REVISION OF THE DOCUMENTATION FOR A MODEL FOR CALCULATING EFFECTS OF LIQUID WASTE DISPOSAL IN DEEP SALINE AQUIFERS

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Details of additions and modifications to a computer code described in an earlier report entitled "A model for calculating effects of liquid waste disposal in deep saline aquifers," USGS WRI 76-61, NTIS-PB256 903/AS are documented. These additions and modifications include free water surface, vertical recharge, equilibrium controlled linear adsorption and a first order irreversible rate reaction. These, plus additional modifications, make this model more adaptable to general hydrologic problems and those involving waste disposal with simple chemical reactions.

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REVISION OF THE DOCUMENTATION FOR A MODEL FOR CALCULATING EFFECTS OF LIQUID WASTE DISPOSAL IN DEEP SALINE AQUIFERS

By INTERA Environmental Consultants, Inc.

U.S. Geological Survey

Water-Resources Investigations 79-96

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1.0 ABSTRACT

The model developed under this contract is a modified version of the deep well disposal model developed by INTERCOMP Resource Development and Engineering, Inc., for the U.S. Geological Survey (A model for calculating effects of liquid waste disposal in deep saline aquifers). The model is a finite-difference numerical solution of the partial differential equations describing

(1) single phase fluid flow in the aquifer,
(2) energy transport by convection and conduction, and
(3) contaminant transport dissolved in the fluid by convection and dispersion.

Both the energy and the contaminant transports include molecular diffusion and hydrodynamic dispersion.

The objective of the contract was to modify the original version of the model for more general applications. Some of the major features of the model are as follows:

(1) Fluid density is permitted to be a function of fluid pressure, temperature and contaminant concentration, the viscosity can be described as a function of pressure and temperature.

(2) Aquifer heterogeneities in hydrological properties can be described on a numerical grid block basis.

(3) Free water surface is permitted to exist in the aquifer for shallow ground water applications.

(4) Contaminant may adsorb on rock surface or decay according to a first order reaction. The adsorption is described by a linear adsorption isotherm function of rock type in the aquifer.

(5) The model is extremely flexible in providing a wide choice of boundary conditions. These include natural flow in the aquifer, aquifer influence functions around the perimeter of the grid in recognition that the gridded region does not have no-flow boundaries, heat losses into the overlying impermeable strata, and the wellbore heat and pressure drop calculations coupled to the aquifer flow equations.

(6) The model offers the option of selecting an iterative or direct solution technique, and selecting central or backward finite-difference approximations in both time and space.

(7) Virtually any aquifer shape can be modeled by proper grid block description in three dimensions. In addition, the model is fully transient.

The major limitation of the model arises using second-order correct (central-difference) finite-difference approximation in space. To avoid numerical oscillations in the solution, the user must restrict grid block and time step sizes depending upon the magnitude of the dispersivity.

2.0 INTRODUCTION

During the fiscal year 1974-1975, the U.S. Geological Survey awarded a contract to INTERCOMP Resource Development and Engineering, Inc., to develop a three-dimensional transient mathematical model which would accurately simulate the behavior of liquid waste injection into deep saline aquifers. The contract report and the model documentation are available from the National Technical Information Service (INTERCOMP Resource Development and Engineering, Inc., 1976). That development was performed by a former INTERCOMP subsidiary company, INTERA Environmental Consultants, Inc. The objective of this contract to INTERA was to revise the deep well disposal model to provide some additional capabilities such as use of the model for shallow ground water conditions, include adsorption and radioactive decay of contaminant on rock surface.

The basic model remains the same as developed under the previous contract. This model should be considered only as a revised version of the deep well disposal model. An understanding and proper use of this version will require this revision document as well as the original model development report and documentation.

Section 3 of this report describes the fluid flow system and the physical laws applicable to the transport of momentum, energy and mass within the system. It includes the development of mathematical equations from these laws, numerical approximations of the partial differential equations and basic assumptions contained in the revised version of the model.

Section 4 lists user options available and basic model limitations. Efficient use of the model requires an understanding of the manner in which the boundary conditions are handled. Proper simulation of the aquifer system includes selecting the appropriate sets of model options to describe the physical boundary conditions.

Section 5 is the basic program user documentation. Input data forms and the definitions of each of the variables are listed. User entered data errors that can be detected by the program are also listed in this section.

This report does not include detailed descriptions 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 instead to the original report (INTERCOMP Resource Development and Engineering, Inc., 1976) for a complete description of the above.

3.0 TECHNICAL APPROACH

The numerical model developed under the contract is a modified version of the deep well disposal model calculating transport of momentum, energy and a contaminant mass in a porous medium. The model consists basically of two parts: (1) a three-dimensional finite-difference aquifer model, and (2) a wellbore model relating surface pressure and enthalpy to aquifer pressure and enthalpy. The two models are coupled together, and are indistinguishable to the user.

The deep well disposal aquifer 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) conservations of total liquid mass;
(2) conservation of energy; and
(3) conservation of the mass of a specific contaminant dissolved in the waste injection fluid.

