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RISK METHODOLOGY FOR GEOLOGIC DISPOSAL OF RADIOACTIVE WASTE: THE SANDIA WASTE ISOLATION FLOW AND TRANSPORT (SWIFT) MODEL

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RISK METHODOLOGY FOR GEOLOGIC DISPOSAL OF RADIOACTIVE WASTE: THE SANDIA WASTE ISOLATION FLOW AND TRANSPORT (SWIFT) MODEL

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ABSTRACT

This report describes the development of a three-dimensional finite difference model (SWIFT) to simulate the transport by ground water of trace concentrations of radioisotopes. The model was developed for use by NRC in the analysis of deep geological nuclear waste disposal facilities. It is based upon an existing model which treats the injection of liquid chemical wastes into deep saline aquifers. Complete documentation of SWIFT is provided. Comparison of SWIFT results with the analytical solution for constant velocity and diffusivity condition and with the ORIGEN code results for static conditions is presented. A discussion of possible future developments is given.

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DEVELOPMENT OF RADIOACTIVE WASTE DISPOSAL MODEL

1.0 INTRODUCTION

In late 1975, Sandia Laboratories (SL) entered into an agreement with the U.S. Nuclear Regulatory Commission (NRC) to undertake the problem of the development of a methodology for use in the risk evaluation of nuclear waste disposal facilities. The primary objective of this program was the development of a procedure (or methodology) to be used for the analysis of the properties of nuclear waste disposal facilities. This objective was recognized as involving both the development of a workable conceptual approach and the problem of providing the appropriate building blocks to support the conceptual approach. The objective of the work described in this report is to develop a mathematical model for the building block "Radionuclide Transport by Groundwater."

For the benefit of the reader the background of the Sandia Waste Isolation Flow and Transport (SWIFT) model development and how it fits in the overall methodology development are presented below.

1.1 Background of the Methodology Development

After considering several alternative approaches, it appeared that the methodology could be reduced to a structure which contained six problem areas. Models would then have to be found or constructed to provide the necessary inputs and outputs relative to these particular problem areas. These problem areas were:

1) Site Description.

   Information about and the ability to model a waste disposal depository.

2) Waste Description.

   Data about and the necessary modeling to describe the radionuclide waste put into the site.

3) Potential Release Mechanisms.

   Models to indicate the likelihood of possible mechanisms of release from the depository.

4) Radionuclide Transport by Groundwater

   A model which could use available data to describe radionuclide movement from the depository to the biosphere.

5) Pathways to Man.

A model which could use available data to describe radioisotopic movement through the biosphere to man.

6) Dosimetry and Health Effects.

A model to estimate the health effects of radioisotopes to man.

Thus, the methodology concept was viewed as the combination of six problem areas of major concern. These were considered to be functionally related as in Figure 1 below:

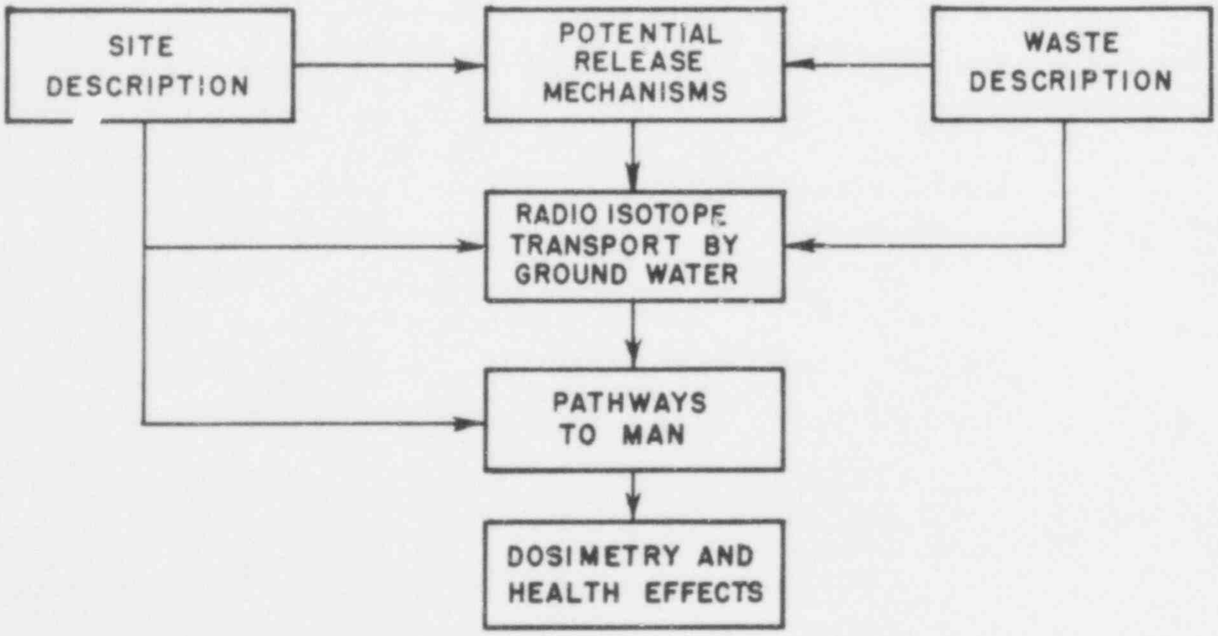

FIGURE 1. Conceptual Approach to Development of Methodology for Analysis of Deep Geological Disposal of Radioactive Waste.

Once the concept had been formulated, the next step was to develop adequate models to be used in the framework of Figure 1. While doing this, the relevant uncertainties were to be kept in mind. These included both the statistical uncertainty the available data and the consequent implied uncertainty resulting from the model as well as the potential of treating some of these uncertainties by classicial techniques of sensitivity analysis.

1.2 Background of Model Development

As discussed above, it became apparent during the initial analysis at SL that there were a number of areas critical to the development of a nuclear waste disposal methodology. One of these major portions was the simulation of radionuclide transport through the geosphere by groundwater.

There were a few models to simulate the transport. One was the theoretical study of Lester, Jansen, and Burkholder (Ref. 1) at Battelle Northwest Laboratories (BNWL) which solved the transport equations under a restricted set of assumptions. Another perhaps more significant study was the examination of a large amount of field data from the National Reactor Testing Station in Idaho, now Idaho National Engineering Laboratory, by means of an extensive digital simulation of radionuclide migration (Ref 2). This study was done by J. B. Robertson of the U.S. Geological Survey (USGS). Another model had been developed by Duguid and Reeves (Ref. 3) of Oak Ridge National Laboratory (ORNL) which was somewhat limited in the treatment of radioisotopes.

In addition, there were a few limited analytical studies such as the one by Holly et al (Ref. 4). These were usually based upon the work of Ogata and Banks (Ref. 5). In general, these studies contained very restrictive assumptions and, moreover, dealt with only one radioisotope. Complete analytical solution to the radioactive decay equations were published by Bateman in 1910 (Ref. 6).

The most promising work of all the reviewed models was the Liquid Chemical Waste Injection Model (Ref. 7) developed for the USGS Water Resources Division (WRD) by INTERA Environmental Consultants, Inc. under a contract from USGS to INTERCOMP, which was a parent company of INTERA at that point in time.

The Liquid Waste Injection Model was developed as a three-dimensional transient mathematical simulation which would accurately simulate the behavior of liquid industrial wastes or saline fronts in a deep saline aquifer. It is a finite-difference model solving simultaneously the partial differential equations describing:

1) Conservation of total liquid mass,
2) Conservation of energy, and

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3) Conservation of the mass of a specific contaminant dissolved in the injection fluid.

In addition, the model in its development was not restricted to just the examination of liquid waste disposal but was designed so that there was considerable flexibility in its application. In addition to being able to deal with very large and complex problems (limited by the computational facilities available), the model could be limited by the user to efficiently address the problem at hand. That is, it can be operated as a one, two, or three dimensional simulation with the degree of complexity elected by the user.

Thus, the USGS waste injection model (now often referred to as Survey Waste Injection Program or SWIP) possessed a number of advantages for the NRC methodology with only one significant disadvantage. This was the fact that it did predict only an inert solute but not dissolved radionuclides. A contract was placed with INTERA Environmental Consultants, Inc. to modifty the basic SWIP in order to include radionuclides transport.

The documentation prepared for SL by INTERA under this contract is reproduced, with minor changes, as the sections 2.0 through 5.0.

1.3 Scope of Model and the Report

The SWIFT Model can be used to calculate high level waste migration. It can also be used for low level radioactive waste discharge and accidental release of radioactive material below the water table.

In this model, fluid properties are assumed to be independent of the concentration of radioactive isotopes. Since these isotopes are likely to be present in aquifer fluids only in small quantities, this is probably a good assumption. However, this model includes the deep well disposal model in its original form. Solution of radioactive nuclide equations are additions to the model and may be selected only if their use is desired.

This report describes modifications made in the model, some of the validation of the model and a program user documentation. The report does not include detailed description of various boundary conditions available to a user, fluid property models used internally, numerical truncation errors associated with the use of the model, solution techniques and computer code organization. The user is referred to the original report to USGS for a complete description of the above.

Section 2 of this report describes the fundamental fluid flow system and the physical laws applicable to the system. It includes the development of mathematical equations from these laws, numerical approximations of the developed equations and basic assumptions contained in the model.

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Numerical solution of a one-dimensional system is compared with known analytical solutions in Section 3. Exact solutions of three component radioactive decay chains in one-dimensional geometry for certain boundary conditions are known.

Section 4 is the basic program user documentation. This section describes the procedure to define decay chains and lists all model options available in the model. Input data forms and the definitions of each of the variables are listed. Program user errors in the entered data that can be detected by the program are also listed in this section.

Section 5 compares the ORIGEN and INTERA model results for static conditions. It also discusses the results of hypothetical heat simulation cases to study the thermal effects.

Proposed future activities and conclusions are presented in Section 6.0.

The computer code for SWIP is available from NTIS.

SWIP documentation available from NTIS in paper
or microfiche
I.D.# PB256903/AS

SWIP code on tape available from NTIS
I.D.# PB256902/AS

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2.0 TECHNICAL APPROACH

The numerical model developed under the contract with INTERA is based on the deep well disposal model which was modified to calculate transport of radioactive nuclides in a porous medium. The basic structure of the model remains unchanged. A wellbore model is coupled to the reservoir transport model. The wellbore model relates surface pressure and enthalpy to bottom-hole pressure and enthalpy.

The deep well disposal reservoir model solves three coupled partial differential equations describing the behavior of a liquid phase injected into an aquifer system. The three differential equations are:

(1) conservation of total liquid mass;

(2) conservation of energy, and

(3) conservation of the mass of a specific contaminant dissolved in the injection fluid.

The radioactive waste disposal reservoir model, in addition to the above three equations, solves the following equation for each of the radioactive constituents:

(4) conservation of mass of the species dissolved in fluid phase and adsorbed on the rock medium including its radioactive decay and generation from other constituents.

2.1 Description of the Basic Equations for the Reservoir Model

The first equation describes the three-dimensional Darcy flow of a single-phase liquid in a porous aquifer. The density of the liquid phase can be a function of temperature, pressure and concentration. The second equation describes the convection and dispersion of energy due to injection of a fluid of different temperature (and pressure) than the resident aquifer fluid. The third equation describes the convection and hydrodynamic dispersion of an inert component present in the system. This allows flow of different salinity or chemical composition fluid from the resident aquifer water.

The fourth equation describes the convective dispersion and adsorption of a radioactive constituent present in trace amounts. The end result is a prediction of the following: (1) decaying trace components, (2) specific chemical contaminant concentrations, (3) of liquid waste and/or discharge of radioactive waste in an aquifer. The aquifer fluid properties are permitted to be functions of liquid chemical waste concentration and temperature.

In addition to the three-dimensional rectangular Cartesian grid, we also have provided a two-dimensional (r, z) grid system. This cylindrical coordinate system is extremely well suited to single source interpretive or predictive calculations.

Basic assumptions contained in the reservoir model are:

(a) Three-dimensional, transient, laminar (Darcy) flow.

(b) Fluid density can be a function of pressure, temperature and concentration of the inert component. Fluid viscosity can be a function of temperature and concentration.

(c) Miscibility of the injected wastes with the in-place fluids.

(d) Aquifer properties vary with position (i.e. porosity, permeability, thickness and elevation can be specified for each grid block in the model).

(e) Hydrodynamic dispersion is described as a function of fluid velocity.

(f) Radioactive constituents are present in trace quantities only, that is fluid properties are independent of the concentrations of these contaminants.

(g) The energy equation can be described as "enthalpy in - enthalpy out = change in internal energy of the system". This is rigorous except for kinetic and potential energy which have been neglected.

(h) Boundary conditions allow natural water movement in the aquifer, heat losses to the adjacent formations and the location of injection, production and observation points anywhere within the system.

The wellbore model provides the boundary conditions for the reservoir model. The reservoir model calculates pressure, temperature and contaminant concentrations at the numerical grid block centers. However, the grid block centers may not correspond to the physical boundary conditions specification points. Energy losses or gains and fluid pressure difference between these points and the corresponding grid block centers are calculated by use of the wellbore model. Depending upon the wellbore model option selected, the model may calculate total fluid mass fluxes across horizontal grid block boundaries and allocate the total flow rate between each vertical layer. As in the original deep well disposal model, the wellbore may refer to a physical well drilled from surface to the aquifer formation. In that case, the user may specify surface pressure and temperature conditions and the wellbore model will calculate the bottom-hole conditions that correspond to the boundary conditions for the reservoir model.

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Source and sink rates of the radioactive components are independent of well rates. This permits discharge of contaminant or energy into the aquifer without being accompanied by fluid.

2.2 Derivation of the Reservoir Model Equations

Suppose x, y, z to be a Cartesian coordinate system and let $Z(x, y, z)$ be the height of a point above a horizontal reference plane. Then the basic equation describing single-phase flow in a porous media results from a combination of the continuity equation

$$\nabla\cdot\rho\underline{u} \quad + \quad q' \quad = \quad -\frac{\partial}{\partial t}(\phi\rho)^* \qquad (2\text{-}1)$$

Net Convection   Source   Accumulation

and Darcy's law in three dimensions.

$$\underline{u} = -\frac{\underline{\underline{k}}}{\mu}(\nabla p - \rho g \nabla Z). \qquad (2\text{-}2)$$

The result is the basic flow equation,

$$\nabla\cdot\frac{\rho\underline{\underline{k}}}{\mu}(\nabla p - \rho g \nabla Z) - q' = \frac{\partial}{\partial t}(\phi\rho). \qquad (2\text{-}3)$$

The energy balance defined as [enthalpy in - enthalpy out = change in internal energy] is described by the energy equation,

$$\nabla\cdot\left(\frac{\rho\underline{\underline{k}}}{\mu}H(\nabla p - \rho g \nabla Z)\right) + \nabla\cdot\underline{\underline{E}}_H\cdot\nabla T \quad - \quad q'_L$$

Net energy convection   Conduction   Heat loss to surrounding strata

$$- \quad q'H \quad - \quad q'_H$$

Enthalpy in with fluid source q'   Energy in without fluid input

$$= \frac{\partial}{\partial t}[\phi\rho U + (1-\phi)(\rho C_p)_R T] \qquad (2\text{-}4)$$

Accumulation

*Detailed definitions of all terms are given in the Nomenclature.

A material balance for the solute results in the solute or concentration equation.

$$\underbrace{\nabla\cdot\left(\rho\hat{C}\frac{\underline{\mathbf{k}}}{\mu}(\nabla p - \rho g\nabla Z\right)}_{\text{Net solute convection}} + \underbrace{\nabla\cdot\rho\underline{\underline{E}}_c\cdot\nabla\hat{C}}_{\text{Diffusion}} - \underbrace{q'\hat{C}}_{\text{Source}}$$

$$= \underbrace{\frac{\partial}{\partial t}(\rho\phi\hat{C})}_{\text{Accumulation}} \qquad (2\text{-}5)$$

A similar material for N radioactive components results in N component equations

$$\underbrace{\nabla\cdot\left[\rho C_i\frac{\underline{\mathbf{k}}}{\mu}(\nabla p - \rho g\nabla Z)\right]}_{\text{Net component i convection}} + \underbrace{\nabla\cdot\rho\underline{\underline{E}}_c\cdot\nabla C_i}_{\text{Diffusion of component i}} - \underbrace{q_i'}_{\text{Source of component i}}$$

$$+ \underbrace{\sum_{j=1}^{N} k_{ij}K_j\rho\phi C_j}_{\text{Generation of component i by decay of other isotopes}} - \underbrace{\sum_{k=1}^{N} k_{ki}K_i\rho\phi C_i}_{\text{Net decay of component i to other isotopes}}$$

$$= \underbrace{\frac{\partial}{\partial t}(\phi\rho K_i C_i)}_{\text{Accumulation}} \qquad (2\text{-}6)$$

where

$$k_{ki}K_i\rho\phi C_i = k_{ki}\rho\phi C_i + k_{ki}\rho_s(1-\phi)C_s \qquad (2\text{-}7)$$

and assumes the approximation

$$\frac{\partial}{\partial t} (\phi\rho K_i C_i) = \frac{\partial}{\partial t} (\phi\rho C_i) + \frac{\partial}{\partial t} [(1-\phi)\rho_s C_s] \qquad (2\text{-}8)$$

where t, the equilibrium adsorption constant, is defined by

$$K_i = 1 + \frac{\rho_B k_{d_i}}{\phi} . \qquad (2\text{-}9)$$

The system of equations (3), (4), (5) and (6) along with the fluid property dependence on pressure, temperature and concentration describe the reservoir flow due to discharge of wastes into an aquifer. This is a nonlinear system of partial differential equations which must be solved numerically using high speed digital computers. Equations (3), (4) and (5) are coupled with each other through fluid property dependence. Since we have assumed that the radioactive components are present in trace quantities only and the fluid properties are independent of these concentrations, Equation (6) is uncoupled from the other equations.

