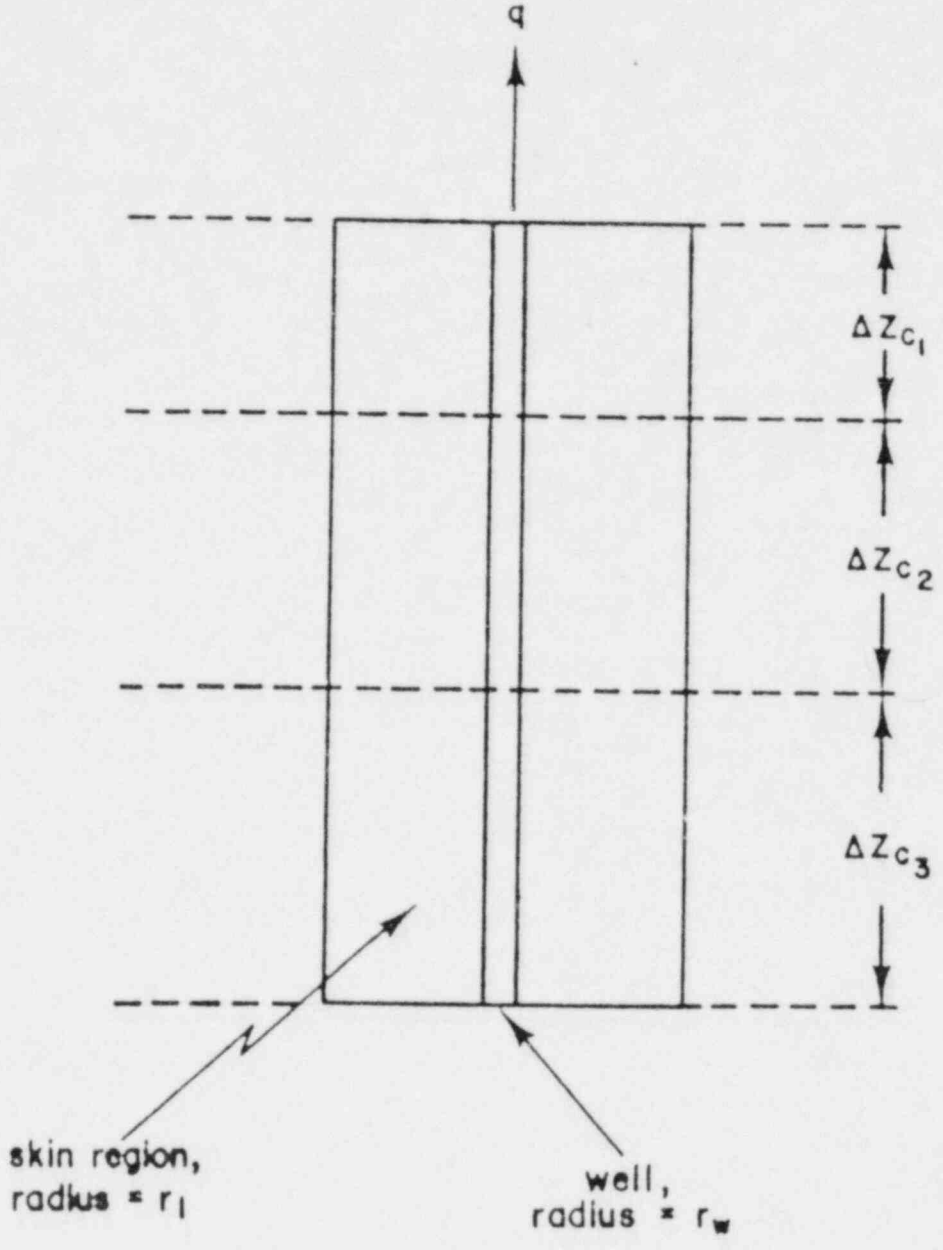

Figure 3-1. Characterization of the Skin Region Surrounding a Well.

values of fluid properties μ_o and ρ_o, well index may be defined in terms of head drop rather than pressure drop:

$$q = WI_o \Delta H \tag{3-3}$$

where WI_o = [ft^2/day] or [m^2/sec] is defined

$$WI_o = \rho_o (g/g_c) WI/\mu_o \tag{3-4}$$

The SWIFT code requires WI_o as input, where μ_o and ρ_o 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) in a cylindrical geometry, which yields

$$WI_o = 2\pi K_s \sum_k \Delta z_k / \ln(r_1/r_w) \tag{3-5}$$

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

$$\bar{r} = (\Delta x \Delta y/\pi)^{1/2} \tag{3-6}$$

Here the radius r_1 is taken to be the point corresponding to the average pressure of the draw-down curve within the equivalent block radius $\bar{r}$. Such a definition is therefore consistent with the assumption that the average draw-down pressure within the grid block is equal to the grid-block pressure. Mathematically, this relation is given by

$$\ln(r_1/r_w) = r_w \left\{ 1 + (\bar{r}/r_w) \left[\ln(\bar{r}/r_w) - 1 \right] \right\} / (\bar{r} - r_w) \tag{3-7}$$

In this case the pressure drop Δp of Eq. (3-2) is the difference in pressures between the well and the average grid-block pressure present at the periphery of the skin. An alternate approach to Eq. (3-7) 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, the well index may be related to the transmissibility, as depicted in Figure 3-2 for a block bounded on one side by a river. The well index in that case would be

$$WI_o = K_o \Delta y \Delta z / (\Delta x/2) \qquad (3\text{-}8)$$

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

Mobility. For 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

$$M_k = (k_\ell / \mu) WI \qquad (3\text{-}9)$$

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 IINDWI is specified in the input. The first option (IINDWI = 1) is that of rate allocation on the basis of mobilities alone, i.e.

$$q_k = M_k \, q / \sum_\ell M_\ell \qquad (3\text{-}10)$$

A second option (|IINDWI| = 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

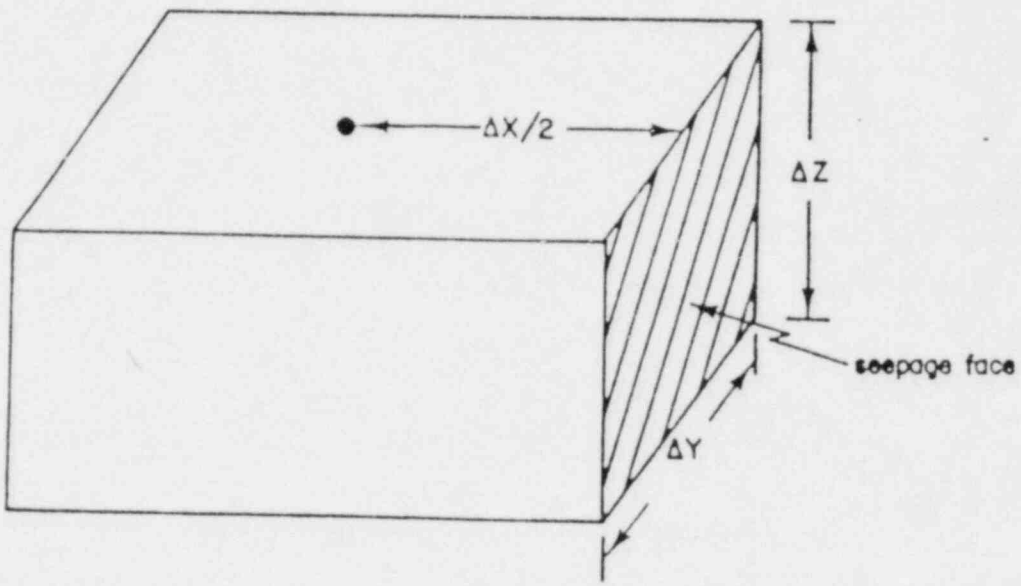

Figure 3-2. Use of a Well to Simulate Seepage to a River.