The first equation describes the three-dimensional Darcy flow of a single-phase liquid in a porous aquifer. The aquifer may be confined, or unconfined. A confined aquifer is bounded vertically by relatively impermeable rock. An unconfined aquifer implies presence of water table or free water surface in the aquifer. The density of the liquid phase can be a function of fluid pressure, temperature and contaminant concentration. The second equation describes the convection and dispersion of energy in a confined aquifer 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 a component in the aquifer system. The contaminating fluid may be of a different salinity, chemical composition or radioactivity.

The model offers the user flexibility to describe the aquifer system in a three-dimensional rectangular cartesian or a two-dimensional cylindrical grid system. The cylindrical coordinate system is well suited to single source interpretive or predictive calculations.

Basic assumptions contained in the aquifer model are:

(a) Fluid flow in the aquifer can be described by Darcy's law for flow through a porous medium.

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

(c) The waste or contaminating fluid is totally miscible with the in-place fluid.

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

(e) 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.

(f) Water table conditions in an unconfined aquifer can be approximated by no capillarity and no residual water saturation (specific retention).

(g) Contaminant reaction can be described by a first order reaction - similar to radioactive decay.

(h) Contaminant adsorption on rock surface can be described by linear adsorption isotherms.

(i) Aquifer properties vary with position-porosity, permeability, thickness, depth, specific heat and adsorption distribution coefficient.

(j) Boundary conditions allow natural water movement in the aquifer, vertical recharge in the uppermost layer; heat losses to the adjacent formations, and the location of injection, withdrawals and observation wells anywhere within the aquifer 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. 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.

3.1 Aquifer Model Equations

Let x,y,z be the coordinates in a Cartesian grid system, and let Z(x,y,z) be the depth of a point below a horizontal reference plane. The basic equation describing single-phase flow in a porous media results from a combination of the continuity equation

$$\underset{\text{Net Convection}}{\nabla \cdot \rho \underline{u}} \qquad \underset{\text{Source}}{q'} \qquad = \qquad \underset{\text{Accumulation}}{-\frac{\partial}{\partial t}(\phi \rho)} \qquad (3\text{-}1)$$

and Darcy's law in three dimensions.

$$\underline{u} \quad = \quad -\frac{k}{\mu} (\nabla p - \rho g \nabla Z). \qquad (3\text{-}2)$$

Variable definitions are given in the nomenclature.

Combining the two equations above, one obtains the basic flow equation

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

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

$$\nabla\cdot\left(\frac{\rho k}{\mu} H(\nabla p - \rho g\nabla Z)\right) + \nabla\cdot\underline{\underline{E}}_H\cdot\nabla T - q_L$$

Net energy convection — Conduction — Heat loss to surrounding strata

$$- q'H - q_H$$

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

$$= \frac{\partial}{\partial t}[\phi\rho U + (1-\phi)(\rho C_p)_R T] \qquad (3\text{-}4)$$

Accumulation

A material balance for the solute results in the concentration equation

$$\nabla\cdot[\rho C\frac{k}{\mu}(\nabla p - \rho g\nabla Z)] + \nabla\cdot\rho\underline{\underline{E}}_C\cdot\nabla C - q'C$$

Net convection — Dispersion — Sources

$$-\lambda\phi\rho K_e C = \frac{\partial}{\partial t}(\phi\rho K_e C) \qquad (3\text{-}5)$$

Reaction/decay — Accumulation

where $\phi\rho K_e C = \phi\rho C + (1-\phi)\rho_s C_s$ (3-6)

and makes the approximation

$$\frac{\partial}{\partial t}(\phi\rho K_e C) = \frac{\partial}{\partial t}(\phi\rho C) + \frac{\partial}{\partial t}[(1-\phi)\rho_s C_s] \quad (3-7)$$

The equilibrium adsorption coefficient K_e is defined as

$$K_e = 1 + \frac{\rho_B K_d}{\phi} \quad (3-8)$$

where ρ_B is the bulk density of the rock, and K_d is the adsorption distribution coefficient. The above derivation is analogous to that given by Grove (1977).

The system of equations 3, 4, and 5 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. These equations are coupled with each other through fluid property dependence. The set of partial differential equations is 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, and 5.

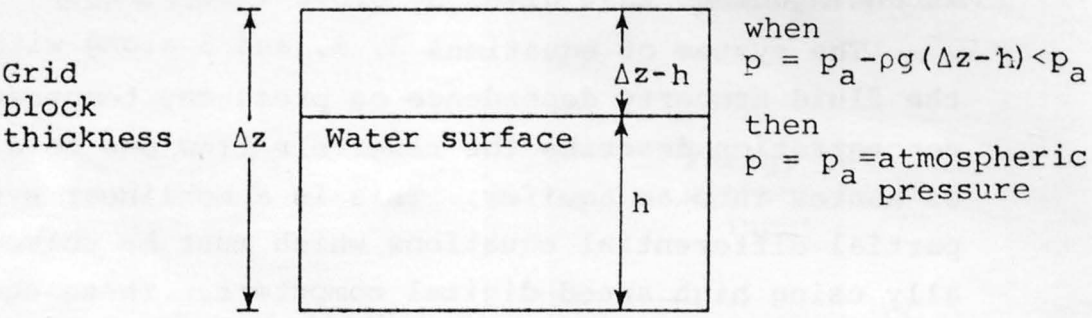
The finite-difference approximations of the above equations are shown in the original deep well disposal report. The only significant change is handling of the free water surface in this version of the model. The energy equation is not solved if the unconfined aquifer option is selected.