These equations are solved by dividing the region of interest into a three-dimensional grid and developing finite-difference approximations for this grid. Once the region of interest is divided into grid blocks, finite-difference equations are developed whose solution closely approximates the solution of Equations (3), (4), (5) and (6). These finite-difference approximations are:

Basic Flow Equation

$$\Delta[T_w(\Delta p - \rho g\Delta Z)] - q = \frac{V}{\Delta t} \delta(\phi\rho) \qquad (2\text{-}10)$$

Energy Equation

$$\Delta[T_w H(\Delta p - \rho g\Delta Z)] + \Delta(T_H\Delta T) - q_L - q\ H - q_H$$

$$= \frac{V}{\Delta t} \delta[\phi\rho U + (1-\phi)(\rho C_p)_R T] \qquad (2\text{-}11)$$

Solute Equation

$$\Delta[T_W \hat{C}(\Delta p - \rho g \Delta Z)] + \Delta(T_c \Delta \hat{C}) - \hat{C}q = \frac{V}{\Delta t}\,\delta(\rho \phi \hat{C}) \qquad (2\text{-}12)$$

Trace Component Equation

$$\Delta[T_w C_i(\Delta p - \rho g \Delta Z)] + \Delta(T_c \Delta C_i) - q_i + V\rho \Sigma k_{ij} K_j C_J$$

$$- V\rho K_i C_i \Sigma k_{ik} = \frac{VK_i\rho}{\Delta t}\,\delta C_i \qquad (2\text{-}13)$$

where the difference operators are defined by

$$\Delta(T_w \Delta p) = \Delta_x(T_w \Delta_x p) + \Delta_y(T_w \Delta_y p) + \Delta_z(T_w \Delta_z p) \qquad (2\text{-}14)$$

with

$$\Delta_x(T_w \Delta_x p) = T_{w,i+1/2,j,k}\,(p^{n+1}_{i+1,j,k} - p^{n+1}_{i,j,k})$$

$$- T_{w,i-1/2,j,k}\,(p^{n+1}_{i,j,k} - p^{n+1}_{i-1,j,k}) \qquad (2\text{-}15)$$

and

$$\delta\chi = \chi^{n+1} - \chi^{n} \qquad (2\text{-}16)$$

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The terms

$$T_w = \frac{kA\rho}{\mu\ell} \qquad (2\text{-}17)$$

$$T_H = \frac{E_H A}{\ell} \qquad (2\text{-}18)$$

$$T_C = \rho\frac{E_C A}{\ell} \qquad (2\text{-}19)$$

have been introduced for notational convenience. Since all of the terms in Equations (17) through (19) are position dependent, a further expansion is illustrated as

$$T_{w,i+1/2,j,k} = \frac{2\Delta y_j \Delta z_k}{(\frac{\Delta x}{k_x})_i + (\frac{\Delta x}{k_x})_{i+1}} (\rho/\mu)_{i+1/2,j,k} \qquad (2\text{-}20)$$

For radial geometry, the term $\frac{2\Delta y_j \Delta z_k}{\Delta x_i + \Delta x_{i+1}}$ becomes $2\pi\Delta z_k/\ln(r_{i+1}/r_i)$. The volume term is written as $\pi\Delta r_i^2\Delta z_k$.

Two terms, the constituent dispersion tensor, E_c, and the effective heat conductivity tensor, E_H, need additional description. Both are taken in the present model as dependent upon the hydrodynamic dispersivity. This dispersivity is a function of the local fluid velocity. Scheidegger (Ref. 8) has shown that for an isotropic porous medium there can be no more than two independent dispersivity factors. This requirement is essential so that the dispersion tensor is invariant under coordinate transformations. These two dispersivities are longitudinal, in the direction of flow, and transverse, perpendicular to flow. Generally, both are functions of the magnitude of the flow velocity. These values can be expressed as:

$$D_1 = \alpha_1|\bar{u}|$$

and

$$D_t \;=\; \alpha_t |\bar{u}|$$

When the velocity vector is divided into components along the coordinate axes, nine components of both the dispersivity and conductivity tensors occur.

The more general expressions for the dispersivity and conductivity tensors in terms of the molecular properties, as well as hydrodynamic dispersivity, can be written as

$$E_C \equiv \phi\alpha v + D_m$$

$$E_H \equiv \phi\alpha v/(\ C_p)_w + K_m$$

$$\text{where} \quad v = \frac{u}{\phi} \tag{2-21}$$

where the dispersivity, α, is either longitudinal or transverse. Note that the apparent conductivity due to hydrodynamic dispersion in the porous media has been taken as the product of the dispersivity and velocity divided by fluid volumetric heat capacity. The ordinary molecular heat conductivity of fluid plus rock, K_m, has been treated as an additive constant.

The concept expressed in the two equations listed is that the microscopic heterogeneity in convective flow creates the same dispersive effect in temperature as it does in a constituent concentration.

3.0 COMPARISON WITH ANALYTICAL SOLUTION

The programmed trace component equations were tested against known one-dimensional analytical solutions for short chains. Solutions for two and three component chains for two sets of boundary conditions have been worked out by Lester *et al*[3] of the following type:

① → ② → ③

where ①, ② and ③ are the component numbers.

boundary conditions used were

(a) impulse release which is a mathematically idealized boundary condition of a point source being released in an infinitesimal time;

(b) decaying band release where concentrations at $x = 0$ are given by

$$
\begin{aligned}
C_1 &= C_{10} && \text{at } t = 0 \\
C_2 &= C_{20} && \text{at } t = 0 \qquad (3\text{-}1) \\
C_3 &= C_{30} && \text{at } t = 0
\end{aligned}
$$

For time $t > 0$, concentrations at the boundary are obtained by decay and generation of the three components in a batch reactor according to the decay chain.

As discussed in the deep well disposal model report (Ref 7), flux boundary conditions, as opposed to concentration boundary conditions, are physically more realistic. The flux boundary conditions are easier to represent in a numerical model. Therefore, decaying flux boundary condition was used for comparison with the analytical solution. The initial and boundary conditions for the band release were as follows:

$$
\text{All } x,\ t \leq 0 \qquad
\begin{aligned}
C_1 &= 0 \\
C_2 &= 0 \qquad (3\text{-}2) \\
C_3 &= 0
\end{aligned}
$$

At $x \to \infty$, $t > 0$

$$\begin{aligned} C_1 &\to 0 \\ C_2 &\to 0 \\ C_3 &\to 0 \end{aligned} \tag{3-3}$$

At $x = 0$, $t > 0$

$$\begin{aligned} uC^1_{1_0} &= uC_1 - E_c \frac{\partial C_1}{\partial x} \\ uC^1_{2_0} &= uC_2 - E_c \frac{\partial C_2}{\partial x} \\ uC^1_{3_0} &= uC_3 - E_c \frac{\partial C_3}{\partial x} \end{aligned} \tag{3-4}$$

where

$$C^1_{1_0} = C_{1_0} e^{-k_1 t}$$

$$C^1_{2_0} = C_{2_0} e^{-k_2 t} + \frac{k_1 C_{1_0}}{k_1 - k_2} (e^{-k_2 t} - e^{-k_1 t})$$

$$\begin{aligned} C^1_{3_0} = {} & C_{3_0} e^{-k_3 t} + \frac{k_2 C_{2_0}}{k_2 - k_3} (e^{-k_3 t} - e^{-k_2 t}) \\ & + k_1 k_2 C_{1_0} \{ \frac{e^{-k_1 t}}{(k_1 - k_2)(k_1 - k_3)} - \frac{e^{-k_2 t}}{(k_1 - k_2)(k_2 - k_3)} \\ & + \frac{e^{-k_3 t}}{(k_1 - k_3)(k_2 - k_3)} \} \end{aligned}$$

For equal adsorption equilibrium constants, reaction and flow solutions can be separated and the total solution is a product of the solutions. Therefore, based upon Lester et al (Ref. 1) and Coats and Smith's (Ref. 9) analytical solutions, for the one-dimensional linear case, the solution for conditions (2) to (4) is as follows:

$$
\begin{aligned}
C_i = \frac{1}{2} C^1_{i_0} [& \operatorname{erfc}(\frac{\sqrt{\gamma}}{2} \frac{x^\star - I}{\sqrt{I}}) - e^{\gamma x^\star} \operatorname{erfc}(\frac{\sqrt{\gamma}}{2} \frac{x^\star + I}{\sqrt{I}}) \\
& - \frac{\gamma}{2} (x^\star + I) e^{\gamma x^\star} \operatorname{erfc}(\frac{\sqrt{\gamma}}{2} \frac{x^\star + I}{\sqrt{I}}) \qquad (3\text{-}5) \\
& + \sqrt{\frac{\gamma I}{\pi}} \exp\{- \frac{\gamma}{4I} (x^\star - I)^2\}]
\end{aligned}
$$

where

$$I = \frac{ut}{K_i \phi L}$$

$$\gamma = \frac{uL}{E}$$

$$x^\star = \frac{x}{L}$$

Since the analytical solution is available for constant velocity and diffusivity conditions only, the numerical solution must be calculated for the same conditions. If compressibility of the medium (fluid and rock) is made negligible, the flow solution result for constant one-dimensional cross section and constant flow rate gives a constant value of the velocity everywhere in the system.

The aquifer and fluid properties used for the test are summarized in Table I.

TABLE I

Aquifer and Fluid Properties used for
the Comparison with Analytical Solutions

Half Life	
Component - 1	433 years
Component - 2	15 years
Component - 3	6,540 years

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Adsorption Distribution Constant	10.39 ft^3/lb
Rock Density	100 lb/ft^3
Fluid Density	62.4 lb/ft^3
Porosity	0.1 (fractional)
Compressibility	
Fluid	Incompressible
Rock	2×10^{-7}/psi
Hydraulic Conductivity	2 ft/day
Darcy Velocity	0.656 ft/day (0.2 m/day)
Initial Concentrations	
Component - 1	1.0 (mass fraction)
Component - 2	0
Component - 3	0
Longitudinal Dispersivity Factor, α	8.5 ft

A total length of 200 m (656 feet) with 40 blocks of equal size were used for the test. Second order numerical space truncation error was eliminated by using a central-difference approximation. Two types of solution comparisons were made:

(a) C vs. x for one t value (10^5 days)

(b) C vs. t for one x value (100 m).

Since the component concentrations in the input stream ($C^1_{1_0}$, $C^1_{2_0}$ and $C^1_{3_0}$) are continuous functions of time and the model input is in terms of constant concentrations over a "time step", average values of $C^1_{1_0}$, $C^1_{2_0}$ and $C^1_{3_0}$ over each time step were used. The results are shown in Figures 2 and 3, respectively. The figures show a good match of the analytical and numerical concentration values in the higher concentration regions. However, relatively low concentrations do not show as good a fit. This could possibly be due to two reasons -- (i) third and higher order truncation errors in the numerical model and (ii) errors associated with numerical approximation of complementary error function in the analytical solution. It must be pointed out that the concentrations have been plotted on semi-log scale which tend to magnify the differences in analytical and numerical results at low concentrations.

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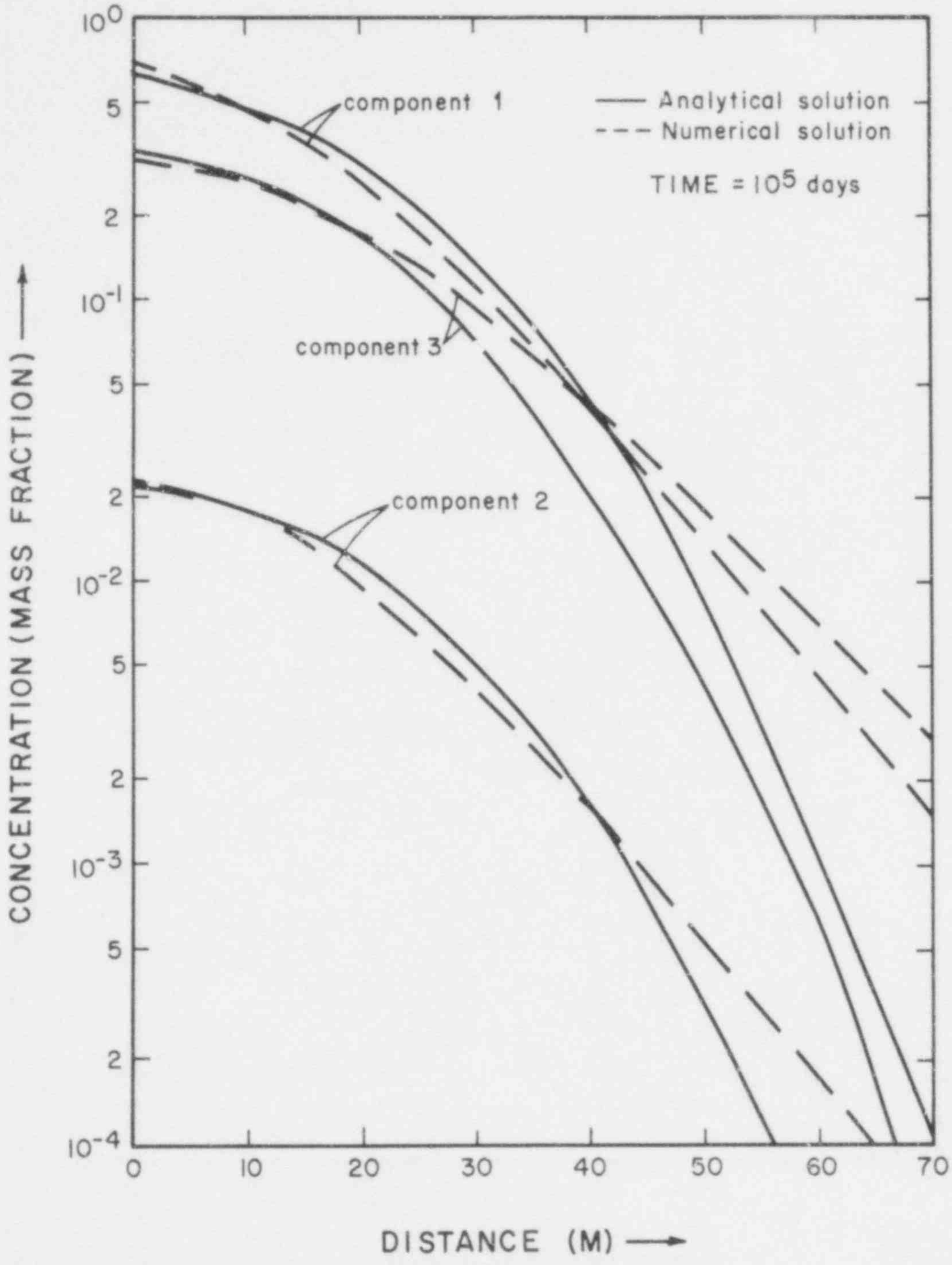

Figure 2. Comparison of Numerical and Analytical Solutions.

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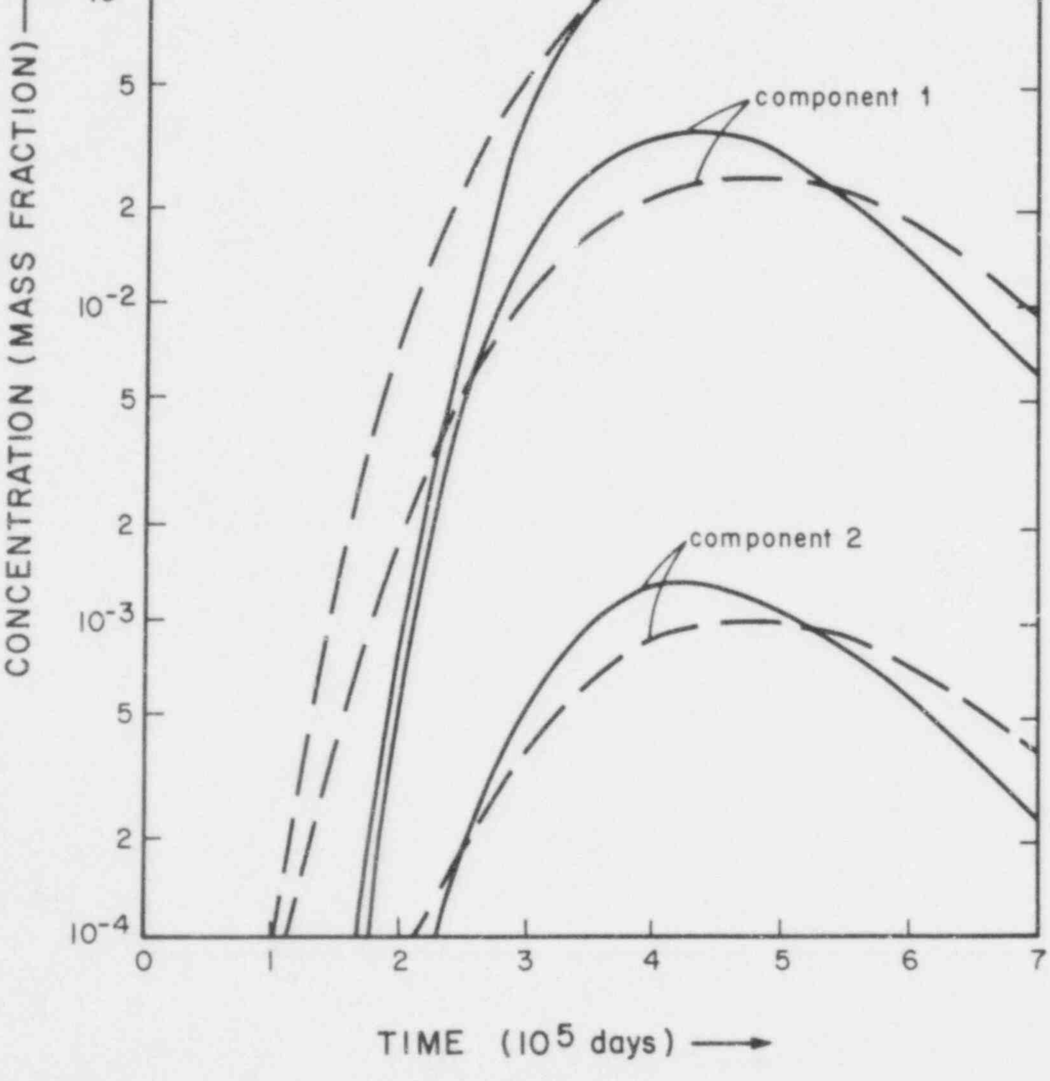

Figure 3. Comparison of Numerical and Analytical Solutions

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The objective of comparing the numerical solution with an analytical solution is to test the programming of finite-difference equations, representation of physical conditions and delineating the magnitude of errors involved in numerical approximations. In our opinion, the solution comparisons prove that the computer programs are error free. The excellent match of numerical and the analytical results near the x = 0 boundary shows that the numerical boundary conditions do represent the physical/analytical conditions extremely well. The shape of the curves, the magnitudes and locations of the maxima show that the numerical model accurately represents the physical behavior of the radioactive waste transport in a porous medium. As discussed in the report to USGS, the magnitude of second order truncation errors may restrict selection of numerical grid block and time step sizes. However, higher order truncation errors are not likely to result in any program use limitations because of the accuracy in available model input data such as adsorption coefficients of radioactive isotopes and physical properties of the geological strata that may be used for radioactive waste disposal.