$$q_k = -\left\{\left[p_{bh} + (\rho g/g_c)(h_k - h_{c_1})\right] - p_k\right\} M_k \qquad (3\text{-}11)$$

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

$$q = \sum_k q_k \qquad (3\text{-}12)$$

Subscript c_1 denotes the first layer in which the well is completed (see Figure 3-1). The bottom-hole pressure is defined to be the well pressure at h_{c_1}, the depth of the top of this layer.

The SWIFT code applies Eq. (3-11), for a rate limitation 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. (3-11) is lagged by one time step relative to the most current calculation. For a steady-state simulation, the explicit option should be used with caution since the right-hand side of Eq. (3-11) is then evaluated with initial pressures, which may not be physically meaningful. In the latter semi-implicit case, each q_k is expanded by the relation

$$q_k = q_k^{\,it} + (dq/dp)_k \, p_k \qquad (3\text{-}13)$$

Here the derivative is taken to be

$$(dq/dp)_k = M_k \qquad (3\text{-}14)$$

and term $q_k^{\,it}$ is evaluated iteratively:

$$q_k^{\,1} = -\left[p_{bh}^{\,n} + (\rho g/g_c)(h_k - h_{c_1})\right] M_k \qquad (3\text{-}15)$$

and

$$q_k^{\,it} = q_k^{\,it-1} \, q / \sum_\ell q_\ell^{\,it-1} \qquad it>1 \qquad (3\text{-}16)$$

In Eq. (3-15) $p_{bh}^{\,n}$ is the bottom-hole pressure resulting from grid-block pressures at time level n, i.e., from initial grid-block pressures.

Another useful option based on Eq. (3-11) is that of pressure limitation. Here a bottom-hole pressure p_{bh} is specified. In addition to its usefulness in simulating wells, the facility is also useful in simulating recharge, where the "bottom-hole" pressure, i.e. the surface pressure, cannot exceed atmospheric pressure. It may also be used for simulating discharge to a river, where pressure is also controlling. In an explicit (IINDW1 = 3) implementation, the specified bottom-hole pressure p_{bh} and the time-lagged pressures p_k are used to evaluate the right-hand side of Eq. (3-11). Here, just as in the rate-limited case, this procedure should be viewed with caution since, for a steady-state calculation, time-lagged pressures are obtained from the initial conditions. Equation (3-12) is then used to determine the total flow, which is variable. In an implicit (IINDW1 = -3) implementation, Eqs. (3-13) - (3-15) are used, just as in the rate-limitation case. In this case, however, because of the specification of a bottom-hole pressure, q_k^{it} in Eq. (3-13) is determined exactly, by Eq. (3-15), after only one iteration.

In summary, then, all sources of fluid and sinks of fluid are called wells regardless of whether they refer to physical wells or to artifices for imposing known flow or pressure conditions. Furthermore, all such wells are characterized by position, completion layer, well indices WI_o, layer allocation factors k_ℓ, 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 rate control ($|$ IINDW1$|$ = 2) or pressure control ($|$IINDW1$|$ =3) will be applied, and also whether the source-sink term will be applied explicitly (IINDW1 > 1) or implicitly (IINDW1 < -1).

3.3 Waste Leach

Another submodel which is present in the SWIFT model is that for waste leach. The purpose of this model is to determine the source rate q_{oi} (see Eq. (2-2)) 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 implemention. Phases (2) and (3) above are coupled by the solubilities. Very simply, the source rate q_{oi} for dissolving Phase (2) is kept sufficiently small so 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 considered, specifically, the unleached radionuclides within the waste matrix m_i, the undissolved nuclides no longer in the waste matrix S_i, and the dissolved nuclides C_i. The appropriate conservation equations may be written in the following manner: For the dissolved phase of component i:

$$-\nabla \cdot(\rho C_i \underline{u}) + q_{oi} + \sum_j k_{ij}\lambda_j K_j \phi \rho C_j - \lambda_i K_i \phi \rho C_i \qquad (3\text{-}17)$$

$$= \frac{\partial}{\partial t}(\phi \rho K_i C_i)$$

for the undissolved, but leached, component i:

$$-R_i + q_{oi} + \sum_j k_{ij}\lambda_j S_j - \lambda_i S_i = \frac{dS_i}{dt} \qquad (3\text{-}18)$$

and for the unleached component i:

$$\sum_j k_{ij}\lambda_i m_j - \lambda_i m_i = \frac{dm_i}{dt} \qquad (3\text{-}19)$$

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

$$R_i = \begin{cases} -m_i(t)\rho_w/a, & b \leq t \leq b+a \\ 0 \quad , \text{ otherwise} \end{cases} \qquad (3\text{-}20)$$

It is understood that $j \neq i$ in each summation in the radioactive decay and production terms of Eqs. (3-17) - (3-19). Equations (3-17) and (3-18) are always solved numerically by the SWIFT/SSP code. Furthermore, they are solved in such a manner that the fluid concentrations never exceed the solubility limits.

Two comments are appropriate for the waste-leach equations, Eqs. (3-17) - (3-20). First of all, for the unleached component, Eq. (3-19) 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 which case power-law interpolation from tabular input data is used by SWIFT. Secondly, it may be noted that Eq. (3-17) is a simplified version of Eq. (2-2), the general transport equation for a radionuclide. Dropping the source term qC_i is immaterial, if there are no withdrawal wells in the depository. Neglecting dispersion, i.e. the E term, however, deserves some explanation. Equations (3-17) - (3-20) are solved only for depository blocks and not for the entire system. The purpose is only to determine q_{oi}, and in order to make the algorithm as efficient as possible, physical dispersion is neglected. Furthermore, in order to calculate q_{oi} most easily, an explicit algorithm is used for the convective-transport term in Eq. (3-17). 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. (3-17) 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.

CHAPTER 4

APPLICATION NOTES

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

4.1 Numerical Criteria for Dispersion and Overshoot

One source of difficulty in the numerical solution of a transport equation, such as the radionuclide equation, Eq. (2-2), 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 disadvantages 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 transport equation, which contains a convective term, is 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.

Table 4-1 below contains information on numerical dispersion and overshoot. It is based on a simple analogue of Eq. (2-2), namely

$$D \frac{\partial^2 C}{\partial x^2} - v \frac{\partial C}{\partial x} = \frac{\partial C}{\partial t} \qquad (4\text{-}1)$$

where

$$v = u/\phi \qquad (4\text{-}2)$$

is the interstitial velocity and where

$$D = E_c/\phi = \alpha v \qquad (4\text{-}3)$$

is now the dispersion. In spite of the simplicity of Eq. (4-1), space- and time-step criteria derived from it, i.e., from Table 4-1, have proven to be quite useful in practice. They are reprinted here from INTERCOMP [1976] for easy reference.