Under these conditions, the finite-difference approximations of the flow and concentration equations become:

$$\Delta[T_w(\Delta p-\rho g\Delta Z)] - q' = \frac{\delta(V\rho)}{\Delta t} \qquad (3\text{-}9)$$

$$\Delta[T_w C(\Delta p-\rho g\Delta Z)] + \Delta(T_E\Delta C) - Cq - \lambda V\rho C = \frac{\delta(V\rho C)}{\Delta t} \qquad (3\text{-}10)$$

In the model, the grid block pressures are the fluid pressures at the top of the blocks. Therefore, as shown in the figure, the magnitude of this pressure relative to the atmospheric pressure determines whether the free water surface exists in the block or not.



If the free water surface exists in the grid block, the volume of the fluid in the block is given by

$$V = \Delta x\Delta y h\phi$$

$$= \frac{h}{\Delta z} V_o \qquad (3\text{-}11)$$

Otherwise

$$V = \Delta x\Delta y\Delta z\phi[1+C_r(p-p_o)]$$

$$= V_o\,[1+C_r(p-p_o)] \qquad (3\text{-}12)$$

The right hand sides of Equations (9) and (10) can be expanded as follows:

$$\delta(V\rho) = V^n\delta\rho + \rho^{n+1}V_oC_r\delta p \qquad \text{if } p>p_a$$

$$= V_o\delta\rho + \frac{V_o}{g\Delta z}\delta p \qquad \text{if } p<p_a \qquad (3\text{-}13)$$

$$\delta(V\rho C) = V^nC^n\delta\rho + \rho^{n+1}C^nV_oC_r\delta\rho + \rho^{n+1}V^{n+1}\delta C \qquad \text{if } p>p_a \qquad (3\text{-}14)$$

$$= V_oC^n\delta\rho + \frac{V_oC^n}{g\Delta z}\delta p + V_o\left(\frac{p^{n+1}-p_a}{g\Delta z}+\rho^{n+1}\right)\delta C \qquad \text{if } p<p_a$$

On the left-hand sides of the equations, the horizontal transmissibilities are changed to reflect less than total grid block cross-sectional area available for flow and dispersion. The vertical transmissibilities are also changed to account for the saturated water thickness being different from the grid block thickness.

4.0 MODEL CHANGES

As a part of this contract, major updates made in the model and their implementation are discussed in this section. Changes that do not require explicit explanations are not listed here. The updates were as follows:

1. Water Table Conditions - As discussed in Section (3.1), free water surface conditions are handled in a similar method as used by Trescott (1975). Trescott adjusts the accumulation terms in the flow equation according to eq. (3.13). Also, the horizontal transmissibilities are adjusted to reflect less than total grid block cross-section area for flow in partially saturated blocks.

   In this model, water table conditions are permitted if solution of energy equation is not desired. The reason is that for partially saturated blocks, both saturated and dry parts of the block must be included in the equations for energy transport. For the same reason, the user is recommended not to use contaminant adsorption and water table conditions simultaneously.

   Therefore, the model solves total flow and contaminant transport equations or total flow equation only for free water surface conditions. In addition to the two changes similar to Trescott, the model includes adjustment of vertical transmissibilities as well to reflect a changed distance between centers of the two blocks under water table conditions. Similar adjustments including the accumulation term (eq. 3-15) are also made in the concentration equation.

   Under these conditions, the set of two equations is different than under saturated conditions. The equations and the Gaussian elimination are worked out in the same manner as described in Appendix, Vol. I of the original report.

2. Vertical Recharge at Selected Nodes. User may enter vertical recharge rates (ft/day) in the uppermost layer of the numerical system. The recharge rate is converted internally to mass source rate for each of the recharge blocks using block area and recharge fluid temperature and concentration. The pressure is assumed to be atmospheric.

3. Hydraulic Head Printout. Previously grid block pressures were printed out in absolute pressure units (psia) only. Now, user may generate hydraulic heads. Depending upon the user option selected, heads are calculated by using either a constant density, or the grid block fluid density.

4. Carter-Tracy Function Tables. An infinite or a large finite aquifer, not feasible to include in the numerical grid system, can be simulated by using Carter-Tracy method. Dimensionless time versus pressure change at the numerical grid boundary for an infinite aquifer is programmed in the model. The user may enter this data for any size aquifer. Data are included here for four ratios of the external radius of the aquifer to the numerical grid radius.