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4.0 DOCUMENTATION

4.1 DESCRIBING DECAY CHAINS

Three coupled partial differential equations describing conservation of total fluid mass, energy and an inert solute are solved until convergence is reached. This flow solution is then used to solve radioactive/trace component equations one at a time. This solution procedure dictates that during the solution of a component equation, "new" (at time level n+1) concentrations of *all* the parent components be available. From the above, it follows that all the daughter component equations be solved *after* the parent component equation. The natural radioactive decay process proceeds only in one direction and is irreversible. An alpha decay is accompanied by a decrease in mass of the isotope and a beta decay is a loss of an electron (conversion of a neutron to a proton). Therefore, the component with the highest mass number containing the highest number of neutrons does not have any parent components in the series. Obviously this component should be assigned the lowest component number--one. The component which has no daughter components should be assigned the highest component number. In fact, the user is permitted to be more flexible in numbering the components. The only real requirement is that for every decay step, the parent component must be assigned a lower component number than the daughter component. As an illustration, an ordered numbering scheme is shown in Figure 4.

The user is required to provide half-life of each component and identify parent and daughter components for each decay step. If more than one daughter components are formed from one parent component, then the user must provide the parent component fractions decaying to each daughter component.

4.2 USER OPTIONS

The model options available to the user are simply listed here. The use of each of the options is described in the following section along with the input data required.

1. *Problem Size*. There is no upper limit placed on the actual problem size as long as the total core storage required is available on the machine. The program uses a variable dimensioning scheme for all large arrays. After the program dimensions have been specified, the dimensions on arrays and total array storage required are calculated.

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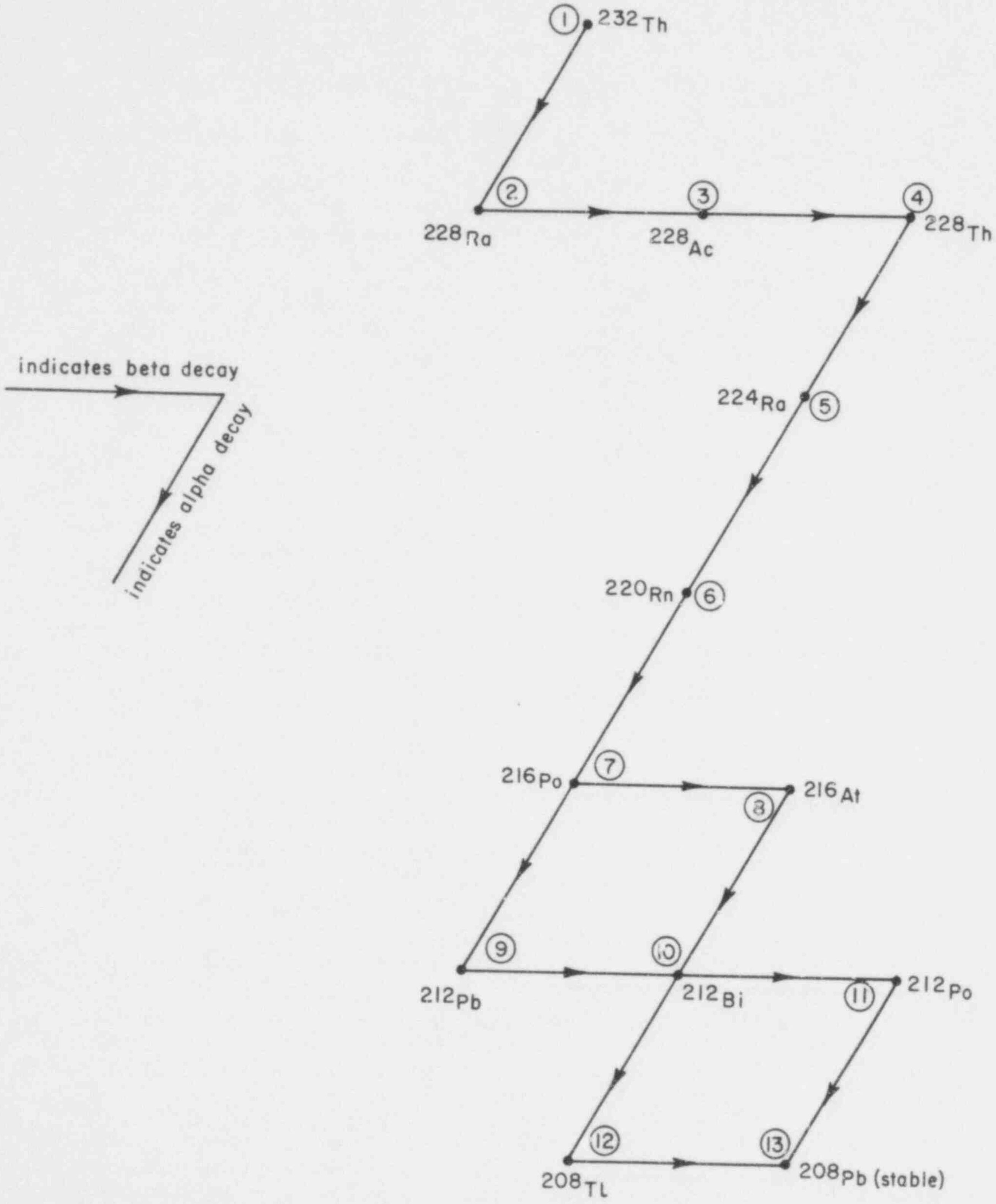

Figure 4. Ordered Component Numbering for the Thorium Series.

2. Coordinate System. The model offers the use of three-dimensional Cartesian coordinates (x, y, z) or two-dimensional radial coordinates with angular symmetry (r, z). Problems can be solved in simpler one- or two-dimensional geometry as well.

3. Decay Chain. There are no restrictions to the total number of components in the decay chain or to the number of parent or daughter components that a component in the decay chain may have. Component numbering procedure is described in Section 4.1.

4. Adsorption Coefficients. The user may enter a regional description of formation type. The numerical grid system may encompass a number of rock or formation types and adsorption coefficients for each isotope may be different for each rock type.

5. Fluid Properties. Formation fluid density is permitted to be a function of pressure, temperature and the inert component concentration. Fluid viscosity may be specified a function of temperature and concentration.

6. Heterogeneities. A user option is available to describe heterogeneities in the aquifer to the extent of each grid block having different horizontal and vertical permeabilities, porosity and rock heat capacity.

7. Geometry. Based upon the selected coordinate system, block pore volumes can be zeroed out to describe the actual aquifer geometry. Individual grid block thicknesses and depths can be adjusted. In addition to that, if Cartesian coordinate system has been selected, dip angles in x and y directions can be specified.

8. Wellbore Model. The wellbore model calculates pressure and temperature differences between physical boundary condition points and corresponding grid block centers.

9. Heat Loss. Gain and loss of heat to overburden and underburden can be included in energy calculation by specifying numerical grid blocks in overlying and underlying strata.

10. Aquifer Influence Functions. Through the use of aquifer influence functions, fluid, energy and contaminant transport across numerical grid boundaries may be permitted. Carter-Tracy aquifer presentation can be used if the total dimensions of the aquifer are larger than the numerical grid system. Steady state aquifer representation is used to specify constant pressure boundaries--initial conditions.

Pot aquifer representation is sometimes useful for empirical history matching purposes. In all the three options mentioned above, the fluid coming into the aquifer is assumed to be at the initial conditions in the peripheral blocks. The fluid leaving the aquifer boundary is assumed to leave at the "current" conditions in the peripheral blocks. An additional option is available to specify constant pressure, temperature and concentration boundaries--not necessarily the initial conditions in the peripheral blocks.

11. Initialization. Initial inert component and radioactive isotope concentrations in each grid block may be specified. The model also offers an option to specify temperature gradients in the vertical direction.

12. Well Specification. The well specification option is very useful in expressing various types of pressure and flux boundary conditions by specifying wells at those grid block locations. The user has the choice to specify injection/withdrawal rates in one of the following ways:

(a) (i) Constant flux boundary condition.
    (ii) Combination of constant flux and pressure boundary condition. The lower of the two flux rates is used--specified and calculated from the specified pressure.

(b) (i) Flux allocation between different layers is based upon layer mobilities alone. Mobility is (fluid density/viscosity) x (a layer allocation factor entered by the user).
    (ii) Flux allocation between different layers is done on the basis of layer mobility and pressure difference between the wellbore (bottom-hole) and the grid block.

(c) (i) Flux is expressed explicitly (calculated at the old time level--beginning of the time step) in the aquifer model equations.
    (ii) Flux is expressed in a semi-implicit manner. A term taking into account the effect of change in grid block pressure is added to the explicit rate.

13. Source Rate. Well rates are specified in terms of total fluid volume (ft^3/day) at temperature and concentration. Enthalpy input is calculated from the bottom-hole pressure and temperature. Inert component input rate is obtained from total fluid rate and concentration of injection (mass fraction). However, radioactive waste may be in solidified form from which energy and trace components will be discharged into the geologic formation without being accompanied by any fluid. Therefore, radioactive component sources are specified in terms of fluid rate (lb/day), energy rate (Btu/day) and components (lb/day).

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14. Automatic Time Step. This option is very useful in minimizing computer processing time. Maximum pressure, temperature and concentration changes desired per grid block per time step can be specified and the program internally calculates the time step required to obtain those changes. The value of the new time step is calculated from the previous time step and the changes over the previous time step. Three values of automatic time step from pressure, temperature and concentration changes will be calculated. The "smallest" value of the three calculated time steps is actually used.

Whether the time step is user specified or internally calculated, a limiting time step for solution of each of the radioactive component equations is calculated internally from user specified component concentration change. If this value is larger than the time step used for p, T and $\hat{C}$ equations, then the same time step is used in solution of the radioactive component equation. However, if the limiting time step is smaller than the time step used for p, T and $\hat{C}$ equations, the time step is subdivided to solve the radioactive component equation. Under this procedure, conceivably each of the component equations could use a different time step.

15. Method of Solution. The model offers the user an option to select a direct or an iterative method of solution for solving the difference equations. The direct method includes an ordered Gaussian elimination scheme and the iterative method is a two-line overrelaxation (L2SOR) method.

16. Plotting Calculated Versus Observed Results. This portion of the model enables the user to plot comparative values of observed (measured) pressure, temperature or inert component concentration with calculated values of the same variable as a function of time for any specified well. Since the wellbore is made an integral part of the calculation, the user can compare these variables at surface conditions, at bottom-hole conditions or both.

17. Contour Mapping. To make the visualization of multidimensional results more comprehensible, two-dimensional contour maps can be prepared on the line printer of pressure, temperature or inert component concentration. These maps can be presented at any time during the calculation. The mapping program presents a diagram of up to 20 contours of the dependent variable. Each contour is described with a different mapping character.

18. Restart Capability. The program includes an optional restart feature which will reduce the total computing time and expense. By retaining intermediate results and data on a magnetic tape or disc area, a problem may be interrupted and restarted at specified convenient times in the simulation run.

4.3 DATA INPUT FORMS

READ M-1 (20A4/20A4)

LIST: TITLE

TITLE	Two cards of alphabetic 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 (8I5)

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

NCALL	Control parameter for solving the basic partial differential equations. If you desire to simulate a solution of all three equations, enter zero. The pressure equation is always solved. The solutions of the temperature and inert component concentration equations may be bypassed, if desired. 0 - All three equations will be solved. -2 - The concentration equation will not be solved. The simulated solution will consist of solving a set of two coupled equations only (pressure and temperature). 1 - Only the pressure equation will be solved. The model is simplified to solving one independent partial differential equation. 2 - The temperature equation will not be solved.
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 tape mounted on Tape Unit Number 4.

ISURF	Control parameter for wellbore calculations. 0 - This means only rates or aquifer formation level pressures will be specified. 1 - Surface values will be specified. The wellbore model will calculate changes from the surface to the aquifer level.
IIPRT	Transmissibility printing key. The value entered here is not used. This version of the model has been modified to read IIPRT in READ R2-13 which activates printing of several intermediate parameters on a one time step basis.
NPLP	Control parameter for plotting pressures in the wells. 1 - Bottom-hole and surface pressures are plotted if wellbore calculations are performed. Only the bottom-hole pressures are plotted if no wellbore calculations are performed. For an observation well, the bottom-hole pressure is the grid block pressure. 0 - If no pressure plots are desired. -1 - If pressure plots are desired for a previous run. Skip READ M-3 through R2-17 and proceed to READ P-1.
NPLT	Control parameter for plotting temperatures in the well. 1 - For an observation well, the grid block temperature is plotted. For an injection well, the bottom-hole temperature is plotted if wellbore calculations are performed. For a production well, the bottom-hole temperature is always plotted. In addition, the surface temperature is plotted if the wellbore calculations are performed. 0 - If no temperature plots are desired. -1 - If temperature plots are desired for a previous run. Skip READ M-3 through R2-17, and proceed to READ P-1.

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NPLC	Control parameter for plotting concentration in the well. 1 - The concentration in the well is plotted for observation and production wells only. 0 - If no concentration plots are desired. -1 - If concentration plots are desired for a previous run. Skip READ M-3 through R2-17, and proceed to READ P-1.

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

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

READ M-3 (12I5)

LIST: NX, NY, NZ, HTG, NCP, NRT, KOUT, PRT, NSMAX, NABLMX, METHOD, NARR

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. If you desire to specify a heterogeneous aquifer, you may either enter HTG=2 and enter data for each aquifer region, or specify a homogeneous linear or radial geometry aquifer and modify the blocks or regions in which heterogeneity is desired. 1 - Homogeneous aquifer, linear geometry. 2 - Heterogeneous aquifer, aquifer data entered on regional basis, linear geometry. 3 - Radial geometry. The aquifer may be heterogeneous in the vertical direction.
NCP	Number of radioactive/trace components in the system.

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NRT	Number of rock types. Adsorption coefficients for each rock or strata type for each component must be entered as input data. Rock type description is entered in READ R1-26.
KOUT	Output control. 0 - All program output activated. 1 - All program output except initial arrays (concentrations, pressures, etc.) are activated. 3 - No program output is activated. KOUT is read again in recurrent data READ R2-13. A value of KOUT here of 3 can be used to omit printing of most initialization data as is sometimes desirable in making a sequence of many history matching runs.
PRT	Output array orientation control. -1 - Print output arrays as areal layers (x-y). Block numbers in the x direction increase from left to right and decrease down the computer page in the y direction. +1 - Printout is similar to above except that J-block numbers increase down the computer page. 2 - Print output arrays as vertical sections (x-z).
NSMAX	Maximum number of radioactive/trace component sources that will be used during the run.
NABLMX	Maximum number of aquifer influence function blocks. This data is used for dimensioning the aquifer influence function arrays. This number is equal to the number of peripheral blocks, if aquifer influence functions are to be used.
METHOD	The method of solution that you will use for the current run. The method of solution entered here is used to dimension the working arrays in numerical solution subroutines (direct solution or L2SOR). The method

to be used is read again in READ R2-2. Since the amount of storage required for direct solution is always larger than for L2SOR, you may specify direct solution on this card and may actually use L2SOR, but you may <u>not</u> specify L2SOR on this card and use direct solution.

0, ±1 - Allocate storage for direct solution. You may specify direct solution or L2SOR in READ R2-2. The dimension of a working array "A" is printed out at this point. If you specify direct solution again in READ R2-2, the minimum length required for the array "A" will be printed. If you desire to use the direct solution method, then this length must be smaller than the dimension of array "A".

±2 - Allocate storage for L2SOR method. You may not specify direct solution in READ R2-2.

NARR Storage allocation for working array ("A") in direct solution routine.

0 - Length of "A" array will be calculated internally using an approximate formula. Later in the program the minimum length will be calculated exactly.

>0 - Storage allocation for "A" array. If you intend to use direct solution, this number must be equal to or greater than the minimum length required which is printed later in the program.

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

READ R0-1 (LIST 1: I3, 2A4, 4X, 3I5, E10.1,
LIST 2: 4(I5, 5X, E10.0)
NOTE: Enter NCP (No. of Components) sets of R0-1 data.
LIST 1: MASS (I), DI(I), 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 according to EQ (r-3) (Section 5.1, Model Documentation, September 1977) 0 - Do not modify rate constant
DEC	Half life of component I in years. For stable components, enter zero.

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

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

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

<u>READ R0-2</u> (8E10.0)

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

DIS	Adsorption distribution coefficient in ft^3/lb. 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.

<u>READ M-4</u> (I10)

LIST: ILAST

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

<u>READ M-5</u> (F10.0)

LIST: TMCHG

TMCHG	Time in days at which the next set of recurrent data is to be read. If TMCHG is less than or equal to the time corresponding to the restart time step number, a set of recurrent data will be read immediately to resume the previous simulation.

NOTE: Proceed to READ R2-1 if you entered M-4 and M-5.

<u>READ R1-1</u> (5E10.0)

LIST: CW, CR, CTW, CPW, CPR

CW	Compressibility of the aquifer fluid, (psi)$^{-1}$

CR	Compressibility of pore structure, pore volume/pore volume/psi.
CTW	Coefficient of thermal expansion of the aquifer fluid, $(°F)^{-1}$.
CPW	The fluid heat capacity, Btu/lb-°F.
CPR	The rock heat capacity per unit volume of solid, Btu/ft^3-°F.

READ R1-2 (7E10.0)

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

UKTX	Thermal conductivity of the fluid saturated porous medium in the x direction (Btu/ft-°F day; see CONV).
UKTY	Thermal conductivity of the porous medium in the y direction.
UKTZ	Thermal conductivity of the porous medium in the z direction.
CONV	Conversion factor for the thermal conductivities. The entered values of the thermal conductivities are multiplied by CONV to obtain Btu/ft-day-°F units. If entered as zero, thermal conductivities should be read in Btu/ft-day-°F.
ALPHL	Longitudinal dispersivity factor, ft. The net hydrodynamic dispersion term in a porous medium is $\phi\alpha_{\ell}u/\phi$, where u is Darcy velocity.
ALPHT	Transverse dispersivity factor, ft.
DMEFF	Molecular diffusivity in the porous medium, includes porosity and tortuosity effects (porosity x fluid molecular diffusivity/tortuosity), ft^2/day.

READ R1-3 (5E10.0)

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

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LIST: BROCK, PBWR, TBWR, BWRN, BWRI

BROCK	Actual rock density (solid particle), lb/ft^3.
PBWR	Reference pressure at which the densities are to be entered, psi.
TBWR	Reference temperature at which the densities are to be entered, °F.
BWRN	The density of the natural aquifer fluid (concentration=0) at PBWR and TBWR, lb/ft^3.
BWRI	The density of the contaminated fluid (concentration=1) at PBWR and TBWR, lb/ft^3.