4.2 Adjustment of the Rate Constant

Program SWIFT will adjust the rate constant if input parameter LADJ, READ RO-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. (2-2) becomes, for the parent nuclide,

$$\frac{dC}{dt} = -\lambda C \qquad (4\text{-}4)$$

(The component subscript has been dropped for convenience.)

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

$$C^{n+1} = C^n e^{-\lambda \Delta t} \qquad (4\text{-}5)$$

TABLE 4-1. Numerical Criteria for Radionuclide Transport

Scheme[+]	Numerical Dispersion	Dispersion Criterion	Overshoot Criteria
CIT-CIS	None	None	$\frac{v\Delta t}{2\Delta x} + \frac{\alpha v \Delta t}{\Delta x^2} \leq 1$, $\frac{\Delta x}{2\alpha} \leq 1$
CIT-BIS	$\frac{v\Delta x}{2}$	$\frac{\Delta x}{2\alpha} << 1$	$\frac{v\Delta t}{2\Delta x} \leq 1$
BIT-CIS	$\frac{v^2\Delta t}{2}$	$\frac{v\Delta t}{2\alpha} << 1$	$\frac{\Delta x}{2\alpha} \leq 1$
BIT-BIS	$\frac{v\Delta x}{2} + \frac{v^2\Delta t}{2}$	$\frac{\Delta x + v\Delta t}{2\alpha} << 1$	None

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

which yields

$$\delta C = -C^n(1-e^{-\lambda\Delta t}) \tag{4-6}$$

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

$$\delta C = -\lambda'(w)\ (C^n + w\delta C)\Delta t \tag{4-7}$$

where

$$w = \begin{cases} 1/2 & \text{CIT} \\ 1 & \text{BIT} \end{cases} \tag{4-8}$$

To see that quantity $\lambda'(w)$, the adjusted rate constant, is indeed a function of the time-weighting constant w, we solve Eq. (4-7) for δC and substitute into Eq. (4-6). The result is

$$\lambda_i'(w) = \frac{e^{\lambda_i\Delta t} - 1}{\Delta t\ [(1-w)e^{\lambda_i\Delta t} + w]} \tag{4-9}$$

where the component subscript has been reintroduced. For the BIT algorithm w = 1, Eq. (4-9) 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. (4-9) is appropriate for decay-dominant transport of a daughter nuclide providing that

$$\tau_{i-1}/\tau_i > 100 \tag{4-10}$$

Without adjustment the time step must be controlled by the criterion

$$\Delta t < \begin{cases} \tau_i/7 & \text{BIT} \\ \tau_i & \text{CIT} \end{cases} \tag{4-11}$$

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 and READ R1-23. Automatic generation is based on a special steady-state solution of the flow equation which gives, for the pressure difference between two points,

$$p_2 - p_1 \sim \ln(r_2/r_1) \tag{4-12}$$

This same relation is the basis for the well index given in Eq. (3-5) 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 interpreted as the outer radius of the disturbed skin zone, (3) the wellbore radius $\hat{r}_1$ = RWW, and (4) the grid-block boundary $\hat{r}_{n+1}$ = 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. (4-12). Using the notation of Figure 4-1, this means that

$$\frac{r_{i+1}}{r_i} = A \tag{4-13}$$

and

$$\frac{\hat{r}_i}{r_i} = A^{1/2} \tag{4-14}$$

A combination of Eqs. (4-13) and (4-14) gives

$$\frac{\hat{r}_{n+1}}{r_1} = A^{n-1/2} \tag{4-15}$$

Equation (4-15) is solved by SWIFT for the common ratio A, and then Eqs. (4-13) and (4-14) are used as recursion relations to define all r_i and $\hat{r}_i$.

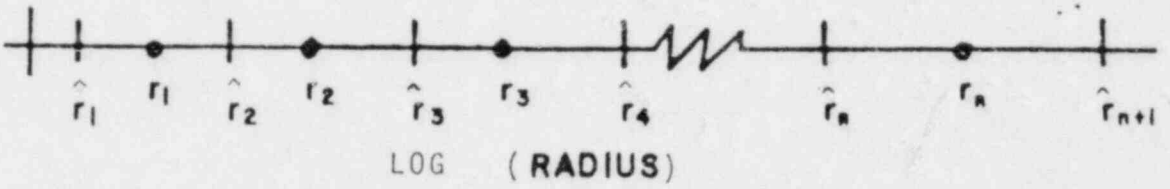

Figure 4-1. Schematic of Radial Mesh Including Grid-Block Centers, r_j, and Grid-Block Boundaries, $\hat{r}_j$.

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. (4-15) be extended by taking

$$\frac{r_1}{\hat{r}_1} = A^{1/2} \tag{4-16}$$

and

$$\frac{\hat{r}_{n+1}}{\hat{r}_1} = A^n \tag{4-17}$$

Equation (4-17) may be solved for A. This parameter may then be used in Eq. (4-16) to calculate the skin radius r_1 from the wellbore radius $\hat{r}_1$. In such a case in which the skin thickness is chosen somewhat arbitrarily, the properties of the skin are reflected solely by the well index.

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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, two integration subroutines, and about 50 supporting subroutines. In this chapter four 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 two integration subroutines ITERS and ITERC. Generally speaking, subroutines READ1 through PRINTP perform the functions of input, initialization, parameter definition, and output in support of ITERS to integrate the steady-state flow equation. In a similar manner, subroutines READ0 and VELS through PLOTC perform the same functions in support of ITERC to integrate the transient state equation for radionuclide transport.

The second and third items presented show the structure of the two integration subroutines ITERS and ITERC in Figure 5-2. As given, these routines have similar structures. Both invoke a subroutine, either SRHP or SRHC, to set up matrix coefficients arising from the finite differencing. Also both ITERS and ITERC use one of three different routines, depending upon user specification, to solve the resulting matrix equations. The only difference in general structure arises in the material balance. ITERC invokes a material-balance subroutine MBAL directly; whereas ITERS does not compute material-balance quantities at all. For fluid flow such quantities are computed in PRINT2 just prior to their being printed.

The final item presented in this chapter is Table 5-1. There the functions of the major subroutines are given very briefly. This brief introduction to the SWIFT/SSP code is presented in order to permit both intelligent usage and perhaps some user modification of the peripheral functions of the code. For more detailed information on the numerical algorithms the reader is referred to INTERCOMP [1976], Part I, Appendix A.