In the following table, the dimensionless time is defined as follows:

$$t_D = \frac{kt}{\mu\phi c_T r_g^2}$$

where k = aquifer permeability

ϕ = porosity

c_T = total compressibility, fluid and rock

μ = fluid viscosity

Table 1.--Carter-Tracy Functions

$r_e/r_g = 2$		$r_e/r_g = 3$		$r_e/r_g = 5$		$r_e/r_g = 10$	
Dimensionless Time	Pressure Change	Dimensionless Time	Pressure Change	Dimensionless Time	Pressure Change	Dimensionless Time	Pressure Change
0.22	0.443	0.5	0.627	3.0	1.167	12.0	1.732
0.24	0.459	0.54	0.636	3.2	1.192	13.0	1.768
0.26	0.476	0.56	0.645	3.4	1.215	14.0	1.801
0.28	0.492	0.60	0.662	3.6	1.238	15.0	1.832
0.30	0.507	0.65	0.683	3.8	1.259	16.0	1.862
0.32	0.522	0.70	0.703	4.0	1.281	17.0	1.890
0.34	0.536	0.75	0.721	4.2	1.301	18.0	1.917
0.36	0.551	0.80	0.740	4.4	1.321	19.0	1.943
0.38	0.565	0.85	0.758	4.6	1.340	20.0	1.968
0.40	0.575	0.90	0.776	4.8	1.360	22.0	2.017
0.42	0.593	0.95	0.791	5.0	1.378	24.0	2.063
0.44	0.607	1.0	0.806	5.5	1.424	26.0	2.108
0.46	0.621	1.2	0.865	6.0	1.469	28.0	2.151
0.48	0.634	1.4	0.920	6.5	1.513	30.0	2.194
0.50	0.648	1.6	0.973	7.0	1.556	32.0	2.236
0.60	0.715	2.0	1.076	7.5	1.598	34.0	2.278
0.70	0.782	3.0	1.328	8.0	1.641	36.0	2.319
0.80	0.849	4.0	1.578	9.0	1.725	38.0	2.360
0.90	0.915	5.0	1.828	10.0	1.808	40.0	2.401
1.0	0.982			11.0	1.892	50.0	2.604
2.0	1.649			12.0	1.975	60.0	2.806
3.0	2.316			13.0	2.059	70.0	3.008
5.0	3.649			14.0	2.142		
				15.0	2.225		

The pressure change is the pressure at the internal boundary of the numerical grid system.

5. Printer Contour Maps. The model now includes options to print areal (x-y) and/or vertical (r-z or x-z) pressure, temperature and contamination concentration maps. Twenty contours of the dependent variable are printed between a range specified by the user. The map scale and region to be mapped are also user entered quantities providing additional flexibility.

6. Temperature Initialization. Previously the user could specify temperature gradients within the aquifer in the vertical direction only. Now initial temperatures within the numerical grid system may be specified on a regional basis. A region consists of a contiguous group of blocks. Pressures are initialized according to hydrostatic equilibrium. The effect of temperature on fluid density is computed for initializing the aquifer pressure.

7. Radioactive Decay and Adsorption. As discussed in the previous section, radioactive decay and adsorption are now included in the model. Natural alpha or beta decay is equivalent to a first order chemical reaction, and therefore any first order reaction of the contaminant can be described. Contaminant adsorption on rock surfaces is described by a linear adsorption isotherm. In radioactive contaminant transport, linear adsorption isotherm is generally described by adsorption coefficient K_d, which is a ratio is contaminant adsorbed on rock and contaminant present in fluid phase. The function K_d is assumed constant for each rock type.

5.0 USER OPTIONS

The user options available in the present version of the model are described here. The options refer to description of boundary conditions, initial conditions, aquifer rock and fluid property description, visual aids to the user, and efficient program execution. These options are as follows:

(1) Variable Dimensioning. 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. These arrays are located in the blank common. Redimensioning of the arrays can be done by recompiling only the Main routine. On Control Data machines, dynamic storage allocation allows the flexibility of no redimensioning.

(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) 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.

(4) 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.

(5) 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.

(6) 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 may be different for each rock type.

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

(8) 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.

(9) 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. The constant pressures along the edges are the initial grid block pressures in the boundary blocks. 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.

(10) Vertical Recharge. The user may specify vertical recharge rates into the aquifer as functions of time.

(11) Water Table Conditions. Free water surface may exist in the uppermost layer of the aquifer. This option coupled with vertical recharge option permits a user to use the model for near surface ground water aquifer systems.

(12) Well Specifications. 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) multiplied by (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. Contaminant rate is obtained from total fluid injection rate and contaminant concentration in the injection fluid.

(14) Initial Conditions. The user may specify fluid temperature and concentration in each grid block. However, fluid pressure is specified at one point within the aquifer, and the model initializes all grid block pressures assuming existence of static equilibrium.

(15) 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.

(16) Finite-Different Approximations. The model offers an option to select either central or backward (upstream) difference approximations in space. Also, the user may select time implicit (backward-in-time) difference approximations.

(17) 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.

(18) 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-hold conditions or both.

(19) 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. The user may generate areal (x-y) maps, or vertical (x-z, r-z), or both types of contour map.

(20) 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.