READ R1-4 (I5)

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

LIST: NOUT

NOUT	Output control parameter for wellbore calculations. 0 - No output is activated. 1 - Iteration summary (number of outer iterations, flow rate and the bottom-hole pressure) is printed for each well. 2 - The well pressure and temperature (at the surface for an injection well and at the bottom-hole for a production well) and the flow rate are printed every time subroutine WELLB is called. 3 - The pressure and temperature in the well are printed over each increment (see DELPW in READ R1-5).

READ R1-5 (3E10.0)

LIST: PBASE, DELPW, TDIS

PBASE	Atmospheric or reference pressure at the wellheads, psi. This is used to convert absolute pressure to gauge pressure.
DELPW	Incremental value of pressure over which wellbore calculations are to be performed. The pressure and temperature calculations in the wellbores proceed in increments. The length increment corresponding to DELPW is calculated, and the temperature change over each increment is evaluated.

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TDIS	Thermal diffusivity of the rock surrounding the wellbores, ft^2/hr.

READ R1-6 (4I5)

The number of entries in the viscosity and temperature tables are entered here. You should enter as much viscosity data as is available. You are required to enter at least one viscosity point for the resident fluid (concentration=0) and one for the injection fluid (concentration=1). These reference viscosity points should preferably be at the middle of the expected temperature range and, if possible, both the reference viscosities should be entered at the same temperature. If only one viscosity point is available, the program obtains viscosity at other temperatures according to Lewis and Squires' generalized chart (Ref. 10). If you desire to enter a constant viscosity for any of the two fluids, you must enter one more viscosity point in addition to the reference viscosity. For example, if you desire to enter constant viscosity of 0.9 cp for the injection fluid, enter NTV. 1, the reference viscosity of the injection fluid VISIR=0.9 and VISI(1)=0.9.

The temperature table describes the initial temperatures existing in the aquifer.

NOTE: Number of entries in the viscosity tables refer to the viscosity values to be entered in addition to the reference viscosities.

LIST: NCV, NTVR, NTVI, NDT

NCV	Number of entries in the concentration-viscosity table. This table is for viscosities other than at the reference temperature TRR. The table should contain the viscosities of the fluid mixture at concentrations other than 0 and 1, since these two values are entered as reference viscosities. If only the two pure fluid viscosities are available, enter zero and read in the viscosities of the pure fluids as reference viscosities.
NTVR	Number of entries in the temperature-viscosity table for the aquifer resident fluid.
NTVI	Number of entries in the temperature-viscosity table for the contaminated fluid.
NDT	Number of entries in the depth versus temperature table.

READ R1-7 (4E10.0)

LIST: TRR, VISRR, TIR, VISIR

The reference viscosities of the contaminated and the resident fluids are to be entered here.

TRR	Reference temperature for the resident viscosity fluid, °F.
VISRR	Viscosity of the resident fluid at the reference temperature TRR, cp.
TIR	Reference temperature for the contaminated fluid viscosity, °F. If possible, this temperature should be taken equal to TRR.
VISIR	Viscosity of the contaminated fluid at TIR, cp.

READ R1-8 (8F10.0)

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

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

SC	Concentration, fraction.
VCC	Viscosity (cp) of a fluid mixture at concentration SC, and temperature TRR.

READ R1-9 (8F10.0)

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

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

TR	Temperature, °F.
VISR	Viscosity (cp) of the resident fluid at the temperature TR. Do <u>not</u> re-enter the reference viscosity at TRR (READ R1-7).

READ R1-10 (8F10.0)

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

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

TI	Temperature, °F.
VISI	Viscosity (cp) of the contaminated fluid at the temperature TI. Do <u>not</u> enter the reference viscosity at TIR (READ R1-7).

READ R1-11 (2F10.0)

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

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

ZT	Depth, ft.
TD	Temperature, °F.

READ R1-12 (2I5)

LIST: NZOB, NZUB

NZOB	Number of overburden blocks. If $NZOB \leq 2$, overburden heat loss calculations are not performed.
NZUB	Number of underburden blocks. If you desire the underburden heat loss calculations to be performed, a value of 3 or greater should be entered. If the number of aquifer blocks (NZ) is equal to one, the underburden heat loss is assumed to be equal to the overburden heat loss.

READ R1-13 (4E10.0)

LIST: KOB, CPOB, KUB, CPUB

KOB, KUB	Vertical thermal conductivities of the overburden and the underburden blocks, respectively. These conductivities should also be entered in the same units as in READ R1-2.
CPOB, CPUB	Overburden and underburden heat capacities per unit volume, Btu/ft^3-°F.

READ R1-14 (7E10.0)

NOTE: Skip this READ if NZOB=0.

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

DZOB	Thickness of each overburden block. The first overburden block is at the upper edge of the aquifer. The overburden block numbers increase as you go away from the aquifer.

READ R1-15 (7E10.0)

NOTE: Skip this READ if NZUB=0.

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

DZUB	Thickness of each underburden block. The block numbers increase as you go away from the aquifer.

READ R1-16 (4E10.0)

LIST: TO, PINIT, HINIT, HDATUM

TO	A standard temperature (°F) for calculating fluid density. Fluid density at any other temperature is calculated as the sum of the density at TO and the deviation from it.
PINIT	Initial pressure at the depth HINIT, psi.
HINIT	An arbitrary depth for setting up initial conditions, ft. HINIT can be any depth within the aquifer. HINIT is used only to set up initial pressures in the aquifer.
HDATUM	A datum depth (ft) for printing the dymanic pressures (p-ρgh). The depth h is measured from the datum depth HDATUM. The fluid density used for conversion is resident fluid density at TO and PINIT. This valve is not used internally except for 'Pressure at Datum' output.

READ R1-17 (7E10.0)

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

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

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

READ R1-18 (7E10.0)

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

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

READ R1-19 (7E10.0)

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

DELZ	Thickness of each vertical layer, ft.

If you use the "homogeneous" aquifer option (HTG=1 in READ M-3) then the reservoir is treated as a rectangular parallelepiped and the grid defined by the DELX, DELY, DELZ values are the cell dimensions in the parallelepiped. The x-y plane of the grid is horizontal only if SINX and SINY of READ R1-20 are both zero. Similarly, the z axis in this case points downward only if SINX and SINY are both zero. DELX and DELY are measured along the x-y plane and DELZ is perpendicular to the x-y plane.

If you use the "heterogeneous" aquifer option (HTG=2 in READ M-3) then the x-y plane is a horizontal plane placed over the aquifer structure. The x-axis should be aligned with the longer dimension of the aquifer and should be as "parallel" as possible with this longer dimension.

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 by using either READ R1-21 instead of R1-20 or by regional modifications in READ R1-26.

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

KX	Hydraulic conductivity in x direction, ft/day. This quantity represents the fluid velocity obtained by a potential gradient of unity (ft of water/ft) of the aquifer fluid at concentration zero and temperature, TO. In terms of permeability this quantity is $(k\rho_o g/\mu_o)$. The parameters ρ_o and μ_o are the density and the viscosity of the aquifer fluid at concentration zero and temperature, TO (READ R1-16).
KY	Hydraulic conductivity in y direction, ft/day.
KZ	Hydraulic conductivity, ft/day.
PHI	Porosity (fraction).

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SINX	Sine of the reservoir dip angle along the x-axis.
SINY	Sine of the reservoir dip angle along the y-axis.
DEPTH	Depth to <u>top</u> of grid block (1,1,1,),ft.

<u>READ R1-21</u> (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, UCPR

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

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

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

KX	x direction hydraulic conductivity for flow, ft/day.
KY	y direction conductivity for flow, ft/day.
KZ	z direction conductivity for flow, ft/day.
PHI	Porosity, fraction.
UH	Depth (ft) measured positively downward from reference plane to top of the cell. If entered zero, the depth is unaltered from the value calculated for a homogeneous aquifer.
UTH	Grid block thickness in the vertical direction, ft. If the layer thickness is equal to DELZ(K) read in under READ R1-19, UTH may be entered as zero.
UCPR	Heat capacity of the rock per unit volume, Btu/ft^3-°F. If the rock heat capacity is equal to CPR (READ R1-1), UCPR may be entered as zero.

<u>READ R1-22</u> (7E10.0)

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

These data are read for a radial geometry aquifer with only one source. The source is located at the center of the numerical grid block system. The grid blocks are divided on an equal $\Delta \log r$ basis, i.e. r_i/r_{i-1} is constant. If you desire to use regions of equal $\Delta \log r$ instead of a constant value of $\Delta \log r$ throughout the aquifer, you should specify the number of blocks in each region (READ R1-24) and the boundaries between the regions (READ R1-25).

LIST: RWW, R1, RE, DEPTH

RWW	Well radius, ft.
R1	The first grid block center, ft.
RE	External radius of the aquifer, ft.
DEPTH	Depth from a reference plane to the top of the aquifer, ft.

READ R1-23 (5E10.0)

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

DELZ	Layer thickness in the vertical direction, ft.
KYY	Horizontal hydraulic conductivity, ft/day.
KZZ	Vertical hydraulic conductivity, ft/day.
POROS	Porosity, fraction.
CPR1	Rock heat capacity, Btu/ft^3-°F. If the rock heat capacity in the layer is equal to CPR (READ R1-1), CPR1 may be entered as zero.

You must punch one card for each vertical layer.

READ R1-24 (5I5)

NOTE: These data are read for obtaining regions of equal $\Delta \log r$. If you desire a constant value of $\Delta \log r$ throughout the aquifer, insert a blank card and proceed to READ R1-26.

LIST: NXR(I), I=1, 5

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NXR	Number of grid blocks in each constant Δlogr region. You may specify as many as five regions. The total number of grid blocks in different regions cannot exceed NX. The number of blocks in the outermost region need not be specified. For example, if you desire a total of 25 radial grid blocks and three regions of 5, 10 and 10 grid blocks, then enter NX=25 (READ M-3) and NXR's may be entered as 5, 10, 0, 0, 0 or as 5, 10, 10, 0, 0.

READ R1-25 (4E10.0)

NOTE: If NXR(1)>0, this card is required.

LIST: RER(I), I=1, 5

RER	Radii of the boundaries between different regions, ft. As an example, if the external radius of the aquifer is 5,000 ft and you desire five grid blocks in the first 1,000 ft, 10 grid blocks from 1,000 to 2,500 ft and 10 blocks from 2,500 to 5,000 ft, and if you entered NXR's as 5 and 10 (and the rest zeros), you should enter RER's as 1,000 ft and 2,500 ft only (the rest as zeros). Alternatively, if NXR's were specified as 5, 10 and 10, then RER's should be entered as 1,000, 2,500 and 5,000.

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

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

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

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	Lower and upper limits inclusive on the J-coordinate of the region to be modified.
K1, K2	Lower and upper limits inclusive on the K-coordinates of the region to be modified.
IRT	Rock type. All blocks are assumed to be rock type 1 unless modified using this option.

Transmissibilities are calculated for block edges. The dimensions and conductivities of the two blocks on either side of the edge are used. The internal program units on transmissibility are (ft^3-cp/psi-day). Conversion from conductivity in ft/day is obtained as follows:

Let ρ_o, μ_o = density and viscosity of the resident fluid respectively (C=0) at TO (entered in READ R1-16).

A = block edge area

Δx = distance between the two block centers

$$\text{Transmissibility in } (ft^3\text{-cp/psi-day}) = \text{conductivity (ft/day)} \times \frac{\mu_o(cp)}{\rho_o(lb/ft^3)} \times \frac{A(ft^2)}{\Delta x(ft)} \times 143.8\left(\frac{lb}{psi\text{-}ft^2}\right)$$

The x transmissibility element (I, J, K) refers to transmissibility at the edge (I-1, J, K) and (I, J, K). Similarly the y transmissibility at (I, J, K) is at the (I, J-1, K) and (I, J, K).

FTX	If <u>positive</u> or zero, this is the factor by which the x direction transmissibilities within the defined region are to be multiplied. If <u>negative</u>, the absolute value of FTX will be used for the x direction transmissibilities within the region to be modified, replacing the values read earlier or determined from the permeability data read earlier.
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 volumes.
HADD	This is an increment that will be added to the depths within the defined region. A positive value repositions the cell deeper and a negative value brings it closer to the surface.
THADD	This is an increment that will be added to the thickness values within the defined region. A positive value makes the cell thicker and a negative value makes it thinner.

This data modification feature of the program provides the user with an easy way to build in reservoir heterogeneities or modify the reservoir description data during history matching. These modifications are applicable regardless of whether the data were read according to READ R1-20, R1-21 or R1-23.

The modifiers in LIST 2 above are independent in that a change effected by any one of them does not affect any of the other properties. For example, an FPV of 1.4 will increase pore volumes by 40%, but will not result in any changes in transmissibilities, depth or thickness.

The data modifications occur over rectangular regions areally as defined by the I1, I2, J1 and J2 limits. The vertical extent of the region is defined by K1 and K2. All six of these limits must be within the limits of the calculation grid. Successive regions may partially or entirely overlap other regions.

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.

A modification to the transmissibilities over the region (I1-I2, J1-J2, K1-K2) will not affect the transmissibilities between columns I2 and I2+1, between rows J2 and J2+1 or between layers K2 and K2+1.

READ R1-27 (2I5)

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

LIST: IAQ, PRTAB

IAQ	Control parameter for selecting the type of aquifer block representation.
	0- No aquifer influence blocks are to be used. Skip to READ I-1.
	1- A pot aquifer representation will be used.
	2- A steady state aquifer representation will be used.
	3- Use the Carter-Tracy representation.
	4- Constant pressure, temperature and inert component concentration 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 or bottom water drive without the expense that would be required to model the aquifer as part of the grid system.

READ R1-28 (LIST 1: 6I5; LIST 2: 4E10.0)

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

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

LIST 2: VAB, P1, T1, C1

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I1, I2	Lower and upper limits, inclusive, on the I-coordinate of the aquifer influx region.
J1, J2	Lower and upper limits, inclusive, on the J-coordinate of the region.
K1, K2	Lower and upper limits, inclusive, on the K-coordinate of the region.

For <u>IAQ=1 or 2</u> (READ R1-27)

VAB	Aquifer influence coefficient for each block within the region defined by I1, I2, etc. The units of VAB are ft^3/psi for a pot aquifer representation and ft^3/psi-day for a steady state representation.
P1, T1, C1	Not used.

For <u>IAQ=4</u> (READ R1-27)

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, T1, C1	Constant values of pressure (psi), temperature (°F) and concentration (fraction) at the block boundary specified according to VAB.

NOTE: <u>Follow the last VAB card of this data group by a blank card.</u>

The READ group consists of two cards or any number of sets of two cards, each set defining a rectangular region and the value of VAB to be assigned that region. Overlapping of regions is permissible. The order of the sets is immaterial except that any overlapping will result in the VAB of the last set read to be assigned to the overlapped subregion. If these data are read, i.e. IAQ≠3, then skip READ R1-29 through R1-32 and proceed to READ R1-33.

READ R1-29 (3I5)

NOTE: If IAQ is not equal to 3, omit these data and proceed to READ R1-33. This section is used to enter data for the Carter-Tracy method of calculating aquifer influence functions.

LIST: NCALC, NPT, PRTIF

NCALC	Control parameter for selecting how the Carter-Tracy aquifer coefficients are to be assigned. 0 - The Carter-Tracy aquifer coefficients (VAB) will be read in as input data. 1 - The VAB will be calculated by the program and assigned to each edge (perimeter) block in each areal plane, K=1, 2, . . . NZ. 2 - The VAB will be calculated by the program and assigned to each grid block in the last areal plane, K=NZ only.
NPT	Number of points in the influence function versus dimensionless time table, ($P(t_D)$ versus t_D). If NPT is zero, the program will select the Hurst-Van Everdingen infinite aquifer solution internally.
PRTIF	Print control key for the influence function table. 0 - Suppress printing. 1 - Print the table of $P(t_D)$ versus t_D.

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

NOTE: Enter these data only if NCALC is zero; otherwise, skip this READ and proceed to READ R1-31.

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

LIST 2: VAB

I1, I2	Lower and upper limits, inclusive, on the I-coordinate of the aquifer influence region.
J1, J2	Lower and upper limits, inclusive, on the J-coordinate of the region.
K1, K2	Lower and upper limits, inclusive, on the K-coordinate of the region.

VAB	Aquifer influence coefficient for each block within the region defined by I1, I2, etc. The aquifer influence coefficient VAB for the Carter-Tracy method is actually the fraction of the total aquifer-reservoir boundary that is represented by the length of any given grid block. For this reason it is possible to calculate the VAB from input data previously read in and the VAB does not have to be calculated externally.

NOTE: <u>Follow the last VAB card of this data group by a blank card</u>.

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

<u>READ R1-31</u> (4E10.0)

LIST: KH, PHIH, RAQ, THETAQ

KH	Conductivity-thickness for aquifer, ft^2/day. An average value of transmissivity along the edges should be used.
PHIH	Porosity-thickness for aquifer, ft.
RAQ	Equivalent aquifer radius, ft. The approximate method of Carter and Tracy is valid for circular aquifers. To retain the validity of usage of circular reservoir influence functions, the numerical grid system should be chosen as square as possible.
THETAQ	Angle of influence, degrees. This angle should indicate the portion of the aqu covered by the aquifer influence boundar If mass flow is permitted across all the boundaries, enter 360°.

<u>READ R1-32</u> (2F10.0)

NOTE: This data is entered if NPT is not equal to zero. If NPT is zero, the program will select the aquifer influence functions for an infinite aquifer and you do not have to read in the influence function data. Omit this READ and proceed to READ R1-33.

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

TD	Dimensionless time, $kt/\mu\phi c_T r_e^2$.
PTD	Terminal rate case influence function as given by Van Everdingen and Hurst.

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

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

LIST 2: FAB

NOTE: These data allow the user to modify the aquifer influx coefficient VAB by the relation

VAB(I,J,K) = VAB(I,J,K) x FAB

This is useful when a reservoir may experience no or limited water influx across one boundary. In this case, in the region where influx is limited, the FAB may be set to zero or a small number to reduce the VAB along the boundary.

I1, I2	Lower and upper limits, inclusive, on the I-coordinate of the VAB to be modified.
J1, J2	Similar definition for the J-coordinate.
K1, K2	Similar definition for the K-coordinate.
FAB	Factor by which the VAB will be modified in the region I=I1, I2, J=J1, J2 and K=K1, K2.

NOTE: Follow these data with one blank card. If no modifications are desired, one blank card is still required.

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 and there is no natural flow, insert a blank card and proceed to READ R2-1.