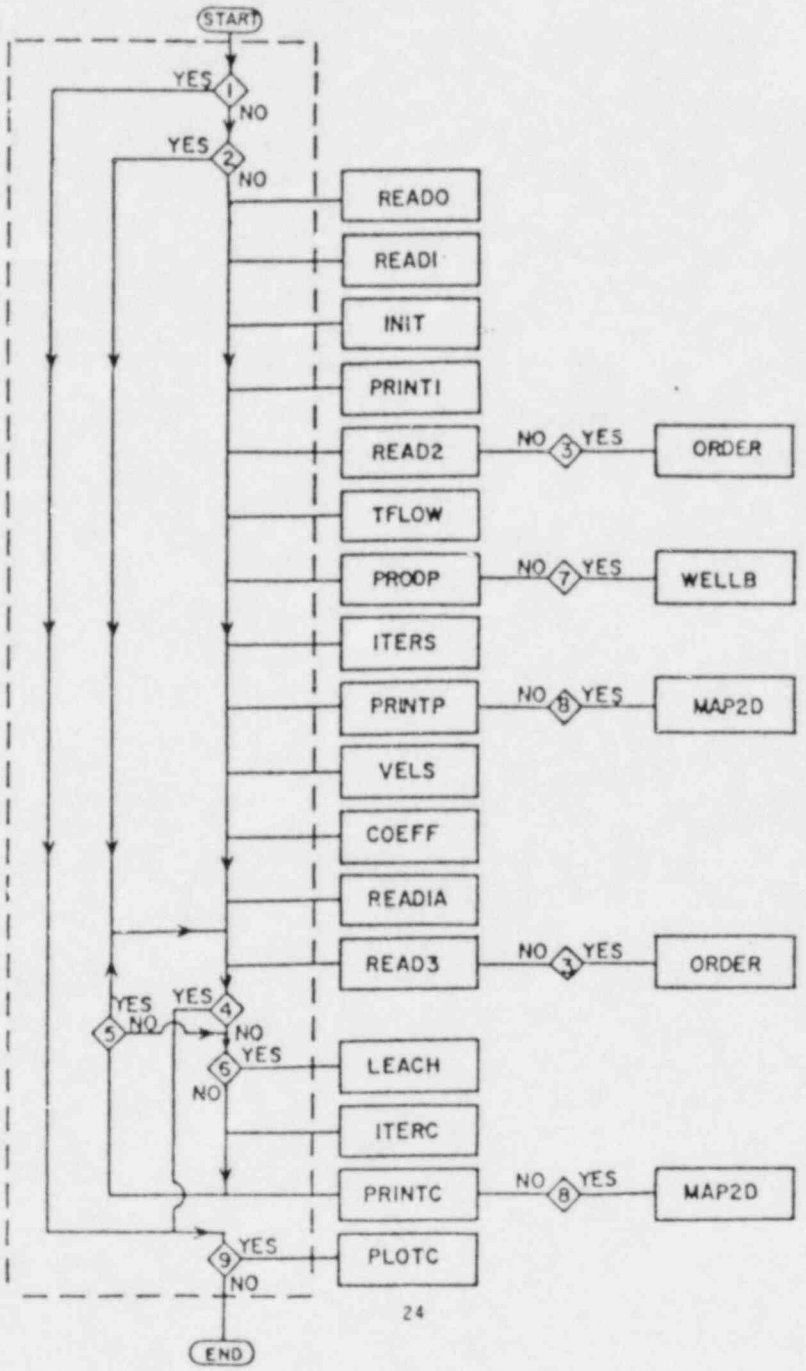
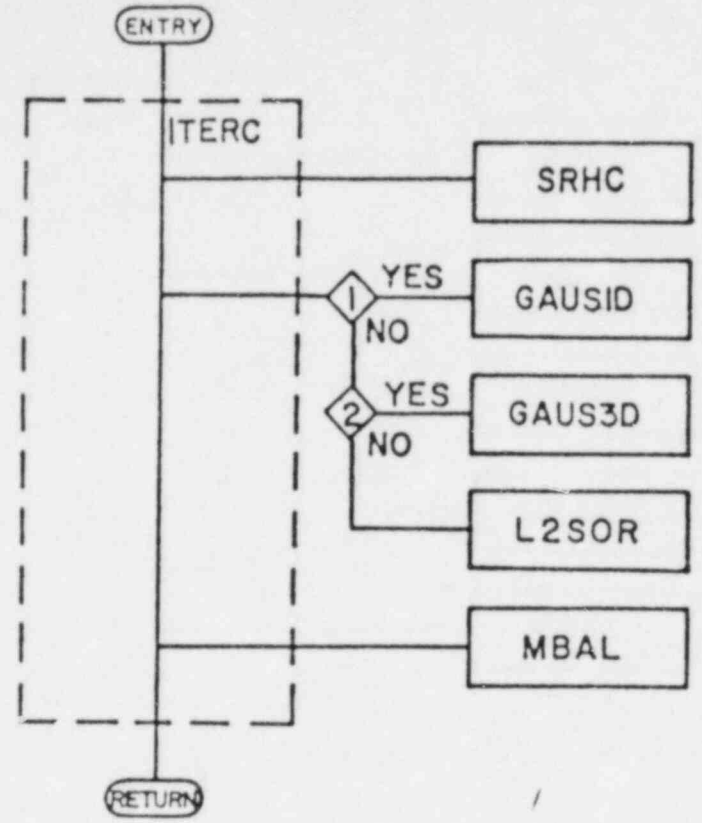
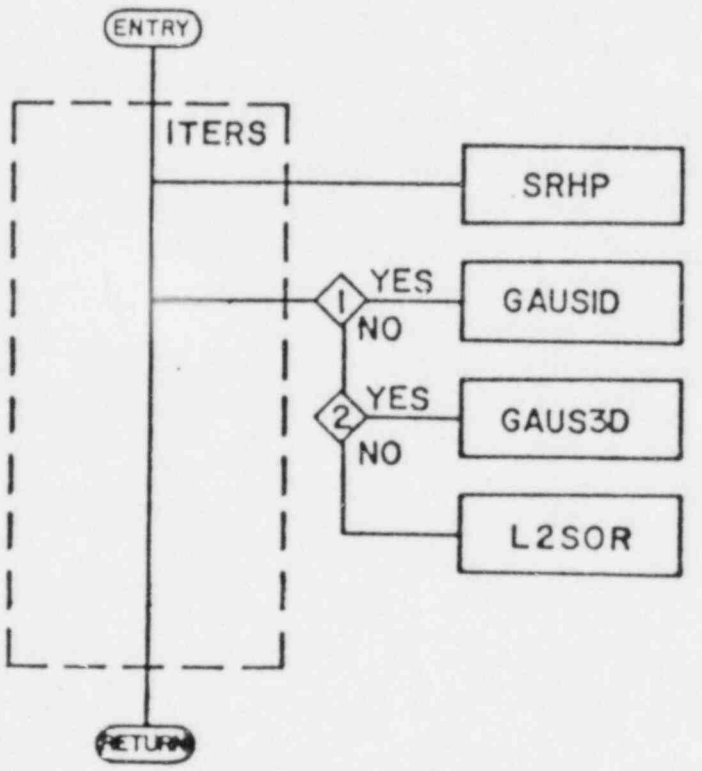


Figure 5-1. Overall Structure of Steady-State Version of SWIFT.



(a)



(b)

Figure 5-2. Breakdown of (a) Radionuclide Transport and (b) Steady-State Pressure Solution Algorithms.

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 here?

(5) Are the recurrent data read at this time step?

(6) Is the waste-leach submodel employed?

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

(8) Are any two-dimensional contours maps desired?

(9) Are any plots desired for this run?