6.0 DATA CARDS

This section defines the order of the input data and the units for each parameter. The user is referred to the original report for definitions of different physical parameters, and the execution control parameters are defined as they appear in the input statements. Each data card (or a group of data cards) is introduced in the order in which it must appear in the data deck and is assigned a reference number. The reference number also indicates the program in which the data is read:

Reference	Program
M	MAIN
R1	READ1
I	INIT
R2	READ2
P	MAIN

The program is organized to use only the actual amount of core storage required. A variable "G" in the main program is used to store all the variables that need to be dimensioned equal to the number of blocks. These variables will be referred to as full size arrays. The array "G" is stored in the blank common. The program is subject to a total of 20 wells, and seven overburden and underburden impermeable blocks. In actual practice, the only limitation on problem size is the core size of the machine used. The program can be easily redimensioned to the size of the actual problem.

The Fortran format associated with each input (or read) group is also noted below. For runs from initial conditions, all data described below must be prepared according to instructions. For any changes in the well rates or specifications, only the recurrent data (reference R2) should be entered. Also, the recurrent data must be entered whenever contour maps are desired or a restart record is to be written. The plotting data is entered after all the recurrent data has been read in. For a restart run, no data is read in READ1 and INIT subroutines. If you desire a plot for a previous run, all the required data is read in the main program.

User entered data errors that can be detected by the program during execution are listed in Section 5.1.

A description of all the input data cards is given on the following pages.

READ M1 (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 (16I5)

LIST: NCALL, RSTRT, ISURF, IFREE, 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 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 — 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.

For a nonrestart run, i.e., a run from initial conditions, read RSTRT as zero.

ISURF — Control parameter for wellbore calculations.

0 - No wellbore calculations will be performed. This means only rates or bottom-hole pressures may be specified.

1 - Wellbore calculations will be performed.

IFREE — Free water surface index.

0 - The physical system is confined aquifer system.

1 - Free water surface may exist in the uppermost vertical layer.

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 R2-15, 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 R2-15, and proceed to READ P-1.

NPLC — Control parameter for plotting concentration in the well.

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

0 - If no concentration plots are desired.

-1 - If concentration plots are desired for a previous run. Skip READ M-3, through R2-15 and proceed to READ P-1.

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

READ M-3 (16I5)

This data will be used to dimension all full size arrays (equal to total number of blocks) for the program as well as many other arrays. Because of the use of this method, very little dimensioning of input parameters and computational arrays is required throughout the remainder of the program.

LIST: NX, NY, NZ, HTG, NRT, KOUT, PRT, NABLMX, MAXRCH, 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 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, linear geometry.
- 3 - Radial geometry. The aquifer may be heterogeneous in the vertical direction.

NRT — Number of rock types. Adsorption distribution coefficients (K_d's) are assumed to be functions of rock type only.

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 R2-12. A value of KOUT here of 3 can be used to omit printing of all initialization data as is sometimes desirable in making a sequence of many history matching runs.

PRT — Output array orientation control.

- -1 - Print output maps 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 - Print out is similar to above except that block numbers in the y direction increase down the computer page.
- 2 - Print output maps as vertical sections (x-z).

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.

MAXRCH — Maximum number of vertical recharge blocks.

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 not 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 also be printed. This length must be smaller than the dimension of array "A". "A" estimated can also be input through NARR.

±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 GAUS3D.

0 - Dimensioning on "A" array will be calculated internally using an approximate formula. Later in the program, the minimum length required is calculated exactly and printed out.

>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.

READ M-4 (7F10.0)

NOTE: This card is read only if the run is a restart, i.e. only if the value read for RSTRT is non-zero.

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 NO. R2-1 if RSTRT is non-zero.

READ R1-1 (7E10.0)

LIST: CW, CR, CTW, CPW, CPR, DLMDA

CW	Compressibility of the aquifer fluid, $(psi)^{-1}$.
CR	Compressibility of rock, $(psi)^{-1}$.
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, Btu/ft^3-°F.
DLMDA	Half life of contaminant, years. For stable contaminants, enter zero.

READ R1-2 (7E10.0)

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

UKTX	Thermal conductivity of the 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.

ALPHT — Transverse dispersivity factor, ft.

DMEFF — Molecular diffusivity in the porous media, including the effect of tortuosity and porosity, ft^2/day.

READ R1-3 (7E10.0)

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

LIST: PBASE, PBWR, TBWR, BWRN, BWRI, BWPRNT

PBASE — Base or atmospheric pressure. This pressure is used for

(i) vertical recharge

(ii) surface pressure for wellbore calculations

(iii) atmospheric pressure for free water surface calculations. If the water pressure at the top of the grid block is below this value, free water surface is below the top of the block.

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 injection fluid (concentration = 1) at PBWR and TBWR, lb/ft^3.

BWPRNT — Density for converting grid block pressures to fluid heads or pressures at datum (for output only).

<0 - Absolute magnitude of BWPRNT is used for calculating pressure at datum

$$P_{datum} = p - |BWPRNT| g(h-h_{datum})$$

0 - Grid block fluid density is used for calculating fluid heads (Φ)

$$\Phi = p/(\rho_{block} g) - (h-h_{datum})$$

>0 - BWPRNT is used for calculating fluid heads (Φ).

$$\Phi = p/(BWPRNT \cdot g) - (h-h_{datum})$$

READ R1-4 (14I5)

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 (7E10.0)

LIST: DELPW, TDIS

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.