LIST: ICOMP, INAT, IRD

ICOMP	Control parameter for initializing inert component concentrations. 0 - Initial concentrations in all the grid blocks are zero. If you enter zero, skip READ I-2. 1 - The initial concentrations are not zero everywhere. Non-zero concentrations will be entered in READ I-2.
INAT	Control parameter for entering initial fluid velocity 0 - The aquifer fluid is static initially. If you enter zero, skip READ I-3. 1 - The resident fluid velocity will be entered in READ I-3.
IRD	Control parameter for initializing radioactive/trace components concentrations. 0 - Initial concentrations in all the grid blocks are zero. If you enter zero, skip READ I-4. 1 - Non-zero concentrations for each component will be entered in READ I-4.

<u>READ I-2</u> (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	Lower and upper limits, inclusive, on the J-coordinate of the non-zero concentration region.
K1, K2	Lower and upper limits, inclusive, on the K-coordinate of the non-zero concentration region.
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. You need to specify only the non-zero concentrations. Follow the last card with a blank card.

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READ I-3 (F10.0)

NOTE: If INAT=0, skip this card.

LIST: VEL

VEL	Initial velocity of the resident aquifer fluid in the x direction, ft/day. The initial velocities in the y and z directions are assumed to be zero. This option can be used only with a steady state aquifer influence function representation. Under this option, boundary pressures corresponding to the initial velocity are calculated and fixed at the boundaries during the run.

READ I-4 (See READ I-2)

NOTE: If IRD=0, skip this READ. Data input is identical to READ I-2. One complete set of input data is required for each component (total NCP).

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RECURRENT DATA

The data described previously are required to describe the aquifer and fluid properties and to establish initial conditions. These data are all read before the first time step and at subsequent time steps when you desire to change the well conditions, time step data or mapping specifications. Note that any of the data entered up to this point cannot be changed. The overburden and underburden blocks specifications or aquifer influence functions cannot be changed in any manner once they have been specified at the beginning.

<u>READ R2-1</u> (8I5)

LIST: INDQ, IWELL, IMETH, ITHRU, IRSS, 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. If you are entering data before the first time step (new run), and you enter IMETH=0, the program selects direct solution backward with time and space finite-difference approximations. The solution, under these conditions, is unconditionally stable. 1 - Read new or altered method of solution.
ITHRU	Run termination control. 0 - Run is to continue.

	1 - Run is to terminate at this point. No more recurrent data will be read after this card. If you do not desire any plots, i.e. NPLP, NPLT and NPLC are all zero, this should be the last card in your data deck.
IRSS	Control parameter for reading radioactive components source data. 0 - Do not read trace component source data. 1 - Read new or altered source data.
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 you desire the wellbore calculations 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.

<u>READ R2-2</u> (I5, F10.0)

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

LIST: METHOD, WTFAC

METHOD	Method of solution. If you enter zero, the program selects METHOD=1. You may select direct solution only if you specified direct solution 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 you enter WTFAC≤ 0, the program selects WTFAC=1.0.

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

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

LIST: NITQ, TOLX, TOLDP, DAMPX, E

NITQ	Maximum number of outer iterations in the wellbore calculations. For example, if the injection rate for a well is specified, the wellhead pressure is calculated iteratively to obtain the bottom-hole pressure necessary to inject the specified rate. If entered as zero or a negative number, the program selects the default value of 20.
TOLX	The tolerance on the fractional change in pressure over an iteration. If entered as zero or a negative number, the default value of 0.001 is selected.

TOLDP	The tolerance on pressure, psi. The default value is 1 psi.
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 this data only if INDQ is equal to one.

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

Q	Production rate, ft^3/day. If it is an injection well, enter the value as a negative production rate. You must enter all the well rates even if all of them have not changed.

READ R2-6 (I5, E10.0)

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

LIST: I, QWELL

I	Well number.
QWELL	Production rate, ft^3/day. Enter negative values for injection rates. You need to enter only the altered well rates.

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

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

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

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 bottom-hole or surface pressure. The lower of the specified and the calculated rate is allocated between layers on the basis of mobilities and the pressure drop between the wellbore and the grid block.

2, 3 - The rate is expressed explicitly [illegible] the aquifer model equations.

-2, -3 [illegible]ne rate is expressed in a semi-implicit manner in the aquifer model equations, e.g.

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

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LIST 2: WI, BHP, TINJ, CINJ

WI	Well index, ft^2/day. (See Section 3.1.2. of Ref. 7)
BHP	Bottom-hole pressure, psi. This must be specified if IINDW1=$\pm$ 3.
TINJ	Temperature of the injection fluid, °F. If surface conditions are being specified, it is the temperature at the surface.
CINJ	Contaminant concentration in the injection fluid, dimensionless.

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

NOTE: Skip this list if ISURF=0.

X	Pipe (wellbore) length to top of perforations, feet.
DW	Inside wellbore (pipe) diameter, feet.
ED	Pipe roughness (inside), ft. Enter zero if it is a smooth pipe.
OD	Outside wellbore (casing) diameter, ft.
TTOPW	Rock temperature surrounding the wellbore at the surface, °F.
TBOTW	Rock temperature surrounding the wellbore at the bottom-hole, °F.
UCOEF	Overall heat transfer coefficient between the inner surface of the pipe and outer surface of the casing, Btu/ft^2-°F-hr.
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. These should be in proportion to total productivity of individual layers, taking into account layer kh (absolute transmissivity x thickness) and layer formation damage or improvement (skin). Only the

relative values of these factors are important. For example, if layers 3 through 6 (IC1=3, IC2=6) are completed then KHL values of .5, 2, 2.5, .1 will give the same result as values of 5, 20, 25, 1. The absolute productivity (injectivity) of completion layer k is computed as

$$\mathrm{WI} \times \mathrm{KHL}(k+1-\mathrm{IC1}) / \sum_{\ell=1}^{\ell=\mathrm{IC2}-\mathrm{IC1}+1} \mathrm{KHL}_{\ell}$$

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. If ISURF is one, THP must be specified for the wells with well option IINDW1=±3. A production (or injection) rate is calculated from THP, and lower of the calculated and specified rate is used for allocation between layers.

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

READ R2-9 (I5)

LIST: NSS

NSS	Number of radioactive component sources/sinks.

READ R2-10 (LIST 1: 4I5; LIST 2: 8E10.0)

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.

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

QWW	Fluid discharge rate, lb/day. A negative rate implies a source and a positive a sink.
QHH	Heat discharge rate, Btu/day.
QCC	Components discharge rates, lb/day.

READ R2-11 (3I5)

NOTE: This data is entered if INDT is not zero. If you desire to use the default values for the data entered on this card, enter INDT as zero and skip this READ. However, if you desire to include the off-diagonal (or cross derivative) dispersion terms in the x-y plane (E_{xy} and E_{yx}), MINITN must be entered greater than or equal to 2. If MINITN is entered as one, or if the default value is used, an approximation is used to include the effect of the off-diagonal dispersion terms by enhancing the diagonal terms.

LIST: MINITN, MAXITN, IMPG

MINITN	Minimum number of outer iterations in the subroutine ITER (see Section 2.2 for explanation). The default values has been programmed as one.
MAXITN	Maximum number of outer iterations in the subroutine ITER. The default value is 5.
IMPG	Number of time steps after which the optimum parameters for the inner iterations are recalculated for the two line successive overrelaxation method. You do not have to enter this data if METHOD is not equal to ±2. The default value for IMPG is 5.

READ R2-12 (8E10.0)

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

TCHG	Time (days) 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.

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DT	Time step specification. If DT is positive it will be the time step (days) used from the current time to TCHG. If DT is zero, the program will select the time step automatically. DT must not be zero for the first time step of a run starting from zero time.
DCMX	Maximum trace component concentration change desired per time step. If a smaller limiting time step is calculated internally for a particular component, then specified as DT, then time step for solving finite-difference equation of that component is reduced. The solution over the specified time step is calculated in a number of steps using the same flow solution. The default value is 0.95.

NOTE The following five parameters are used only if the automatic time step feature is selected, i.e. DT=0.

DSMX	Maximum (over grid) concentration change desired per time step.
DPMX	Maximum (over grid) pressure change desired per time step, psi.
DTPMX	Maximum (over grid) temperature change desired per time step, °F.
DTMAX	Maximum time step allowed (days).
DTMIN	Minimum time step required (days).

If any of the five parameters above is entered as zero, the default value is used. These values are as follows:

DSMX=0.25
DPMX=50.0 psi
DTPMX=10.0°F
DTMAX=30.0 days
DTMIN=1.0 day

These parameters are used only if DT equals zero. The time step DT must not be read as zero for the first time step. If DT is read as zero, the program will automatically increase or decrease the time step size every time step to seek a value such that the maximum changes in the concentration, pressure and temperature are less than or equal to the specified values.

READ R2-13 (11I5)

LIST: IO1, IO2, IO3, IO4, IO5, IO8, RSTWR, MAP, KOUT, MDAT, IIPRT

The program prints five types of output at the end of each time step. The parameters IO1, IO2, IO3, IO4 and IO5 control the frequency of the outputs.

IO1	Control parameter for frequency of the time step summary output. The time step summary gives cumulative field injections and productions, material and heat balances, average aquifer pressure, cumulative heat loss to the overburden and the underburden, cumulative water, contaminant and heat influxes across the peripheral boundaries, and the maximum pressure, concentration and temperature changes in any block during the time step.
IO2	Control parameter for frequency of the well summary output. This summary gives water, heat and contaminant fluid production and injection rates, cumulative production and injection, wellhead and bottom-hole pressures, wellhead and bottom-hole temperatures and the grid block pressure in which the well is located. This summary also gives the total production and injection rates and cumulative production and injection.
IO3	Control parameter for listings of the grid block values of concentration, temperature and pressure.
IO4	Control parameter for injection/production rate in each layer for each well.
IO5	Control parameter for listings of the grid block values of trace component concentrations.

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

-1	Omit printing for all time steps from the current time through TCHG, inclusive.
0	Print at the end of each time step through to the step ending at TCHG.
1	Print only at time TCHG.

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n(>1)	Print at the end of every n^{th} time step and at the time TCHG.
IO8	Control parameter for listings of the grid block values of the dependent variables. The listings are printed according to the frequency specified (IO3). This parameter gives you the option for not printing the tables you do not desire. The parameter requires a three digit specification and the first digit refers to pressure, the second to temperature and the third to concentration. 0 - The grid block values will be printed. 1 - The grid block values (pressure at datum or temperature or concentration) will not be printed. 2 - Refers to the first digit only. Neither the absolute pressure nor the pressure at datum will be printed. e.g. If you desire only temperature grid block values, enter 201.
RSTWR	Restart record control parameter. 0 - No restart record will be written. 1 - Restart record will be written on Tape 8 at time TCHG.
MAP	Parameter for printing contour maps at time TCHG. Only two-dimensional maps are printed. The maps are printed for r-z coordinates in a radial system and x-y coordinates (areal maps) in a linear system. This parameter requires a three digit specification, the first digit referring to mapping pressures, the second for mapping temperatures and the third for concentrations. 0 - The variable will not be mapped. 1 - The variable will be mapped at TCHG. e.g. If you desire the contour maps for pressure and temperature only, enter 110.
KOUT	See READ M-3.
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.
IIPRT	Intermediate parameters printing index. Activated for <u>one</u> time step only. 0 - None of the following output will be activated. 1 - Darcy velocities will be printed. 2 - Flow, thermal dispersion and mass dispersion transmissibilities will be printed in addition to the velocities. 3 - Fluid density, viscosity, enthalpy and net dispersivities will be printed in addition to the quantities listed above.

<u>READ R2-14</u> (I5, 2F10.0)

NOTE: Enter this data only if you desire contour maps (MAP is not equal to 000), <u>and</u> 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) 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.

<u>READ R2-15</u> (6I5, 2F10.0)

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

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

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-coordinate 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 pressure (psi) used to obtain 20 contour maps. 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 maxima and use the value as AMAXP. If you enter AMINP as a large negative number (<-99.0), the program will search for a minima and use the value as AMINP.

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

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

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

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

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

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

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

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

NOTE: This data entered up to this point is sufficient to execute the program until time equal TCHG. The recurrent data is read again at that point. If you desire to terminate a run, enter ITHRU=1 (READ R2-1) after R2-17. If you desire any plots (if NPLP or NPLT or NPLC equals one), you should enter the plotting data (READ P-2 through P-4). If you do not desire any plots, ITHRU=1 will terminate execution at this point.

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PLOTTING DATA

The specifications for the plots and observed data are entered here. You may obtain plots even if you do not have any observed data available. Do not enter any plotting data if you do not desire any plots. Plots can be obtained for the values of the dependent variables in the well (at the wellhead and at the bottom-hole). The quantities plotted depend upon the "type" of the well. The quantities plotted for different wells are as follows:

Type of Well	Quantities Plotted
Observation well	Bottom-hole pressure, temperature and concentration
Injection well-bottom-hole conditions specified (ISURF=0)	Bottom-hole pressure
Injection well-surface conditions specified (ISURF=1)	Bottom-hole pressure and temperature, surface pressure
Production well-bottom-hole conditions specified	Bottom-hole pressure, temperature and concentration
Production well-surface conditions specified	Bottom-hole pressure, temperature and concentration, surface pressure and temperature

You should enter READ P-1 only if you are obtaining plots for a previous run. The plotting data for one well consists of the data from READ P-2 through P-4. Enter as many sets of these data as the wells for which you desire plots. If you desire plots for all the wells, enter NWT sets of these data. If you enter less than NWT sets, follow these cards with a blank card.

READ P-1 (I5)

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

LIST: NWT

NWT	Total number of wells.

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

LIST: KW, ID

KW	The well number.
ID	A title for the plots for well number KW.

READ P-3 (7F10.0)

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

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

TMN	Lower limit on time.
TMX	Upper limit on time.
DT	Time step for each row. For example, if TMN=5, TMX=15 and DT=0.5, the time coordinate axis will be 20 rows long.
PWMN, PSMN, TWMN, TSMN, CMN	Lower limits on bottom-hole pressure, surface pressure, bottom-hole temperature, surface temperature and concentration, respectively.
PWMX, PSMX, TWMX, TSMX, CMX	Upper limits on bottom-hole pressure, surface pressure, bottom-hole temperature, surface temperature and concentration, respectively.

READ P-4 (6F10.0)

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

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

TOX	Observation time.
POW	Bottom-hole pressure.
POS	Surface pressure.
TOW	Bottom-hole temperature.

TOS	Surface temperature.
COS	Concentration.

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

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.

READ M-7 (I5)

LIST: MAP

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

READ R2-15 to R2-17 Map Specifications

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

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4.4 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 exceed the dimensions, you must redimension the array. This requires recompiling the program. The user is referred to Section 2.4 (Ref. 7) for redimensioning 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 55 represent the following errors:

(1) This error refers to READ M-3.
NX is less than or equal to one or
NY is less than one or
NZ is less than one.
The minimum dimensions on the grid block system are 2x1x1. The maximum size is limited only by the available computer storage.

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

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

(5) This error refers to READ R1-3.
Either one or both the fluid densities (BWRN and BWRI) is zero or negative.

(6) This error refers to READ R1-7 through R1-10.
One or more of the viscosity values is entered as zero or negative.

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

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

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

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

(11) This error refers to READ R1-17 through R1-19. One or more of grid block sizes (DELX, DELY, DELX) are zero or negative.

(12) This error refers to aquifer properties for a homogeneous aquifer (READ R1-20).
One or more of KX, KY and KZ is negative or
PHI is less than 0.001 or greater than 1.0 or
SINX or SINY is less than -1 or greater than +1.

(13) This error refers to heterogeneous aquifer data, READ R1-21.
I is greater than NX or
J is less than 1 or greater than NY or
K is less than 1 or greater than NZ or
KX or KY or KZ is negative or
PHI is less than 0.001 or greater than 1.0.

(14) This error refers to READ R1-22.
The first grid block center (R1) is less than or equal to the well radius (RWW) or R1 is greater than or equal to the aquifer boundary radius (RE).

(15) This error refers to READ R1-23.
The layer thickness (DELZ) is less than or equal to zero or
KYY or KZZ is negative or
porosity (PORO3) is less than 0.001 or greater than 1.0.

(16) This error refers to READ R1-24 and R1-25. The sum of NXR's is greater than NX or one or more of RER's is greater than RE.

(17) This error refers to aquifer description modifications, READ R1-26.
One or more of I1, I2, J1, J2, K1, K2 are out of permissible ranges 1-NX, 1-NY and 1-NZ respectively, or
I1 is greater than I2 or
J1 is greater than J2 or
K1 is greater than K2.

(18) This error refers to READ R1-27 and R1-28.
IAQ is greater than 3 or
one or more of I1, I2, J1, J2, K1, K2 are out of permissible ranges 1-NX, 1-NY and 1-NZ respectively or
I1 is greater than I2 or
J1 is greater than J2 or
K1 is greater than K2.

(19) The number of aquifer influence blocks (NABL) are greater than NABLMX specified in READ M-3.

(21) This error refers to READ I-2.
One or more of I1, I2, J1, J2, K1, K2 are out of permissible ranges 1-NX, 1-NY and 1-NZ respectively, or
I1 is greater than I2 or
J1 is greater than J2 or
K1 is greater than K2 or
CINIT is negative.

(22) This error refers to READ I-4.
The description is the same as error 21 for radioactive/trace components.

(23) Some grid block pore volume is non-zero and sum of transmissibilities is zero.

(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 I-NZ or
IIC1 is greater than IIC2 or
the top block of the completion interval (K=IIC1) is a zero pore volume block.

(30) The entered value of IINDW1 is not permissible.
The permissible values are +1, ±2 and ±3.

(32) A well index of zero is permissible only if IINDW1 is equal to one. This error occurs if IINDW1 is not equal to one and WI is zero or negative.

(33) IINDW1 is ±3 and BHP is 0. The specified value of the bottom-hole pressure is a limiting value of the well pressure if IINDW1 is ±3.

(35) All completion layers of a well are in zero pore volume blocks.

(37) One or more of KHL values are negative.

(38) All KHL values are zero for some well. At least one KHL value must be non-zero.

(39) A well number I is negative or exceeds NWT.

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

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

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

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

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

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

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

(45) DTMAX is less than DTMIN.

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

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

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

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

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

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

Error numbers 51 through 54 refer to READ group R0.

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

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

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

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

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4.5 AUXILIARY DISC FILES

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

If the number of components are greater than 4, two disc files (unit 2 and 3) are used for concentration storage. 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 <u>two</u> 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 is written on unit 12. If plots are desired, at the end of the run unit 12 is rewound, plotting data is read in and plots printed. 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 <u>read</u> from unit 4.
5	Card reader
6	Line printer
8	Restart records are <u>written</u> on this unit.
12	Plotting data is written on this unit.