Conditions for Figure 5-2 are as follows:

(1) Is the problem one-dimensional?

(2) Is a direct solution desired?

Table 5-1. Subroutine Functions

Subroutine	Function
COEFF	Determination of dispersion and transmissibilities for radionuclide transport
GAUS1D	Gaussian elimination for a 1-D system
GAUS3D	Gaussian elimination for 2-D and 3-D systems
INIT	Initialization of pressures and concentrations
ITERC	Solution of transient-state radionuclide chains by setting matrix coefficients and invoking matrix solution
ITERS	Solution of steady-state flow equation 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
PRINTC	Output of radionuclide-transport results: material balances and profiles of concentrations
PRINTP	Output of fluid-flow results: well summary, material-balance summary, and profiles of pressure, transmissiblity, and Darcy velocity
PRINTI	Printing of initialized values of pressures, pore volumes, rock types, and transmissibilities

Table 5-1. Subroutine Functions, Continued

Subroutine	Function
READ0	Radionuclide-chain input including distribution coefficients
READ1	Input of geometrical, hydrological and dispersion data. Calculation of constant portion of transmissibilites
READ1A	Reading of rock-type modifications and repository information including solubilities
READ2	Additional input for fluid-flow calculation including solution control, wells, and output control
READ3	Input of time-dependent data for the radionuclide execution including solution control, sources, and output control
SRHC	Determination of load-vector terms for the concentration equation
SRHP	Determination of load-vector terms for the pressure equation
TFLOW	Calculation of fluid transmissibilities for each block interface
VELS	Determination of Darcy velocities
WELLB	Implements the well-bore model to obtain subsurface conditions from surface conditions

5.2 Sample Problems

As mentioned in the introduction, seven sample problems have been developed and published in a companion document by Chu, Finley and Reeves [1981]. The discussion there includes the physical setting along with a description of input and output. The English Engineering system of units is used. In order to complement that work and, at the same time, make this document complete, a listing of input and output for those same seven 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/SSP source code.

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CHAPTER 6

INPUT DATA GUIDE

6.1 Fixed Data

Read M-1 (20A4/20A4)

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)

LIST: RSTRT, ISURF, IUNIT

RSTRT	-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 file denoted as 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.
IUNIT	Unit specification control.	
	0 -	English Engineering System.
	1 -	SI System.

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

READ M-3 (15I5)

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

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 description data.

- 1 - Homogeneous aquifer, cartesian geometry.
- 2 - Heterogeneous aquifer, aquifer data entered on regional basis, cartesian geometry.
- 3 - Radial geometry. The aquifer may be heterogeneous only in the vertical direction.

NCP — Number of radioactive/trace components in the system.

NRT — Number of rock types.

NOTE: Both distribution coefficients and dispersivities are functions of rock 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 is 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. These data are 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, $\pm$1 - Storage is allocated for direct solution.

$\pm$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 either READ R2-2 or READ R3-5 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 RO should be entered only if RSTRT $\leq$ 0 and NCP > 0. Otherwise skip READ RO-1 and RO-2.

READ RO-1 LIST 1: I3, 2A4, 4X, 3I5, E10.0;

LIST 2: 4(I5, 5X, E10.0))

NOTE: Enter NCP (number of components) sets of RO-1 data.

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

MASS — Mass number of the isotope.

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.

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 RO-2 (7E10.0)

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

DIS — Distribution coefficient in ft^3/lb (m^3/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 RSTRT < 0, (READ M-2), this is the end of your data set.

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

READ M-4 (I10)

LIST: ILAST

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

READ M-5 (F10.0)

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 RSTRT (READ M-2), a set of recurrent data will be read to resume the previous simulation.

NOTE: Proceed to READ R3-1 for a restart run, i.e., RSTRT > 0.

READ R1-1 (5E10.0)

LIST: CW, CR, ALPHL, ALPHT, DMEFF

CW	Compressibility of the aquifer fluid, $(psi)^{-1}$ ($(Pa)^{-1}$)
CR	Compressibility of pore structure, $(psi)^{-1}$ or ($(Pa)^{-1}$)
ALPHL	Longitudinal dispersivity factor, ft (m).
ALPHT	Transverse dispersivity factor, ft (m).
DMEFF	Molecular diffusivity in the porous medium, includes porosity and tortuosity effects (porosity x fluid molecular diffusivity/tortuosity), ft^2/day (m^2/sec).

READ R1-2.5 (7E10.0)

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

LIST: ALPHAL (I), ALPHAT (I) (NRT cards, one for each rock type, I)

ALPHAL	Longitudinal dispersivity, ft (m).
ALPHAT	Transverse dispersivity, ft (m).

NOTE: A blank card will assign the values of READ R1-1 to that rock type.

READ R1-3 (5E10.0)

LIST: BROCK, PBWR, BWRN, BWRI

BROCK	Actual rock density (solid particle) lb/ft^3 (kg/m^3).
PBWR	Reference pressure at which the densities are to be entered, psi (Pa).
BWRN	Minimum density of the aquifer fluid (inert compound concentration=0) at PBWR, lb/ft^3 (kg/m^3).
BWRI	Maximum density of the aquifer fluid (inert component concentration=1) at PBWR, lb/ft^3 (kg/m^3).

NOTE: If ISURF=0, omit READ R1-4 and R1-5 and proceed to R1-16.

READ R1-4 (I5)

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 (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 in the well is printed over each increment (see DELPW in READ R1-5).

READ R1-5 (3E10.0)

LIST: PBASE, DELPW

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).

READ R1-16 (4E10.0)

LIST: PINIT, HINIT, HDATUM

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

HINIT	An arbitrary depth for setting up initial conditions, ft (m). HINIT can be any depth within the aquifer. HINIT is used only to set up initial pressures in the aquifer.
HDATUM	A datum depth in ft (m) for printing the dynamic pressures ($p-\rho gh/g_c$). The depth h is measured from the datum depth HDATUM. The fluid density used for conversion is the resident fluid density at TO and PINIT. This value is not used internally except for pressure-at-datum output.

READ R1-17 (LIST DIRECTED)+

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

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

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

READ R1-18 (LIST DIRECTED)+

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

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

READ R1-19 (LIST DIRECTED)+

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

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

+List-Directed Read. Input data consist of a string of values separated by one or more blanks, a comma or slash. To repeat a value, an integer constant is followed by an asterisk and the constant to be repeated.

READ R1-20 (7E10.0)

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 READ R1-20 or by using regional modifications in READ R1-26.

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

KX — Hydraulic conductivity in the x direction, ft/day (m/sec).

KY — Hydraulic conductivity in the y direction, ft/day (m/sec).

KZ — Hydraulic conductivity in the z direction, ft/day (m/sec).

NOTE: Hydraulic conductivities are converted to permeabilities by using the initial pressure and concentration of grid block (1,1,1).

PHI — Porosity (fraction).

SINX — Sine of the reservoir dip angle along the x-axis (positive downward).

SINY — Sine of the reservoir dip angle along the y-axis (positive downward).

DEPTH — Depth to top of grid block (1,1,1), measured from the reference plane (positive downward) ft (m).

NOTE: Since the approximation sin(x) = tan(x) is used, SINX and SINY should be less than about 0.2.