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

READ R1-6 (14I5)

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 (conc. = 0) and one for the injection fluid (conc. = 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' (1934) generalized chart. 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 NTVI=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 injection fluid.

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

READ R1-7 (7E10.0)

LIST: TRR, VISRR, TIR, VISIR

The reference viscosities of the injection 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 injection fluid viscosity, °F. If possible, this temperature should be taken equal to TRR.

VISIR — Viscosity of the injection 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 not re-enter the reference viscosity at TRR.

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 injection fluid at the temperature TI. Do not enter the reference viscosity at TIR.

READ R1-11 (2F10.0)

Initial temperatures in the aquifer and the overburden-underburden blocks are to be entered here. The model requires a user-entered temperature profile. Horizontal variation can be entered in READ I-3.

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

ZT — Depth, ft.

TD — Temperature, °F.

READ R1-12 (8E10.0)

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

ADS — Product of adsorption distribution coefficient (K_d) and solid particle rock density (ρ_{rock}) for each rock type. The adsorption equilibrium coefficient is calculated as

$$K_e = 1 + \frac{1-\phi}{\phi} (\rho_{rock} K_d)$$

All blocks are assumed to be rock type 1 unless modified by READ R1-26.

READ R1-13 (215)

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 R1-14 (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 R1-15 (7E10.0)

NOTE: Skip this READ if NZOB=0.

LIST: DZUB(K), K = I, 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 R1-16 (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 R1-17 (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 an arbitrary depth HINIT, psi. Quantities PINIT and HINIT are used only to set up initial conditions.
HINIT	Depth for setting up initial conditions, ft. HINIT can be any depth within the reservoir.
HDATUM	A datum depth (ft) for printing the dynamic pressures ($p - \rho gh$). The depth h is measured from the datum depth HDATUM.

READ R1-18 (7E10.0)

NOTE: If HTG=3 (radial geometry), skip to READ R1-23.

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

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

READ R1-19 (7E10.0)

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

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

READ R1-20 (7E10.0)

LIST: DELZ(K) K=1, NZ

DELZ — Thickness of each vertical layer, ft.

If you use the linear geometry aquifer description (HTG=1 or 2) 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 R1-21 are both zero. DELX and DELY are measured along the x-y plane and DELZ is perpendicular to the x-y plane.

READ R1-21 (7E10.0)

NOTE: These data by themselves describe a homogeneous reservoir. Heterogeneity may be introduced by using either READ R1-22 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.

KY — Hydraulic conductivity in y direction, ft/day.

KZ — Hydraulic conductivity in z direction, ft/day.

PHI — Porosity (fraction).

SINX — Sine of the reservoir dip angle along the x-axis.

SINY — Sine of the reservoir dip angle along the y-axis.

DEPTH — Depth from arbitrary reference plane (e.g. sea level) to top of grid block (1,1,1), feet.

NOTE: Skip to R1-26 if HTG not equal to 2. All aquifer properties are assumed to be those described in R1-21 unless modified by R1-22.

READ R1-22 (LIST 1 - 6I5, LIST 2 - 6E10.0)

NOTE: Read as many sets of these data as necessary to describe all the aquifer heterogeneities. Follow the last set 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 described.

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

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

KX, KY, KZ Hydraulic conductivities in the x, y and z-directions respectively, ft/day.

PHI Porosity, fractional.

UH Depth to the top of the region. If entered zero, it is not modified.

UTH Thickness of the region. Only positive values of UTM modify grid block thickness within this region; otherwise it is described by R1-20.

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.

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

READ R1-23 (4E10.0)

These data are read for a radial geometry aquifer with only one well. The well is located at the center of the grid block system. The user has the option of dividing the grid blocks on an equal $\Delta \log r$ basis, (i.e., r_i/r_{i-1} is constant) or entering each grid block center value.

LIST: RWW, R1, RE, DEPTH

RWW — Well radius, feet.

R1 — Grid block selection option.

- >0 — The first grid block center in feet, for dividing grid blocks on an equal $\Delta \log r$ basis.
- 0 — Grid block center values will be user entered in READ R1-25.

RE — External radius of the aquifer, feet.

DEPTH — Depth from a reference plane to the top of the aquifer, feet.

READ R1-24 (5E10.0)

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

DELZ — Layer thickness in the vertical direction, feet.

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.

NOTE: If R1>0 (READ R1-23), skip R1-25.

READ R1-25 (7E10.0)

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

RR — Grid block center radius, feet.

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 description modifications desired. Follow the last set with a blank card, which the program recognizes as the end of this data set. Even if no regional modifications are desired, the blank card must nevertheless be included.

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

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.
IMPG	Rock type. If rock type is 1, you may enter zero.
FTX	If positive or zero, this is the factor by which the x direction transmissibilities within the defined region are to be multiplied. If negative, the absolute value of FTX will be used for the x direction transmissibilities within the region to be modified, replacing the values read earlier or determined from the permeability data read earlier.
FTY	This has the same function of FTX, but applies to the y direction transmissibilities.
FTZ	This has the same function FTX, but applies to the vertical transmissibilities.
FPV	This has the same function as 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 R1-21, R1-22 or R1-24.