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5.0 PRELIMINARY RESULTS AND VALIDATION

5.1 COMPARISON WITH ORIGEN MODEL RESULTS

The ORIGEN model is an analytical solution of radioactive nuclides decay equations using a batch reactor concept. No flow or diffusion is permitted. The computer code was written at Oak Ridge National Laboratories (Ref 10). The INTERA radioactive waste migration model was run under similar conditions. The objectives of this comparison were:

(i) To evaluate the effect of numerical truncation errors arising due to isotope decay terms.

(ii) To develop a set of criteria to delete components in numerical simulations without losing any accuracy in the results.

It is important that conclusions derived from such comparisons be fairly general. Model comparisons for two chains were made. The two matches were very similar. However, results for only one chain are included in this report. The chain described here is a relatively long chain (23 components) with significant contrasts in half-lives (10^{-12} to 10^{9} years). The decay chain was CF250 → PB206. All the isotopes and their half-lives are listed in Table II. This is a real chain and major components are present in high level radioactive waste. The other chain was a 19 component decay chain.

The INTERA model runs were made using a two block numerical grid system with zero permeability and dispersivity. The initial amounts present were the same as had been used in the ORIGEN model. The ORIGEN model runs were supplied to us by Sandia. The model calculations were done for a period of 100,000 years. The results are plotted in Figure 5. The match is considered to be excellent.

The criteria derived from the above comparison are as follows:

(1) Delete a component i for which the two conditions listed below are satisfied -

(a) the product of time of interest (t) and rate constant k_i are greater than or equal to 10; i.e.

$$k_i t > 10$$

TABLE II - Decay chain used for ORIGEN and INTERA Model comparisons.

ISOTOPE	HALF-LIFE YEARS	PARENT COMPONENT	FRACTION	INITIAL AMOUNT PRESENT ,g.
CF250	13.08	-	-	1.50×10^{-4}
CM246	4.711×10^{3}	CF250	0.9921	101.0
AM242M	152.0	-	-	319.0
AM242	1.825×10^{-3}	AM242M	1.0	3.83×10^{-3}
CM242	0.446	AM242	0.82	0.784
PU242	3.79×10^{5}	CM246 AM242	0.9997 0.18	6.15×10^{4}
PU238	89.0	CM242	1.0	1.26×10^{4}
U238	4.51×10^{9}	PU242	1.0	5.73×10^{7}
TH234	0.066	U238	1.0	8.32×10^{-4}
PA234M	2.22×10^{-6}	TH234	1.0	1.93×10^{-8}
PA234	7.70×10^{-4}	PA234M	0.001	6.69×10^{-6}
U234	2.47×10^{5}	PA234M PU234 PU238	0.999 1.0 -	1.02×10^{4}
TH230	8.00×10^{4}	U234	1.0	0.405
RA226	1.60×10^{3}	TH230	1.0	2.94×10^{-5}
RN222	0.010	RA226	1.0	0.
PO218	5.80×10^{-6}	RN222	1.0	0.
PB214	5.10×10^{-5}	PO218	1.0	0.
BI214	3.75×10^{-5}	PB214	1.0	0.
PO214	6.34×10^{-12}	BI214	1.0	0.
PB210	21.0	PO214	1.0	6.49×10^{-8}
BI210	0.014	PB210	1.0	2.94×10^{-11}
PO210	0.038	BI210	1.0	7.39×10^{-10}
PB206	Stable	PO210	1.0	0.

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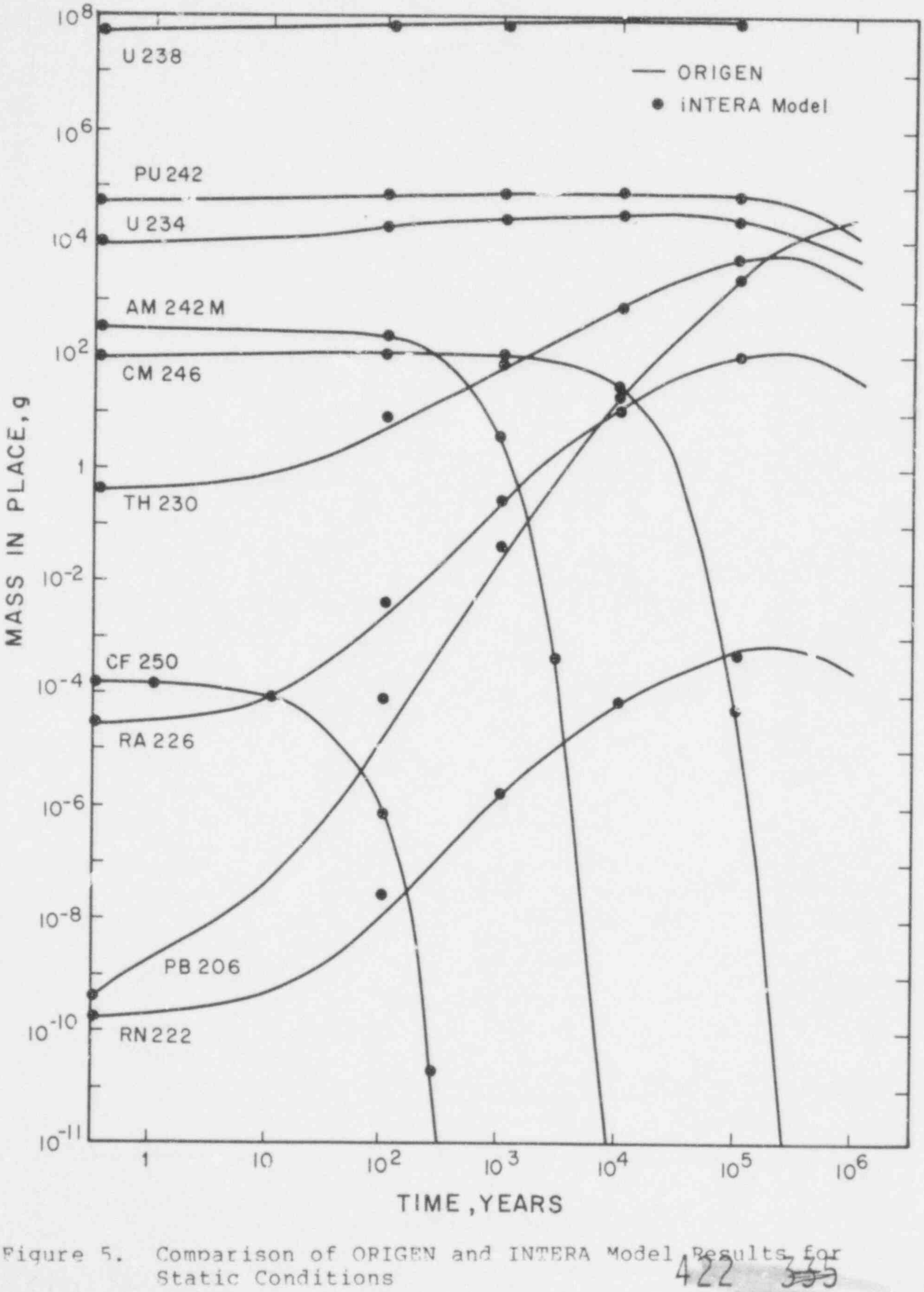

Figure 5. Comparison of ORIGEN and INTERA Model Results for Static Conditions

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(b) the parent component (i-1) has a much smaller decay rate (or larger half-life) than component i,

$$\frac{\tau_{i-1}}{\tau_i} > 100$$

Under these conditions, all of component i present initially has virtually decayed and the amount present at any time is controlled by its parent component.

If component i is deleted from the chain, then

(a) the amount of component i present initially should be transferred to its daughter component accounting for the potential mass change during the decay step.

(b) calculate the amount of component i present at time level n+1 from the amount of i-1 at time level n+1 and amount of i at time level n.

$$C_i^{n+1} = \frac{\tau_i}{\tau_{i-1}} C_{i-1}^{n+1} + C_i^n e^{-k_i \Delta t} \qquad (5-1)$$

If $k_i \Delta t > 10$, this reduces to

$$C_i^{n+1} = \frac{\tau_i}{\tau_{i-1}} C_i^{n+1} \qquad (5-2)$$

(2) For any component i which has no parent component, exact solution under static conditions can be obtained from the finite difference equations by modifying the decay constant as follows:

$$k_i = \frac{e^{k_i \Delta\tau} - 1}{\Delta\tau} \qquad (5-3)$$

(3) For any component i with parent component i-1 having a much larger half life than component i, i.e.:

$$\frac{\tau_i}{\tau_{i-1}} < 100$$

the rate constant should be modified according to Eq. (5-3).

(4) For every component i which is included in the numerical modeling and its rate constant k_i has <u>not</u> been modified, the time step must be limited such that

$$\frac{\Delta t}{\tau_i} < \frac{1}{7}$$

5.2 THERMAL EFFECTS

This model was developed to calculate movement of radioisotopes from a nuclear waste repository. The radioisotopes would move away from a repository only if a water contact with an aquifer is established. There are several ways in which this could occur. In this work we have studied direction and extent of thermal gradients created in the repository by heat generation from the radioactive waste. Thermal stresses can potentially fracture rock media resulting in flow through the repository.

A hypothetical repository site is selected in this work to make heat calculations using the INTERA model. Though the site is entirely hypothetical, its dimensions and properties are realistic. A cross-section of the complete aquifer system is shown in Figure 6. The region modeled here is boxed in. The recharge area is the upstream part of the aquifer and the discharge is into the river downstream. The entire valley cross-section was modeled by the Albuquerque District Office of the U.S. Geological Survey, Water Resources Division using a finite difference flow model. Potentials calculated by this model at the upstream INTERA grid boundary were used as boundary conditions in this work. The aquifer and fluid properties used are listed in Table III.

A total of 790 blocks were used in the numerical model runs. The horizontal distance of 155,000 feet was described by 79 blocks and 10 blocks were used in the vertical direction to describe the 2400 feet thick aquifer region. The grid blocks were smallest at the repository and increased in size away from it. Four horizontal blocks and one vertical block describe the actual repository.

Two kinds of runs were made - conduction only and including convection. The comparison of the two permits one to isolate the effect of convection. The heat input to the aquifer in both the cases was maintained at the same level and was equal in all four repository blocks. As the waste decays with time, generated heat decreases accordingly. The heat input rate was supplied by Sandia and is shown in Figure 7.

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Table III Aquifer and Fluid Properties Used for the Hypothetical Heat Simulation Runs

Hydraulic conductivity, ft/day

	Strata			
	Upper Sandstone	Shale	Salt	Lower Sandstone
Horizontal	50	10^{-2}	10^{-5}	40
Vertical	1.4	10^{-3}	10^{-6}	7
Porosity, fractional	0.3	0.3	0.03	0.3

Thermal conductivity of the porous media, Btu/ft - day - °F	
Horizontal	58.05
Vertical	49.34
Heat capacity	
Solid rock, Btu/ft^3-°F	28.0
Fluid, Btu/ft - °F	1.0
Hydrodynamic dispersity factor, ft	
Longitudinal	500
Transverse	50
Compressibility	
Rock, (pore vol)/ (Pore vol). psi	3×10^{-6}
Fluid, 1/psi	3.2×10^{-6}
Coefficient of thermal expansion of fluid, 1/°F	2.9 10^{-6}
Fluid density, lb /ft^3	73.98

Fluid viscosity	Temperature, °F	Viscosity, °F
	59	1.138
	104	0.6531
	149	0.4342
	194	0.3156

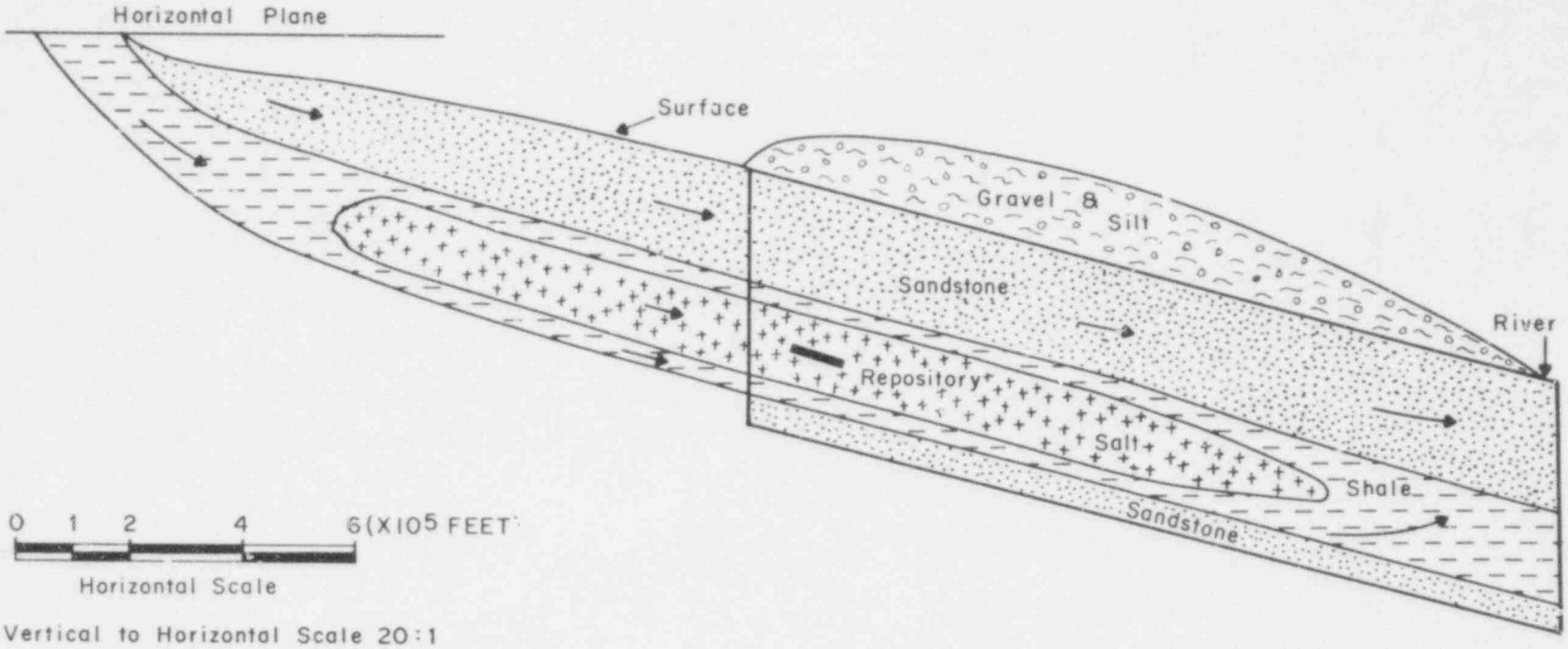

Figure 6. Cross-Section of the Aquifer System Modeled for Studying Thermal Effects

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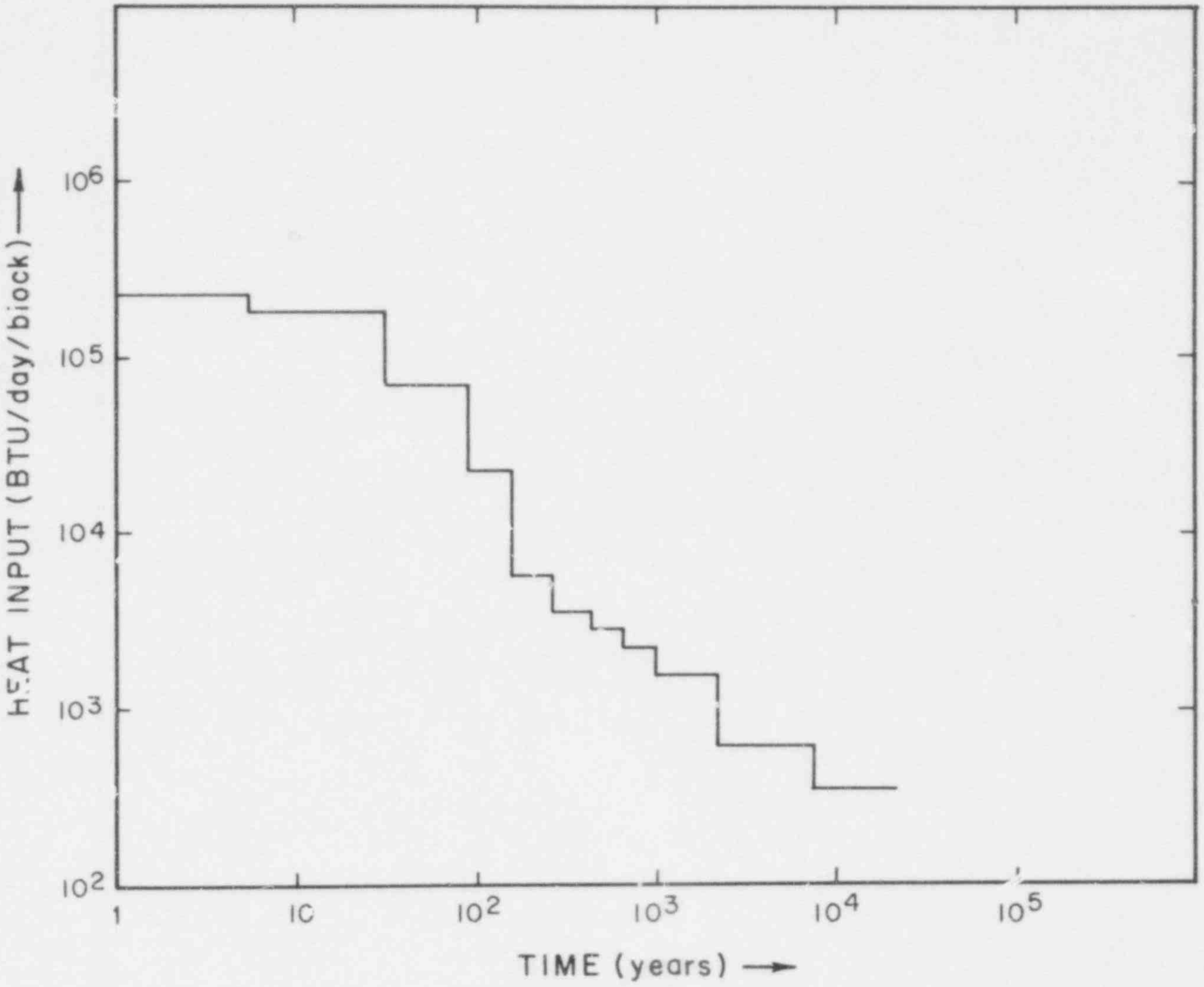

Figure 7. Heat Input Rate Used in Each Repository Block

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The conduction only run was made by no recharge or discharge into or from the aquifer and the coefficient of thermal expansion of the aquifer fluid was set to zero. This way, there is no forced or natural convection present in the aquifer. Heat is conducted through rock and fluid. The run with convection was made by using constant potential boundary conditions in all the blocks at the recharge end, and the uppermost block (representing the river) at the discharge end. The flow solution was run to steady-state before heat was introduced. Both the cases were run to 20,000 years.