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

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.

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	Hydraulic conductivity in the x direction, ft/day (m/sec).
KY	Hydraulic conductivity in the y direction, ft/day (m/sec).
KZ	Hydraulic conductivity in the z direction, ft/day (m/sec).
PHI	Porosity, fraction.
UH	Depth in ft (m) measured positive downward from reference plane to top of the grid block. 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 under READ R1-19, UTH may be entered as zero.

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

READ R1-22 (4E10.0)

NOTE: These data are read for a radial geometry with only one well. The well is located at the center of the grid block system. The grid blocks are divided on an equal $\Delta\log(r)$ basis, (i.e., r_i/r_{i-1} is constant).

LIST: RWW, R1, RE, DEPTH

RWW	Well radius, ft (m).
R1	The center of the first grid block for dividing grid blocks on an equal $\Delta\log(r)$ basis, ft (m). The difference R1-RWW is interpreted as the skin radius.
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)

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

DELZ	Layer thickness in the vertical direction, ft (m).
KYY	Hydraulic conductivity in the radial direction, ft/day (m/sec).
KZZ	Hydraulic conductivity in the vertical direction, ft/day (m/sec).
POROS	Porosity, fraction.

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

READ R1-26 (LIST 1: 6I5, LIST 2: 6E10.0)

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. Ever if no regional modifications are desired, the blank card must nevertheless be included.

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

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

I1, I2	Lower and upper limits inclusive, on the I-coordinate of the region to be modified.
J1, J2	(Similar definition for the J coordinate.)
K1, K2	(Similar definition for the 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 positive or zero, this is the factor by which the x direction transmissibilities within the defined region are to be multiplied. If negative, the absolute value of FTX will be used for the x direction transmissibilities within the region to be modified.

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

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

FPV — This has the same function of FTX, but applies to 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.

READ R1-27 (2I5)

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.

LIST: IAQ, PRTAB

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

- 0 - No aquifer influence blocks are to be used. Skip to READ I-1.
- 4 - Constant pressure boundary conditions will be used at blocks specified in READ R1-28.

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.

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 entire aquifer as part of the grid system.

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

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

LIST 2: VAB, P1

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

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

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

VAB — Boundary block type.

- 1.0 - Block is at I=1 edge.
- 2.0 - Block is at I=NX edge.
- 3.0 - J=1 edge.
- 4.0 - J=NY edge.
- 5.0 - K=1 edge.
- 6.0 - K=NZ edge.

P1 — Constant value of pressure, psi (Pa), at the block boundary specified according to VAB.

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

READ I-1 (3I5)

NOTE: These data are read for initializing concentrations and natural flow in the aquifer. If the initial concentrations are zero everywhere in the aquifer, insert a blank card and proceed to READ R2-1.

LIST: ICOMP, IRD

ICOMP	Control parameter for initializing inert component concentrations. 0 - Initial concentrations in all the grid blocks are zero. 1 - The initial concentrations are not zero everywhere. Non-zero concentrations will be entered in READ I-2.
IRD	Control parameter for initializing radioactive/trace component concentrations. 0 - Initial concentrations in all the grid blocks are zero. 1 - Non-zero concentrations for each component will be entered in READ I-4.

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

NOTE: Skip this READ if ICOMP is zero.

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

I1, I2	Lower and upper limits, inclusive on the I-coordinate of the non-zero concentration region.
J1, J2	(Similar definition for the J-coordinate.)
K1, K2	(Similar definition for the K-coordinate.)
CINIT	Initial 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 the non-zero concentrations need to be specified. Follow the last card with a blank card.

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

NOTE: If IRD=0, skip this READ.

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

I1, I2	Lower and upper limits, inclusive on the I-coordinate of the non-zero concentration region.
J1, J2	(Similar defintion for the J-coordinate.)
K1, K2	(Similar definition for the K-coordinate.)
CINIT	Initial concentration in each of the blocks within the region defined by I1, I2, etc., dimensionless.

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

6.2 Steady-State Flow Data

READ R2-1 (9I5)

LIST: INDQ, IWELL, IMETH, IPROD, IOPT, INDT

INDQ — Control parameter for reading well rates.

0 - Do not read well rates.

1 - Read well rates on one card (READ R2-5). The user must enter all well rates under this option.

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.

NOTE: If data are being entered for the first time step (new run), and IMETH = 0, the program selects direct solution with backward differencing in both time and space. The solution, under these conditions, is unconditionally stable.

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 wellbore iteration data.

0 - Do not read wellbore iterations data. If it is a new run and the wellbore calculations are to be performed, 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.

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

1 - Read new or altered iteration data.

READ R2-2 (I5, F10.0)

NOTE: These data are entered if IMETH is not equal to zero.

LIST: METHOD, WTFAC

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

±1 - Reduced-band-width-direct solution.

±2 - Two-line-successive-overrelaxation (L2SOR) solution

WTFAC — Weighting factor for finite-difference approximation.

1.0 - Backward difference.

0.5 - Central difference.

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

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

NOTE: These data are 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. 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 psi (4.8×10^7 Pa).
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.

READ R2-4 (I5)

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

LIST: NWT

NWT	Total number of wells.

READ R2-5 (7E10.0)

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

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

Q — Production rate, ft^3/day (m^3/sec). For an injection well, enter the value as a negative production rate. All the well rates must be entered even if all of them have not changed.

READ R2-6 (I5, E10.0)

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

LIST: I, QWELL

I — Well number.

QWELL — Production rate, ft^3/day (m^3/sec). Enter negative values for injection rates. You need to enter only the altered well rates.

READ R2-7 (LIST 1: (6I5), LIST 2: (4E10.0); LIST 3: (8E10.0), LIST 4: (7E10.0))

NOTE: These data are 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

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.

IINDW1 — Well specification option.

1 - Specified rate is allocated between layers on the basis of mobilities alone.

±2 - Specified rate is allocated between layers on the basis of mobilities and the pressure drop between the wellbore and the grid block.

±3 - An injection or production rate is calculated from the specified bottomhole or surface pressure and allocated as in the previous option.

2,3 - The rate is expressed explicitly in the aquifer model equations.

-2,-3 - The rate is expressed in a semi-implicit manner in the aquifer model equations, i.e.,

$$q = q_x + \frac{dq}{dp} p$$

where q_x is an explicit rate term.

LIST 2: WI, BHP, CINJ

WI — Well index, ft^2/day (m^2/sec).

BHP — Bottom-hole pressure, psi (Pa). This must be specified if IINDW1=± 3.

CINJ — Brine concentration in the injected fluid, dimensionless.

LIST 3: X, DW, ED, OD, THETA

NOTE: Skip this list if 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).

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

LIST 4: KHL(K), K=IC1, IC2

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)

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). 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.

READ R2-11 (3I5)

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

LIST: MINITN, MAXITN

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.

READ R2-13 (11I5)

LIST: MAP, IIPRT, RSTWR

MAP — Parameter for printing contour maps. Only two-dimensional maps are printed. The maps are printed for r-z coordinates in a radial system and for both x-y and x-z coordinates in a cartesian system.

0 - The variable will not be mapped.

1 - The variable will be mapped.