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 that apply to the region. For the transmissibility and pore volume modifications, the order of multiple changes does not affect the final result if all the modifiers are multiplicative (positive). However, if some or all of the modifications are replacement values (negative) the order of input may affect the final result. For example, consider the following two situations in which the same modification data are applied in different orders to an original value and the final result is different.

	CASE 1	CASE 2
Original Value	100	100
Modification and Result	.50(50)	-70.(70.)
Modification and Result	-70.(70.)	.50(35.)
Modificationand Result	.20(14.)	.20(7.)

READ R1-27 (215)

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 influence 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: 615; 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

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 IAQ=1 or 2 (READ R1-27)

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

For IAQ=4 (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: Follow the last VAB card of this data group by a blank card.

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

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.

READ R1-31 (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.

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

READ R1-32 (2F10.0)

NOTE: These data are 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 (215)

NOTE: These data are read for initializing concentrations, temperatures, and natural flow in the aquifer. If the initial concentrations are zero everywhere in the aquifer, there is no natural flow, and the temperature conditions are not to be changed, insert a blank card and proceed to READ R2-1.

LIST:ICOMP, ITEMP, INAT

ICOMP — Control parameter for initializing the 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.

ITEMP — Control parameter for initializing aquifer temperatures.

- 0 - Initial temperatures in all the grid blocks are set by a vertical temperature profile entered in READ R1-11.
- 1 - Temperature variations from the profile (READ R1-11) will be entered by the user.

INAT — Control parameter for entering natural fluid velocity.

0 - The aquifer fluid is static initially. If you enter zero, skip READ I-4.

1 - The resident fluid velocity will be entered in READ I-4.

NOTE: Skip READ I-2 if ICOMP (READ I-1) is zero.

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

NOTE: Enter as many cards as necessary to describe all non-zero concentrations in the aquifer. Follow the last set with a blank card.

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: Skip READ I-3 if ITEMP (READ I-1) is zero.

READ I-3 (615,F10.0)

NOTE: Enter as many cards as necessary to describe all temperature variations in the aquifer. Follow the last I-3 card with a blank card.

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

I1, I2	Lower and upper limits, inclusive, on the I-coordinate of the temperature initialization region.
J1, J2	Lower and upper limits, inclusive, on the J-coordinate of the temperature initialization region.
K1, K2	Lower and upper limits, inclusive, on the K-coordinate of the temperature initialization region.
TINIT	Initial temperature in all the blocks described above, °F.

READ I-4 (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.

RECURRENT DATA

The data described previously (M, I and R1 data) are to describe the aquifer and fluid properties and to establish initial conditions. The following data (R2 data) are 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.

READ R2-1 (14I5)

LIST: INDQ, IWELL, IMETH, ITHRU, IRCH, 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.

IRCH — Vertical recharge data change parameter

0 - Vertical recharge data will not be entered during this time step.

1 - Vertical recharge data will be read during this time step.

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.

READ R2-2 (I5,F10.0)

NOTE: These data are 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 $\leq$ 0, the program selects WTFAC = 1.0.

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

NOTE: These data are 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, DOLDP, DAMPX, EPS

NITQ	Maximum number of outer iterations in the wellbore calculations. For example, if the injection rate for a well is specified, the wellhead pressure is calculated iteratively to obtain the bottom-hole pressure necessary to inject the specified rate. If entered as zero or a negative number, the program selects the default value of 20.
TOLX	The tolerance on the fractional change in pressure over an iteration. If entered as zero or a negative number, the default value of 0.001 is selected.
TOL DP	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 these 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 these data only if INDQ is equal to two. Read as many cards as necessary to describe all the 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 and 4 - 7E10.0, LIST 3 - 8E10.0)

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

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

I	Well number.
IIW	I-coordinate of grid cell containing the well.
IJW	J-coordinate of grid cell containing the cell.
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 in the aquifer model equations.

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

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

4 - Constant bottom-hole pressure

LIST 2: WI, BHP, TINJ, CINJ

WI — Well index, ft^2/day.

BHP — Bottom-hole pressure, psi. This must be specified if IINDWI = ±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), feet. Enter zero if it is a smooth pipe.
OD	Outside wellbore (casing) diameter, feet.
TTOP	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

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

NOTE: Skip READ R2-8 if IRCH is equal to zero (READ R2-1)

READ R2-8 (4I5, 3E10.0)

NOTE: Enter as many of these cards as necessary to describe all the recharge data. Follow the last R2-8 card with a blank card.

LIST: I1, I2, J1, J2, U1, U2, U3

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

J1, J2 Lower and upper limits, inclusive, on the J-coordinate of the vertical recharge region.

U1 Recharge rate, ft/day.

U2 Temperature of the recharge fluid, °F.

U3 Contaminant concentration in the recharge fluid, dimensionless.

READ R2-9 (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.