Up to about 75 years, both results were very similar except that slightly higher temperatures were reached in the repository with the purely conductive mode. Since flow through the repository is of very small magnitude, the convection effect is small. The maximum temperature in the repository goes up to roughly 240°F at about 30 years. After 75 years, the differences in the two runs are very obvious and rather dramatic. This is illustrated by temperature contours maps at 600 years shown in Figures 8 and 9. The maps show only a part of the aquifer system - only 1 upstream blocks are shown here. These maps clearly indicate the effects of energy transfer by fluid convection. The differences in the two temperature profiles can be listed as follows:

(i) The temperature in the repository for the conduction only case is greater than 105°F, whereas with convection, it is less than 87.5°F.

(ii) Aquifer temperature in the upper aquifer is higher than 72.5°F without convection. When convection is included, this temperature is unchanged from the initial 68°F. A relatively high water flow rate through this aquifer carries away all the energy reaching the aquifer from the repository. The 70° contour is not symmetric and is somewhat extended towards the direction of the flow.

(iii) Aquifer temperature in the lower aquifer is also significantly higher in the conduction only case. The temperature profile is again non-symmetric. Temperatures in the lower aquifer (with convection included) are higher than in the upper aquifer. This shows that the flow rate is lower through the lower aquifer.

Eventually all the heat generated in the repository is transferred away in both the cases. A higher temperature is created with conduction only to achieve the same rate. The results demonstrate how the model can be effectively used to study the effect of various parameters in radionuclide migration calculations.

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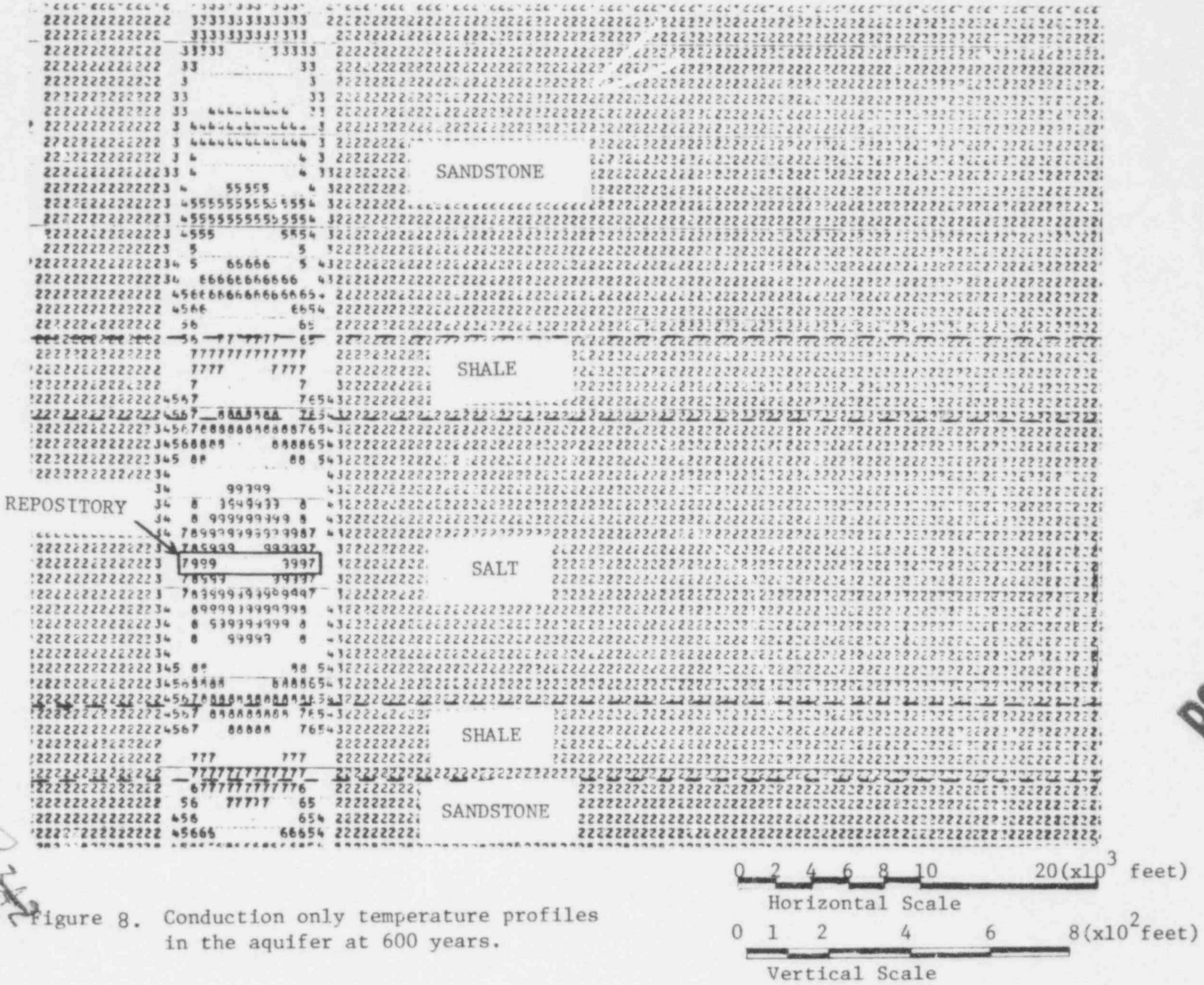

Figure 8. Conduction only temperature profiles in the aquifer at 600 years.

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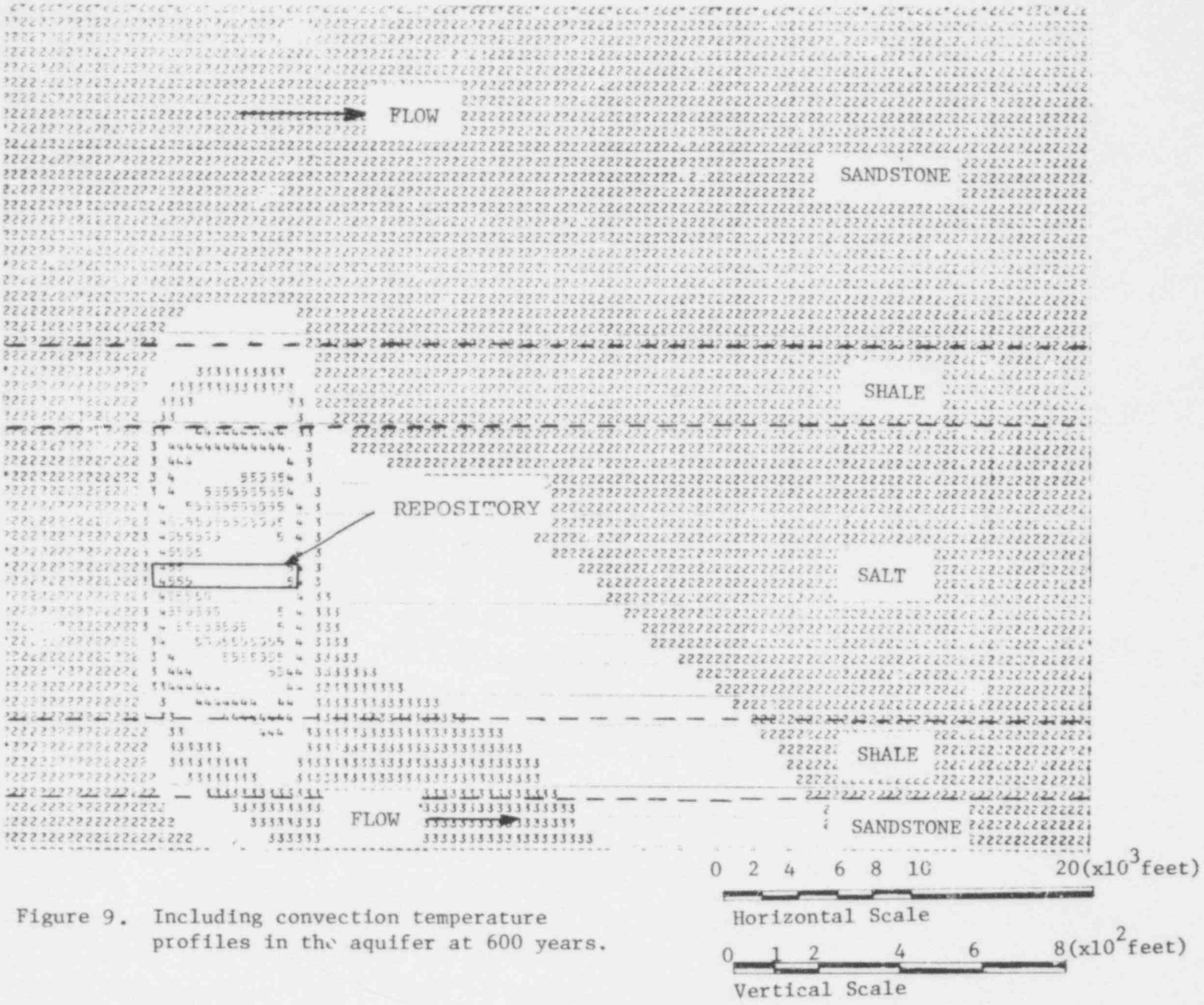

Figure 9. Including convection temperature profiles in the aquifer at 600 years.

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Table IV

MAP LEGEND FOR FIGURES 8 and 9

Temperature Range °F	Map Character
60.0 - 62.5	
62.5 - 65.0	1
65.0 - 67.5	
67.5 - 70.0	2
70.0 - 72.5	
72.5 - 75.0	3
75.0 - 77.5	
77.5 - 80.0	4
80.0 - 82.5	
82.5 - 85.0	5
85.0 - 87.5	
87.5 - 90.0	6
90.0 - 92.5	
92.5 - 95.0	7
95.0 - 97.5	
97.5 -100.0	8
100.0 -102.5	
102.5 -105.0	9
105.0 -107.5	
107.5 -110.0	0

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6.0 SUMMARY AND CONCLUSIONS

The radioisotope transport model, whose documentation was presented in the previous section, represents a very thorough treatment of the transport of radioisotopes by ground water through the geosphere. In fact, concern has been expressed that it is too comprehensive and thus puts too great a burden on user understanding. There is an element of truth in this observation but knowledge of the capabilities and limitations is a natural requirement accompanying any new tool. This particular model is not believed to be either absolutely complete nor even the best possible representation of the processes involved. It is, on the other hand, felt that it does represent a step forward in the ability to predict in this relatively unstudied area.

In addition to the studies referred to, a number of ground water analyses are discussed in Rodda (Ref. 12). A more recent study is that of Cooley (Ref. 13) using a different method of solution of the relevant equations. An indication of the state of the art and some of the difficulties being encountered is provided by the volume edited by Saleem (Ref. 14). There are some problems reconciling laboratory data with field experience as demonstratated by Wood (Ref. 15). On the other hand, there have been very successful commercial applications of models very similar to the one reported here, for example Nolen et al (Ref. 16).

In using this radioisotopic transport model, it should be noted that it is a tool for numerically solving a set of equations. These equations were derived to describe a number of physical processes as described previously. It appears that the solution of the equations quite adequately describes the ground water flow processes within the limits of present knowledge. The new addition to the model is the incorporation of the radioactive decay process and the ion exchange process as described by adsorption distribution coefficients. The first is generally held to be quite well understood while very limited data (and much less consistent) is available for the adsorption process. These concepts were presented and discussed at the 1977 Annual Meeting of the Geological Society of America (Ref. 17).

SWIP has been compared with a number of other programs and analytical solutions of the radioactive decay process in a static environment. The results agree very well. It still remains to establish any but theoretical validation for a dynamic flow adsorption situation. This will be one of the continuing activities necessary in this modeling effort.

In addition, it should be noted that SWIP does not contain any reactive chemistry. In addition, it should be noted that SWIP does not contain any reactive chemistry other than that which is associated with radioactive decay and the adsorption-desorption process. That associated with radioactive decay is simply that described by the decay equations as described on page . The geochemistry is simplified by assuming constant K_d's for each rock type although K_d's are permitted to vary, as functions of rock type.

The model does not contain any chemical interaction involving ionic states of the isotope involved or the solubility. The K_d's are not functions of salinity or the presence of other isotopes in the system.

There is a considerable body of evidence that indicates that adsorption distribution coefficients vary by many orders of magnitude with the chemical environment. This aspect of the simulation is not addressed at all in the present simulation. In fact, there may not be sufficient information about those phenomena to reasonably incorporate such a simulation at the present time.

Subject to the above limitations (and perhaps others) SWIP seems to do what it was intended to do very well, given that the user is careful about possible numerical and hydrogeologic difficulties. These limitations have been evaluated by Lantz (Ref. 18) and are explicitly described in the documentation. Here, documentation means not simply that supplied in the preceding section but especially that of the original survey model, SWIP (Ref. 8). In that document, the limits described in Part 1, paragraphs 3 and 5, and in Part 2, paragraph 3, should be considered. In addition to these numerical-hydrogeologic criteria, those dealing with decay chains should be noted. These are discussed in Section 5.1. Unfortunately, these criteria require that the user have some background in mathematics, geology and physics.

For the convenience of the user, an Appendix to this report has been included. The Appendix lists the data input forms both in the order in which they may be input and also alphabetically in terms of the input variables.

6.1 Proposed Future Activities

In support of the NRC methodology program, continuing effort has been and is being expended in the area of geosphere transport. This effort has included both model application and development.

In the area of model application, the planned activities included calculations to better understand depository properties. A number of one, two, and three dimensional calculations were planned to this end. In addition, some calculations were to be performed to better understand the flow fields in the vicinity of depositories. Associated with the above was an analyses of the sensitivity of transport results to geological and hydrological properties.

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With respect to model developing, the incorporation of a continuous leach model was planned. Further, in view of the work of Tamura (Ref. 19), the effect of salinity on adsorption distribution coefficients is to be examined. Also, in view of the recent report of Means et al (Ref. 20), there appears to be a similar serious problem with organic material.

6.2 Conclusions

The radioisotopic transport model presented here is believed to be almost as advanced as the supporting technology will permit. With the exception of the dynamic transport of radioisotopes with adsorption it has been validated in a number of ways. Furthermore, the equations that are being solved are generally accepted as being an accurate representation of the phenomena being described. It is understood that the USGS intends to attempt indirect validation under flow through the examination of natural aquifers which contain isotopic disequilibria.

This model was the most advanced of three considered by EPA as being applicable to the analysis of nuclear waste disposal facilities (Ref. 21). EPA contracted the Holcomb Research Institute of Butler University, Indiana, to assess the present status of international numerical models. Of the 250 models categorized, the model described in this report was the only one with radioactive decay, adsorption in addition to concentration, temperature dependent density and viscosity and including pressure effects on enthalpy. (Ref. 22).

7.0 NOMENCLATURE

C - concentration of the radioactive/trace component in fluid phase

$\hat{C}$ - concentration of the inert contaminant

C_S - concentration of the radioactive/trace component in adsorbed state

$\underline{\underline{E}}$ - dispersivity tensor (hydrodynamic + molecular)

g - acceleration due to gravity

H - fluid enthalpy

$\underline{\underline{k}}$ - permeability tensor

k - rate of decay

K - equilibrium adsorption constant

K_d - adsorption distribution constant

ℓ - distance between adjacent grid block centers

p - pressure

q' - fluid source rate (withdrawal)

q_L - rate of heat loss

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q_H - rate of energy withdrawal

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t - time

T - temperature

T - transmissibility

$\underline{u}$ - velocity vector

U - internal energy

V - grid block pore volume

Z - height above a reference plane

Greek Letters

ϕ - porosity

μ - viscosity

ρ - fluid density

ρ_S - formation density

ρ_B - bulk density of rock and fluid

τ - radioactive decay half life

Subscripts

c - component (mass)

H - heat (energy)

R - rock (formation)

w - water (fluid)

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9.0 References

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9.0 APPENDIX

In exercising SWIFT, it is sometimes difficult to locate the controlling variables. This leads to much thumbing through the documentation. In an effort to assist the user, the following two tables are provided.

In each table, the first column lists the program variables, the second column lists variables associated with the first. The third column is the page number in the original INTERA document. Finally, the fourth column is the number of the card as mentioned in the documentation.

The first table lists the data variables in order in which they are encountered in setting up a problem. The second table lists the same information alphabetically by program variable. Thus, one can easily determine the page and card number from the variable name. Subscripts of subscripted variables were included.