IIPRT — Intermediate parameters printing index.

0 - none of the following output will be activated.

1 - Darcy velocities will be printed.

2 - Flow transmissibilities will be printed in addition to the velocities.

3 - Fluid density will be printed in addition to the quantities listed above.

RSTWR — Restart record control parameter.

0 - No restart record will be written.

1 - Restart record will be written on Tape 8.

NOTE: Both READ R2-14 and READ R2-15 are read from routine MAPDAT rather than from routine READ2.

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

NOTE: Enter these data only if contour maps are desired, i.e., MAP is not equal to 0.

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 lefthand 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 (radial geometry), direction.

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

NOTE: Enter these data only if pressure contour maps are desired, i.e. if MAP equals one.

NOTE: Read as many cards as necessary for the pressure maps desired. Follow the last card with a blank card.

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

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

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

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

AMAXP, AMINP — The maximum and minimum value of the pressure, psi (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 you enter AMAXP as zero or a negative value, the program will search for a maximum and use the value as AMAXP. If you enter AMINP as a large negative number ($\leq$-99.0), the program will search for a minimum and use that value as AMINP.

READ R1A-1 (7I5) Modification of rock types.

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

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

I1A — Lower limit inclusive on the I-coordinate of region of modified rock type.

I1B	Upper limit of I indices.
J1A, J1B, K1A, K1B	Similarly defined indices used to specify the region in which the rock type is to be changed.
IRT	Rock type.

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 (I5) Waste Type

LIST: ILEVEL

ILEVEL	If ILEVEL = 1, then canister radii and separations are defined. If ILEVEL = 0, then waste-volume density is specified.

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

LIST: SDRIFT, SCNSTR, DCNSTR, HCNSTR

SDRIFT	Separation of rows of canisters, ft (m). Used only for ILEVEL = 1.
SCNSTR	Center-to-center canister separation within each row, ft (m). Used only for ILEVEL = 1.
DCNSTR	For ILEVEL = 1, DCNSTR is the diameter of each canister, ft (m). For ILEVEL = 0, DCNSTR is the volumetric waste density (volume of wastes/bulk volume).
HCNSTR	Canister height, ft (m). Used only for ILEVEL = 1.

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

LIST: CONVL, CONVC, CONVT

CONVL	For ILEVEL = 1, CONVL multiplies SDRIFT, SCNSTR, DCNSTR, and HCNSTR to convert them to ft (m). For ILEVEL = 0, CONVL multiplies only DCNSTR to convert it to volume of wastes per bulk volume.
CONVC	This parameter multiplies the waste concentrations (R1A-8) to convert them to lb/ft^3 (kg/m^3) of wastes.
CONVT	This parameter multiplies the specified interpolation times (R1A-7) to convert them to days (seconds).

NOTE: The default value for CONVL, CONVC and CONVT is one.

READ R1A-6 (6I5) Location of repository

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

I1A	Lower limit of I indices, inclusive.
I1B	Upper limit of I indices, inclusive.
J1A, J1B, K1A, K1B	Similarly defined indices used to specify the repository location.

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 for READ R1A-7 and proceed to READ R1A-8.

READ R1A-7 (7F10.0) Interpolation times.

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

CTIME	Interpolation times, day (sec).

NOTE: The values of CTIME must increase monotonically with increasing index I. No two values may be equal and, to use power-law interpolation, all values of CTIME must be greater than zero.

NOTE: The user should enter NCOMP R1A-8 cards. However, the information will be used only in those cases where CNAME matches DI, as specified in READ RO-1.

READ R1A-8 (2A4, 2X, 6F10.0/(7F10.0)) Interpolation on initial concentrations.

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

CNAME	Identification of radioactive component.
CNDUM	In-place radionuclide concentration, i.e., radionuclide mass per unit waste volume, lb/ft^3 (kg/m^3).

NOTE: 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.

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

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

CS	Solubility limits expressed as mass fractions.

6.3 Recurrent Data

The data described previously are required to describe the aquifer and fluid properties, to establish steady-state flow conditions, and to characterize the repository. The following data are used to simulate time-dependent radionuclide transport. They are all read before the first time step and at subsequent time steps when a change is desired in the radionuclide source data, the time step or the mapping specifications. Note that, except for parameter IMETH, none of the data entered up to this point can be changed.

READ R3-1 (3I5)

LIST: IRSS, IMETH, ITHRU

IRSS — Control parameter for reading radionuclide source data.

- 0 - Do not read trace components source data.
- 1 - Read new or altered rate source data defined by block number.
- 2 - Read time parameters for waste-leach submodel.

IMETH — Control parameter for reading method of solution.

- 0 - Do not read method of solution.
- 1 - Read new or altered method of solution.

NOTE: If data are being entered for the first time step (new run), and IMETH = 0, the program selects direct-solution, backward-with- time-and-space finite-difference approximations. The solution, under these conditions, is unconditionally stable.

ITHRU — Run termination control.

- 0 - Run is to continue.
- 1 - Run is to terminate at this point.

NOTE: If IRSS = 0, skip READ R3-2 and R3-3.

READ R3-2 (I5)

LIST: NSS

NSS	Number of radioactive component sources/sinks.

NOTE: Skip this READ if IRSS ≠ 1.

READ R3-3 (LIST 1: 4I5; LIST 2: 7E10.0)

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

LIST 1: I, IIS, IJS, IKS

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: (QCC(I, J) J=1, NCP)

QCC	Components discharge rates, lb/day (kg/sec). A negative rate implies a source and a positive rate implies a sink.

NOTE: Skip this READ if IRSS ≠ 2.

READ R3-4 (2E10.0)

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 R3-5 (I5, F10.0)

NOTE: These data are entered if IMETH is not equal to zero.

LIST: METHOD, WTFAC

METHOD — Method of solution. If zero, the program selects METHOD = 1. Direct solution may be used here only if direct solution was 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 backward finite-difference approximation in time.

-1 - Reduced-band-width direct solution with Crank-Nicholson approximation in time.

-2 - Two-line-successive-overrelaxation solution with Crank-Nicholson approximation in time.

WTFAC — Weight factor for finite-difference approximation in space.

1.0 - Backward difference.

0.5 - Central difference.

If WTFAC $\leq$ 0, the program selects WTFAC = 1.0.

READ R3-6 (2E10.0)

LIST: TCHG, DT

TCHG — Time in days (secs) at which next set of recurrent data will be read. 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).

READ R3-7 (2I5)

LIST: IO1, IO5, MAP, MDAT, RSTWR

IO1 — Control parameter for frequency of the time step summary output. The time step summary gives mass-conservation information, including amount in place, total sources and sinks, quantities of generated and decayed species, and the material balances.

IO5 — Control parameter for listings of the grid block values of trace component concentrations.

The following values apply to 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.

MAP — Parameter for printing contour maps for the parent radionuclide at time TCHG. Only two-dimensional maps are printed.

0 - The variable will not be mapped.

1 - The variable will be mapped at TCHG.

MDAT — Control parameter for entering the mapping specifications.

0 - The mapping specifications are not to be changed.

1 - Read new mapping specifications. If you are activating the printing of contour maps for the first time during the current run, MDAT must be entered as one.