READ R2-10 (14I5)

NOTE: These data are 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 (original documentation) for explanation). The default value 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 R2-1I (7E10.0)

LIST: TCHG, DT, 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.
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.
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 R2-12 (10I5)

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

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

IO1 — Control parameter for frequency of the time step summary output. The time step summary (7 lines) 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.

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

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

0 — Print at the end of each time step through to the step ending at TCHG.

1 — Print only at time TCHG.

n(>1) — Print at the end of every n^{th} time step and at the time TCHG.

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. 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 - An areal map (x-y) of the variable will be printed.

2 - Vertical (x-z or r-z) contour map will be generated.

3 - Both areal and vertical maps will be printed.

E.G. If desired areal map of pressure and both areal and vertical maps of concentration, enter 103.

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 Velocities, fluid properties and transmissibilities printing index. These quantities are printed only at the beginning of the next time step or at the current time.

0 - Additional printing is not activated

1 - Darcy velocities are printed

2 - Darcy velocities, flow, energy and mass transport transmissibilities are printed

3 - Darcy velocities, transmissibilities, fluid density, viscosity, enthalpy and dispersivities are printed.

NOTE: Skip READ R2-13 to R2-15, if

(i) MAP is equal to zero (READ R2-12) or

(ii) MAP is not equal to zero and MDAT is equal to zero.

READ R2-13 (2I5)

LIST: NORNXY, NORNXZ

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

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

1 - x increases from left to right and y (or z) increases down the computer page. The origin is the upper left hand corner.

READ R2-14 (4E10.0)

LIST: XYXL, XYYL, XZXL, XZZL

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

XZXY, XZZL — The x/r and z map lengths in inches, respectively, for all the vertical maps.

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

NOTE: Enter one card for each map requested on R2-12 card. For example, if MAP = 103, areal pressures, areal concentration and vertical concentration maps will be generated. Therefore, exactly 3 data cards should be entered here for this example.

LIST: I1(I), I2(I), J1(I), J2(I), K1(I), K2(I), AMIN(I), AMAX(I), I=1, Number of MAPS requested (max. of 6)

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

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

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

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

Data entered up to this point are sufficient to execute the program until time equals TCHG(R2-11). The program then goes back to the beginning of the recurrent data (R2-1). Model execution proceeds in this manner until the user enters ITHRU = 1 (R2-1). If any plots are desired, plotting data is entered after all R2 cards. Otherwise, the last card in a data deck should be a R2-1 card with 1 punched in column 20.

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

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 non-zero.

READ M-3 — This card must be identical to the one used for the original run.

READ M-4 — Enter a negative value for TMCHG.

NOTE: Insert as many sets of mapping data (M-5 and M-6) as you desire. Follow the last set with a blank card.

READ M-5 (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-6 (2I5)
LIST: MAP, MDAT

MAP — Requires a three digit specification as in READ R2-12, except that it should be negative.

MDAT — See READ R2-12.

NOTE: If MDAT has been entered as one, you should enter the mapping data R2-13 through R2-15 at this point.

6.1 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 in the original documentation 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 zeroes do not have errors. Error numbers 1 through 50 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, DELZ) 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 thanl or greater than NY or
K is less than 1 or greater than NZ or
KX or KY or KZ is negative or
PHI is less than 0.001 or greater than 1.0.

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

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

(16) This error refers to READ R1-24 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.

(22) Similar to (21) for READ I-3.

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

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

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

(33) IINDW1 is $\pm$3 and BHP is 0. The specified value of the bottom-hole pressure is a limiting value of the well pressure if IIDW1 is $\pm$3.

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

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

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

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

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

Error numbers 41 and 42 refer to READ R2-9.

(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 = $\pm$2) and IMPG is less than or equal to zero.

Error numbers 43 through 46 refer to READ R2-10.

(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 R2-13, R2-14 and R2-15, respectively.

(47) IP2 is greater than NX or
KP2 is greater than NZ or
HTG does not equal 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.

8.0 NOMENCLATURE

C	-	Contaminant concentration in fluid
C_s	-	Contaminant concentration on rock surface
C_p	-	Specific heat
c_r	-	Compressibility of rock
c_t	-	Total rock + fluid compressibility
E_c	-	Total mass diffusivity (hydrodynamic and molecular)
E_H	-	Total thermal conductivity (hydrodynamic and molecular)
g	-	Acceleration due to gravity
H	-	Fluid enthalpy
K_d	-	Adsorption distribution coefficient
K_e	-	Adsorption equilibrium constant
k	-	Permeability
p	-	Fluid pressure
q	-	Source term
r_e	-	External radius of aquifer
r_g	-	Numerical grid radius of aquifer
T	-	Temperature
t_D	-	Dimensionaless time
U	-	Internal energy
u	-	Darcy velocity
V	-	Volume of fluid in a grid
V_o	-	Grid block volume
Z	-	Depth below a horizontal reference plane

8.0 Nomenclature (Continued)

Greek Symbols

ρ	-	Fluid density
ρ_B	-	Bulk density of rock
ρ_S	-	Rock density
ϕ	-	Porosity
μ	-	Viscosity
λ	-	Decay constant

7.0 REFERENCES

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