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TABLE 1

Variables of Data Input Forms in Order of Documentation

Variable	Dependence	Page #	Card #
TITLE		4-6	M-1
NCALL		4-6	M-2
RSTRT		4-6	M-2
ISURF		4-6	M-2
IIPRT		4-6	M-2
NPLP		4-6	M-2
NPLT		4-[illegible]	M-2
NPLC		[illegible]	M-2
NX		4-8	M-3
NY		4-8	M-3
NZ		4-8	M-3
HTG		4-8	M-3
NCP		4-8	M-3
KOUT		4-8	M-3
PRT		4-8	M-3
NSMAX		4-8	M-3
NABLMX		4-8	M-3
MASS(I)		4-10	R0-0-1
DI		4-10	R0-0-1
I		4-10	R0-0-1
NP		4-10	R0-0-1
LADJ		4-10	R0-0-1
DEC		4-10	R0-0-1
BROCK		4-13	R0-0-2
PBWR		4-13	R0-0-2
TBWR		4-13	R0-0-2
BWRN		4-13	R0-0-2
BWRI		4-13	R0-0-2
NOUT	ISURF	4-13	R1-4
PBASE		4-13	R1-5
DELPW		4-13	R1-5
TDIS		4-14	R1-5
NCV		4-14	R1-6
NTVR		4-14	R1-6
NTVI		4-14	R1-6
NDT		4-14	R1-6
TRR		4-15	R1-7
VISRR		4-15	R1-7
TIR		4-15	R1-7
VISIR		4-15	R1-7
SC(I)	NCV	4-15	R1-8
VCC(I)	NCV	4-15	R1-8
TR(I)	NTVR	4-15	R1-9
VISR(I)	NTVR	4-15	R1-9
T[illegible]I)	NTVI	4-15	R1-10
VISI(I)	NTVI	4-15	R1-10
ZT(I)		4-16	R1-11
TD(I)		4-16	R1-11
NDT		4-16	R1-11
NZOB		4-16	R1-12
NZUB		4-16	R1-12
KOB		4-16	R1-13
CPOB		4-16	R1-13
KUB		4-16	R1-13
CPUB		4-16	R1-13
DZOB(K)	NZOB	4-16	R1-14

Variable	Dependence	Page #	Card #
DZUB(K)	NZUB	4-17	R1-15
T0		4-17	R1-16
PINIT		4-17	R1-16
HINIT		4-17	R1-16
HDATUM		4-17	R1-16
DELX(I)	HTG	4-17	R1-17
DELY(J)	HTG	4-17	R1-18
DELZ(K)	HTG	4-18	R1-19
KX	HTG	4-18	R1-20
KY	HTG	4-18	R1-20
KZ	HTG	4-18	R1-20
PHI	HTG	4-18	R1-20
SINX	HTG	4-18	R1-20
SINY	HTG	4-18	R1-20
DEPTH	HTG	4-18	R1-20
I[illegible]	HTG	4-19	R1-21
I2	HTG	4-19	R1-21
J1	HTG	4-19	R1-21
J2	HTG	4-19	R1-21
K1	HTG	4-19	R1-21
K2	HTG	4-19	R1-21
KX	HTG	4-19	R1-21
KY	HTG	4-19	R1-21
KZ	HTG	4-19	R1-21
PHI	HTG	4-19	R1-21
UH	HTG	4-19	R1-21
UTH	HTG	4-19	R1-21
UCPR	HTG	4-19	R1-21
RWW	HTG	4-20	R1-22
R1	HTG	4-20	R1-22
RE	HTG	4-20	R1-22
DEPTH	HTG	4-20	R1-22
DELZ(K)	NZ	4-20	R1-22
KYY(K)	NZ	4-20	R1-22
KZZ(K)	NZ	4-20	R1-22
POROS(K)	NZ	4-20	R1-22
CPR1(K)	NZ	4-20	R1-22
NXR(I)		4-20	R1-24
RER(I)	NXR(1)	4-21	R1-25
I1		4-21	R1-26
I2		4-21	R1-26
J1		4-21	R1-26
J2		4-21	R1-26
K1		4-21	R1-26
K2		4-21	R1-26
IRT		4-21	R1-26
FTX		4-21	R1-26
FTY		4-21	R1-26
FTZ		4-21	R1-26
FPV		4-21	R1-26
HADD	FPV	4-21	R1-26
THADD	FPV	4-21	R1-26
IAQ		4-24	R1-27
PRTAB		4-24	R1-27
I1	IAQ	4-24	R1-28
I2	IAG	4-24	R1-28

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TABLE 1 (continued)

Variable	Dependence	Page #	Card #
J1	IAQ	4-24	R1-28
J2	IAQ	4-24	R1-28
K1	IAQ	4-24	R1-28
K2	IAQ	4-24	R1-28
VAB	IAQ	4-24	R1-28
P1	IAQ	4-24	R1-28
T1	IAQ	4-24	R1-28
C1	IAQ	4-24	R1-28
NCALC	IAQ	4-26	R1-29
NPT	IAQ	4-26	R1-29
PRTIF	IAQ	4-26	R1-29
I1	NCALC	4-26	R1-30
I2	NCALC	4-26	R1-30
J1	NCALC	4-26	R1-30
J2	NCALC	4-26	R1-30
K1	NCALC	4-26	R1-30
K2	NCALC	4-26	R1-30
VAB	NCALC	4-26	R1-30
KH		4-27	R1-31
PHIH		4-27	R1-31
RAQ		4-27	R1-31
THETAQ		4-27	R1-31
TD	NPT	4-28	R1-32
PTD	NPT	4-28	R1-32
I1		4-28	R1-33
I2		4-28	R1-33
J1		4-28	R1-33
J2		4-28	R1-33
K1		4-28	R1-33
K2		4-28	R1-33
FAB		4-28	R1-33
ICOMP		4-28	I-1
INAT		4-28	I-1
IRD		4-28	I-1
I1	ICOMP	4-29	I-2
I2	ICOMP	4-29	I-2
J1	ICOMP	4-29	I-2
J2	ICOMP	4-29	I-2
K1	ICOMP	4-29	I-2
K2	ICOMP	4-29	I-2
CINIT	ICOMP	4-29	I-2
VEL	INAT	4-30	I-3
I1	IRD	4-30	I-4
I2	IRD	4-30	I-4
J1	IRD	4-30	I-4
J2	IRD	4-30	I-4
K1	IRD	4-30	I-4
K2	IRD	4-30	I-4
CINIT	IRD	4-30	I-4
INDQ		4-31	R2-1
IWELL		4-31	R2-1
IMETH		4-31	R2-1
ITHRU		4-31	R2-1
IRSS		4-31	R2-1
IPROD		4-31	R2-1
IOPT		4-31	R2-1
INDT		4-31	R2-1
METHOD	IMETH	4-32	R2-2
WTFAC	IMETH	4-32	R2-2
NITQ	IOPT	4-33	R2-3
TOLX	IOPT	4-33	R2-3

Variable	Dependence	Page #	Card #
TOLDP	IOPT	4-33	R2-3
DAMPX	IOPT	4-33	R2-3
EPS	IOPT	4-33	R2-3
NWT	INDQ	4-34	R2-4
Q(I)	INDQ	4-34	R2-5
I	INDQ	4-34	R2-6
QWELL	INDQ	4-34	R2-6
I	IWELL	4-35	R2-7
IIW	IWELL	4-35	R2-7
IJW	IWELL	4-35	R2-7
IIC1	IWELL	4-35	R2-7
IIC2	IWELL	4-35	R2-7
IINDW1	IWELL	4-35	R2-7
WI	IWELL	4-36	R2-7
BHP	IWELL	4-36	R2-7
TINJ	IWELL	4-36	R2-7
CINJ	IWELL	4-36	R2-7
X	IWELL	4-36	R2-7
DW	IWELL	4-36	R2-7
ED	IWELL	4-36	R2-7
OD	IWELL	4-36	R2-7
TTOPW	IWELL	4-36	R2-7
TBOTW	IWELL	4-36	R2-7
UCOEF	IWELL	4-36	R2-7
THETA	IWELL	4-36	R2-7
KHL(K)	IWELL	4-36	R2-7
THP(I)	IPROD	4-37	R2-8
NSS	IRSS	4-37	R2-9
I	IRSS	4-37	R2-10
IIS	IRSS	4-37	R2-10
IJS	IRSS	4-37	R2-10
IKS	IRSS	4-37	R2-10
QWW(I)		4-38	R2-10
QHH(I)		4-38	R2-10
QCC(I.J)		4-38	R2-10
MINITN	INDT	4-38	R2-11
MAXITN	INDT	4-38	R2-11
IMPG	INDT	4-38	R2-11
TCHG		4-38	R2-12
DT		4-38	R2-12
DCMX		4-38	R2-12
DSMX		4-38	R2-12
DPMX		4-38	R2-12
DTPMX		4-38	R2-12
DTMAX		4-38	R2-12
DTMIN		4-38	R2-12
I01		4-40	R2-13
I02		4-40	R2-13
I03		4-40	R2-13
I04		4-40	R2-13
I05		4-40	R2-13
I08		4-40	R2-13
RSTWR		4-40	R2-13
MAP		4-40	R2-13
KOUT		4-40	R2-13
MDAT		4-40	R2-13
IIPRT		4-40	R2-13
NORIEN	MAP	4-42	R2-14
XLGTH	MAP	4-42	R2-14
YLGTH	MAP	4-42	R2-14
IP1	MDAT	4-43	R2-15

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TABLE 1 (continued)

Variable	Dependenc	Page #	Card #
IP2	MDAT	4-43	R2-15
JP1	MDAT	4-43	R2-15
JP2	MDAT	4-43	R2-15
KP1	MDAT	4-43	R2-15
KP2	MDAT	4-43	R2-15
AMAXP	MDAT	4-43	R2-15
AMINP	MDAT	4-43	R2-15
IT1	MDAT	4-43	R2-16
IT2	MDAT	4-43	R2-16
JT1	MDAT	4-43	R2-16
JT2	MDAT	4-43	R2-16
KT1	MDAT	4-43	R2-16
KT2	MDAT	4-43	R2-16
AMAXT	MDAT	4-43	R2-16
AMINT	MDAT	4-43	R2-16
IK1	MDAT	4-43	R2-17
IK2	MDAT	4-43	R2-17
JK1	MDAT	4-43	R2-17
JK2	MDAT	4-43	R2-17
KK1	MDAT	4-43	R2-17
KK2	MDAT	4-43	R2-17
AMAXK	MDAT	4-43	R2-17
AMINK	MDAT	4-43	R2-17
NWT	NPLP	4-45	P-1
KW		4-46	P-2
ID		4-46	P-2
TMN		4-46	P-3
TMX		4-46	P-3
DT		4-46	P-3
PWMN		4-46	P-3
PWMX		4-46	P-3
PSMN		4-46	P-3
PSMX		4-46	P-3
TWMN		4-46	P-3
TWMX		4-46	P-3
TSMN		4-46	P-3
TSMX		4-46	P-3
CMN		4-46	P-3
CMX		4-46	P-3
TOX		4-46	P-4
POW		4-46	P-4
POS		4-46	P-4
TOW		4-46	P-4
TOS		4-46	P-4
COS		4-46	P-4
IMPT	RSTRT	4-47	M-6
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TABLE 2
Variable of Data Input Forms Alphabetized

Variable	Dependence	Page #	Card #
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AMINK	MDAT	4-43	R2-17
AMINP	MDAT	4-43	R2-15
AMINT	MDAT	4-43	R2-16
BHP	IWELL	4-36	R2-7
BROCK		4-13	R0-0-2
BWRI		4-13	R0-0-2
BWRN		4-13	R0-0-2
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CINIT	ICUMP	4-29	I-2
CINIT	IRD	4-30	I-4
CINJ	IWELL	4-36	R2-7
CMN		4-46	P-3
CMX		4-46	P-3
COS		4-46	P-4
CPOB		4-16	R1-13
CPR1(K)	NZ	4-20	R1-22
CPUB		4-16	R1-13
DAMPX	IOPT	4-33	R2-3
DCMX		4-38	R2-12
DEC		4-10	R0-0-1
DELPW		4-13	R1-5
DELX(I)	HTG	4-17	R1-17
DELY(J)	HTG	4-17	R1-18
DELZ(K)	HTG	4-18	R1-19
DELZ(K)	NZ	4-20	R1-22
DEPTH	HTG	4-18	R1-20
DEPTH	HTG	4-20	R1-22
DI		4-10	R0-0-1
DPMX		4-38	R2-12
DSMX		4-38	R2-12
DT		4-38	R2-12
DT		4-46	P-3
DTMAX		4-38	R2-12
DTMIN		4-38	R2-12
DTPMX		4-38	R2-12
DW	IWELL	4-36	R2-7
DZOB(K)	NZOB	4-16	R1-14
DZUB(K)	NZUB	4-17	R1-15
ED	IWELL	4-36	R2-7
EPS	IOPT	4-33	R2-3
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HADD	FPV	4-21	R1-26
HDATUM		4-17	R1-16
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HTG		4-8	M-3
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I	IWELL	4-35	R2-7
I	IRSS	4-37	R2-10
I1	HTG	4-19	R1-21
I1		4-21	R1-26
I1	IAQ	4-24	R1-28
I1	NCALC	4-26	R1-30
I1		4-28	R1-33
I1	ICOMP	4-29	I-2
I1	IRD	4-30	I-4
I2	HTG	4-19	R1-21
I2		4-21	R1-26
I2	IAQ	4-24	R1-28
I2	NCALC	4-26	R1-30
I2		4-28	R1-33
I2	ICOMP	4-29	I-2
I2	IRD	4-30	I-4
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IINDW1	IWELL	4-35	R2-7
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IIW	IWELL	4-35	R2-7
IJS	IRSS	4-37	R2-10
IJW	IWELL	4-35	R2-7
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IK2	MDAT	4-43	R2-17
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IMPT	RSTRT	4-47	M-6
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I02		4-40	R2-13
I03		4-40	R2-13
I04		4-40	R2-13
I05		4-40	R2-13
I08		4-40	R2-13
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IP1	MDAT	4-43	R2-15
IP2	MDAT	4-43	R2-15
IPROD		4-31	R2-1
IRD		4-28	I-1
IRSS		4-31	R2-1
IRT		4-21	R1-26
ISURF		4-6	M-1
IT1	MDAT	4-43	R2-16
IT2	MDAT	4-43	R2-16
ITHRU		4-31	R2-1
IWELL		4-31	R2-1
J1	HTG	4-19	R1-21
J1		4-21	R1-26
J1	IAQ	4-24	R1-28
J1	NCALC	4-26	R1-30
J1		4-28	R1-33
J1	ICOMP	4-29	I-2
J1	IRD	4-30	I-4
J2	HTG	4-19	R1-21
J2		4-21	R1-26
J2	IAQ	4-24	R1-28
J2	NCALC	4-26	R1-30

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Variable	Dependence	Page #	Card #
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J2	IRD	4-30	I-4
JK1	MDAT	4-43	R2-17
JK2	MDAT	4-43	R2-17
JP1	MDAT	4-43	R2-15
JP2	MDAT	4-43	R2-15
JT1	MDAT	4-43	R2-16
JT2	MDAT	4-43	R2-16
K1	HTG	4-19	R1-21
K1		4-21	R1-26
K1	IAQ	4-24	R1-28
K1	NCALC	4-26	R1-30
K1		4-28	R1-33
K1	ICOMP	4-29	I-2
K1	IRD	4-30	I-4
K2	HTG	4-19	R1-21
K2		4-21	R1-26
K2	IAQ	4-24	R1-28
K2	NCALC	4-26	R1-30
K2		4-28	R1-33
K2	ICOMP	4-29	I-2
K2	IRD	4-30	I-4
KH		4-27	R1-31
KHL(K)	IWELL	4-36	R2-7
KK1	MDAT	4-43	R2-17
KK2	MDAT	4-43	R2-17
KOB		4-16	R1-13
KOUT		4-8	M-3
KOUT		4-40	R2-13
KP1	MDAT	4-43	R2-15
KP2	MDAT	4-43	R2-15
KT1	MDAT	4-43	R2-16
KT2	MDAT	4-43	R2-16
KUB		4-16	R1-13
KW		4-46	P-2
KX	HTG	4-18	R1-20
KX	HTG	4-19	R1-21
KY	HTG	4-18	R1-20
KY	HTG	4-19	R1-21
KYY(K)	NZ	4-20	R1-22
KZ	HTG	4-18	R1-20
KZ	HTG	4-19	R1-21
KZZ(K)	NZ	4-20	R1-22
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MAXITN	INDT	4-38	R2-11
MDAT		4-40	R2-13
METHOD	IMETH	4-32	R2-2
MINITN	INDT	4-38	R2-11
NABLMX		4-8	M-3
NCALC	IAQ	4-26	R1-29
NCALL		4-6	M-1
NCP		4-8	M-3
NCV		4-14	R1-6
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NDT		4-16	R1-11
NITQ	IOPT	4-33	R2-3
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NPLP		4-6	M-1

Variable	Dependence	Page #	Card #
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NSS	IRSS	4-37	R2-9
NTVI		4-14	R1-6
NTVR		4-14	R1-6
NWT	INDQ	4-34	R2-4
NWT	NPLP	4-45	P-1
NX		4-8	M-3
NXR(I)		4-20	R1-24
NY		4-8	M-3
NZ		4-8	M-3
NZOB		4-16	R1-12
NZUB		4-16	R1-12
OD	IWELL	4-36	R2-7
P1	IAQ	4-24	R1-28
PBASE		4-13	R1-5
PBWR		4-13	R0-0-2
PHI	HTG	4-18	R1-20
PHI	HTG	4-19	R1-21
PHIH		4-27	R1-31
PINIT		4-17	R1-16
POROS(K)	NZ	4-20	R1-22
POS		4-46	P-4
POW		4-46	P-4
PRT		4-8	M-3
PRTAB		4-24	R1-27
PRTIF	IAQ	4-26	R1-29
PSMN		4-46	P-3
PSMX		4-46	P-3
PTD	NPT	4-28	R1-32
PWMN		4-46	P-3
PWMX		4-46	P-3
Q(I)	INDQ	4-34	R2-5
QCC(I.J)		4-38	R2-10
QHH(I)		4-38	R2-10
QWELL	INDQ	4-34	R2-6
QWW(I)		4-38	R2-10
R1	HTG	4-20	R1-22
RAQ		4-27	R1-31
RE	HTG	4-20	R1-22
RER(I)	NXR(1)	4-21	R1-25
RSTRT		4-6	M-1
RSTWR		4-40	R2-13
RWW	HTG	4-20	R1-22
SC(I)	NCV	4-15	R1-8
SINX	HTG	4-18	R1-20
SINY	HTG	4-18	R1-20
T1	IAQ	4-24	R1-28
[illegible]TW	IWELL	4-36	R2-7
TBWR		4-13	R0-0-2
TCHG		4-38	R2-12
TD	NPT	4-28	R1-32
TD(I)		4-16	R1-11
TDIS		4-14	R1-5
THADD	FPV	4-21	R1-26
THETA	IWELL	4-36	R2-7
THETAQ		4-27	R1-31
THP(I)	IPROD	4-37	R2-8
TI(I)	NTVI	4-15	R1-10
TINJ	IWELL	4-36	R2-7
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TITLE		4-6	M-1
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TOLX	IOPT	4-33	R2-3
TOS		4-46	P-4
TOW		4-46	P-4
TOX		4-46	P-4
TR(I)	NTVR	4-15	R1-9
TRR		4-15	R1-7
TSMN		4-46	P-3
TSMX		4-4	P-3
TTOPW	IWELL	4-36	R2-7
TWMN		4-46	P-3
TWMX		4-46	P-3
UCOE	IWELL	4-36	R2-7
UCPR	HTG	4-19	R1-21
UH	HTG	4-19	R1-21
UTH	HTG	4-19	R1-21
VAB	IAQ	4-24	R1-28
VAB	NCALC	4-26	R1-30
VCC(I)	NCV	4-15	R1-8
VEL	INAT	4-30	I-3
VISI(I)	NTVI	4-15	R1-10
VISIR		4-15	R1-7
VISR(I)	NTVR	4-15	R1-9
VISRR		4-15	R1-7
WI	IWELL	4-36	R2-7
WTFAC	IMETH	4-32	R2-2
X	IWELL	4-36	R2-7
XLGTH	MAP	4-42	R2-14
YLGTH	MAP	4-42	R2-14
ZT(I)		4-16	R1-11

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