RSTWR — Restart-record control parameter.

0 - No restart record will be written.

1 - Restart record will be written on Tape 8 at time TCHG.

NOTE: Both READ R3-8 and READ R3-9 are read from routine MAPDAT rather than from routine READ3.

READ R3-8 (I5, 2F10.0)

NOTE: Enter these data only if you desire parent radionuclide concentration contour maps (MAP is not equal to 0), 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 R3-9 (6I5, 2F10.0)

NOTE: Enter these data only if MDAT equals one.
LIST: IP1, IP2, JP1, JP2, KP1, KP2, AMAXP, AMINP

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

JP1, JP2 — Lower and upper limits, inclusive, on the J-coordinate of the region to be mapped.

KP1, KP2 — Lower and upper limits, inclusive, on the K-coordinates of the region to be mapped. For a linear system you will get (KP2-KP1+1) areal maps.

AMAXP, AMINP The maximum and minimum value of the parent radionuclide concentration used to obtain 20 contour intervals. If the concentration in any grid block is higher than AMAXP, it will be indicated as AMAXP, and similarly a concentration 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 ($\leq$-99.0), the program will search for a minimum and use the value as AMINP.

NOTE: The data entered up to this point are sufficient to execute the program until time equals TCHG. The recurrent data are read again at that point. If you desire to terminate a run, enter ITHRU=1 (READ R3-1) after R3-9.

6.4 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 TMCHG.

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. Enter IMPT = 1 for pressure maps.

READ M-7 (I5)

LIST: MAP

MAP — Same as R2-13 or R3-7.

READ R2-15 or R3-8 Map Specifications

NOTE: Insert as many sets of mapping data (M-6, M-7, R2-15 (or R3-8)) as you desire. Follow the last set with a blank card.

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CHAPTER 7

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 dimensioned array exceeds the dimensions, you must redimension the array. 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 two 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.

(2) This error refers to READ M-3.
The L2SOR option has been selected for a two-dimensional x-y system, which is not permitted in the current implementation.

(3) This error refers to READ R1-1.
One or more of CW and CR is negative. Physically, compressibilities are always equal to or greater than zero.

(4) This error refers to READ R1-2.
One or more of ALPHL, ALPHT and DMEFF is negative.

(5) This error refers to READ R1-3.
The fluid density (BWRN) is 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 is outside the permissible range of -1 to +2.

(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.
I1 is greater than I2 or
J1 is greater than J2 or
K1 is greater than K2
KX or KY or KZ is negative or
PHI is 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.

(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 R1-28.
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.
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.

(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 location 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, $\pm$2 and $\pm$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 $\pm$3 and BHP is 0. The specified value of the bottom-hole pressure is a limiting value of the well pressure if IINDW1 is $\pm$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 and to R3-5.
The L2SOR option has been selected for a two-dimensional x-y system, which is not permitted in the current implementation.

(41) This error refers to READ R2-11
Minimum number of outer iterations (MINITN) is less than 1 or
MINITN is greater than maximum number of outer iterations (MAXITN).

Error numbers 43 and 44 refer to READ R3-6.

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

(44) DT is zero.

(46) This error refers either to READ R2-13 or R3-7.
The value entered for MAP is not permissible. It must be either 0 or 1.

(47) This error refers either to READ R2-15 or R3-9.
IP2 is greater than NX or
KP2 is greater than NZ or
HTG is not equal to 3 and JP2 is greater than NY.

(50) This error refers to READ R3-2 and R3-3.
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 RO.

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

(53) This error refers to READ RO-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 RO-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.

(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 rnages 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 or two values of CTIME are equal.

(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.

(65) This error refers to READ R2-2 and R3-5. METHOD is less than -2 or greater than +2 or WTFAC is greater than 1.0.

CHAPTER 8

AUXILIARY DISC FILES

The program uses disc files for restart records, plotting data and radioactive component concentrations, if the number of components is greater than 4.

If the number of components is greater than 4, two disc files (unit 2 and 3) are used for storage of radionuclide concentrations. As the program execution proceeds, concentrations at the end of the previous time step are read and used. Concentrations at the end of the current time step are calculated and written on a disc file. At the end of the time step, both files are rewound. During this time step, concentrations which were written during the previous time step are read and vice-versa. Therefore two disc files are required for concentration storage.

Similarly, 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 are read in and plots printed. However, if the user desires to save tape 12 data for subsequent plotting, unit 12 should be saved.

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 below:

Unit No.	Function
2	Radioactive component concentrations
3	Radioactive component concentrations
4	For a continuation run, restart record is read from unit 4.
5	Card reader
6	Line printer
8	Restart records are written on this unit.
12	Plotting data are written on this unit.

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NOTATION

Roman

a	total leach time
b	time of initiation of leach process
C	concentration of the radioactive/trace component
$\hat{C}$	concentration of the brine component
c_R	compressibility of rock (formation)
c_w	compressibility of the fluid
$\underline{\underline{D}}$	dispersion tensor
D_m	molecular diffusion
$\underline{\underline{E}}$	dispersivity tensor (hydrodynamic + molecular)
f	fractional saturation
F	fractional transmissibilities
g	acceleration due to gravity
g_c	units factor, equals unity for SI system and 32 lbm.ft/lbf. sec^2 in English Engineering System
h	depth
$\underline{\underline{I}}$	unit tensor
$\underline{\underline{k}}$	permeability tensor
k_{di}	equilibrium adsorption distribution constant for radioactive component i
k_{ij}	branching factor for radioactive component j transforming to component i
k_ℓ	fractional allocation factor
K_i	equilibrium retardation factor for radioactive component i
K_o	hydraulic conductivity

K_s	hydraulic conductivity of the skin region surrounding a well
m	mass density of nuclide waste, i.e., mass of nuclide per volume of waste
M	mobility
N	number of parent radionuclides
p	pressure
p_o	reference pressure
q	rate of fluid withdrawal through wells
q_{ci}	rate of radionuclide withdrawal through wells
q_{oi}	source rate for dissolved radionuclides due to leaching
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	source term for release of a nuclide from the waste matrix, i.e., mass of radionuclide per bulk volume per time
R_s	brine source rate due to salt dissolution
R_s'	fluid source rate due to salt dissolution
S	concentration of undissolved radionuclide leachate, i.e., mass of undissolved radionuclide per bulk volume
t	time
T	transmissibility
$\underline{u}$	Darcy velocity vector
u	magnitude of $\underline{u}$
v	interstitial velocity
w	weighting parameter for numerical time integration
WI	well index
z	depth below a reference plane

Greek Letters

α_L	longitudinal dispersivity
α_T	transverse dispersivity
δ	Kroenecker 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_o	porosity at the reference pressure
ρ	fluid density
ρ_o	fluid density at the reference pressure
ρ_R	formation density
ρ_W	volumetric waste density, i.e., volume of waste per bulk volume
μ	viscosity
τ	radioactive half-life

Subscripts

c	component
R	rock (formation)
w	water (fluid)

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APPENDIX A

ENGLISH AND SI UNITS

Variable	English	SI
Area	ft^2	m^2
Compressiblity	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 transmissiblity	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 B

CONVERSION OF ENGISH TO SI UNITS

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*F-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