A DUAL-FOROSITY MODEL FOR SIMULATING
SOLUTE TRANSPORT IN OIL SHALE

U.S. GEOLOGICAL SURVEY
Water-Resources Investigations Report 85-4281
A DUAL-POROSITY MODEL FOR SIMULATING
SOLUTE TRANSPORT IN OIL SHALE

By Kent C. Glover

U.S. GEOLOGICAL SURVEY
Water-Resources Investigations Report 85-4281

Cheyenne, Wyoming
1986
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CONVERSION DATUM

For those readers interested in using the metric system, the following table may be used to convert the inch-pound units of measurement used in this report to metric units:

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<th>Multiply</th>
<th>By</th>
<th>To obtain</th>
</tr>
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<tbody>
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<td>meter</td>
</tr>
<tr>
<td>foot per day</td>
<td>0.3048</td>
<td>meter per day</td>
</tr>
<tr>
<td>foot squared per day</td>
<td>0.09290</td>
<td>meter squared per day</td>
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A DUAL-POROSITY MODEL FOR SIMULATING SOLUTE TRANSPORT IN OIL SHALE

By Kent C. Glover

ABSTRACT

A model is described for simulating three-dimensional ground-water flow and solute transport in oil shale and associated hydrogeologic units. The model treats oil shale as a dual-porosity medium by simulating flow and transport within fractures using the finite-element method. Diffusion of solute between fractures and the essentially static water of the shale matrix is simulated by including an analytical solution that acts as a source-sink term to the differential equation of solute transport. While knowledge of fracture orientation and spacing is needed to effectively use the model, it is not necessary to map the locations of individual fractures.

The computer program listed in the report incorporates many of the features of previous dual-porosity models while retaining a practical approach to solving field problems. As a result the report does not extend the theory of solute transport in any appreciable way. The emphasis in the report is on bringing together various aspects of solute-transport theory in a manner that is particularly suited to the unusual ground-water flow and solute-transport characteristics of oil-shale systems.
INTRODUCTION

Digital models of ground-water flow and solute transport have been used to predict possible impacts of oil-shale development on the ground-water resource (Robson and Saulnier, 1981). Unfortunately, modeling techniques used in the past either were not developed for use in rock, such as oil shale, where porosity depends on fracturing, or required data that usually are not available. From 1980 to 1983 the U.S. Geological Survey studied migration of solute from an in situ oil-shale retort near Rock Springs, Wyo. (fig. 1). The emphasis of the study was to identify geo-

Figure 1.—(caption on next page) belongs near here.

logic, hydraulic, and chemical factors that control the process of solute transport in oil shale. During the study, it became apparent that no existing model was well suited for the unusual flow and transport characteristics of oil-shale systems. Therefore, as part of the study, a model was developed.

This report describes two digital-computer programs that are used to simulate ground-water flow and solute transport in oil shale with interbedded tuff or sandstone. The U.S. Department of Energy experimental, in situ, oil-shale retort near Rock Springs, Wyo., was used as the prototype flow system of the model. The application of modeling techniques to this flow system is described in a report by K. C. Glover, U.S. Geological Survey, written commun. (1985). The model is designed for use in site-specific studies and consequentially includes many features, such as diffusion of solute between fractures and the shale matrix, that may not be important to basin-wide or regional investigations.
Figure 1.--Location of in situ oil-shale retort near Rock Springs, Wyoming.
A wide array of ground-water flow and solute-transport models have become available in recent years. Konikow and Bredehoeft (1978), and INTERCOMP Resource Development and Engineering, Inc. (1976) describe two of the more commonly used programs. Other models that are potentially useful in studies of oil-shale hydrology are described by Bibby (1981), Noorishad and Mehran (1982), and Rasmuson and others (1982). The model described in this report incorporates many of the features of the above models while retaining a practical approach to the solution of field problems. Boundary conditions can be applied easily and mapping of individual fractures is not necessary. As a result of this approach, the present model does not extend the theory of solute transport in fractured media in any appreciable way. Instead, various aspects of this theory are brought together in a manner that is particularly suited to the unusual ground-water flow and solute-transport characteristics of oil-shale systems.

Throughout the remainder of this report it is assumed that the reader is familiar with the basics of solute-transport modeling in porous media, such as sand-and-gravel aquifers, as well as the finite-element method of numerical analysis. It is believed that most hydrologists faced with a problem of solute migration in oil shale will have faced similar problems in unfractured media. For those readers unfamiliar with applications of solute transport modeling using the finite-element method, it is suggested that teaching references such as Freeze and Cherry (1979), Konikow and Bredehoeft (1978), and Zienkiewicz (1971) be consulted.
OIL SHALE AS A DUAL-POROSITY MEDIUM

Porosity in oil-shale formations may be classified on the basis of its relationship to hydraulic conductivity. Porosity may be considered effective for increasing hydraulic conductivity if the pores are interconnected or not effective, as in shale, if the pores are relatively isolated.

Porosity due to faults, joints, collapse breccia, and solution cavities is the major source of permeability in oil shale with otherwise low permeability (Robson and Saulnier, 1981). Persistent layers of permeable tuff or sandstone, ranging in thickness from less than an inch to several inches, also are common in oil shale (Bradley, 1964) and contribute to the hydraulic conductivity. The porosity of the shale and marlstone matrix, although relatively high, does not contribute significantly to hydraulic conductivity.

Any attempt to simulate ground-water flow and solute transport in oil shale must include consideration of the dual-porosity nature of these sediments. The solute-transport processes of hydrodynamic dispersion and advection are related directly to seepage velocity and therefore are related to the effective porosity of the formation. However, several investigators including Grisak and Pickens (1980) and Bibby (1981) have noted that dispersion and advection alone cannot account for the distribution of non-reacting solute in fractured formations. The extremely low seepage velocity of water within the shale matrix minimizes dispersion and advection, increasing the relative importance of diffusion. The porosity of the shale matrix, although not contributing to hydraulic conductivity, is important to dispersion.
METHODS OF SIMULATION

Ground-Water Flow

Only the part of formation porosity that contributes to hydraulic conductivity needs to be considered in analysing ground-water flow systems. For most practical purposes this porosity in oil shale, whether resulting from faulting, solution channels, or thin beds of permeable tuff and sandstone, can be analysed using the techniques of Snow (1969). He showed that many problems of flow through dual-porosity media can be solved using an anisotropic hydraulic-conductivity tensor in conjunction with standard porous-media techniques. His approach to the problem of ground-water flow is valid if the formation has a fracture density that is high compared to the scale of the problem. In such a case, the hydraulic characteristics of the fractured formation are similar to those of granular media. If fracture spacing is irregular in a given direction, the formation will exhibit heterogeneity. Because mapping of individual fractures is impractical for most field problems, the approach of Snow (1969) is used in this model. From a practical viewpoint the model described in this report may be useful when the hydrologist has some knowledge of the average spacing, aperture size, and directions of fracturing, but accurate mapping of individual fractures is not possible. Through proper alignment of the model cartesian coordinate axes with principal directions of fracturing and use of heterogeneous hydraulic conductivity values, many different fracture geometries can be simulated.
The three-dimensional nature of a fracture system, along with the essentially horizontal bedding plane of most formations, generally results in a three-dimensional flow system in oil-shale strata. Three-dimensional flow systems in oil shale have been observed on both a regional scale by Robson and Saulnier (1981) and on a local scale by the author at the Department of Energy in situ oil-shale retort near Rock Springs, Wyo. Therefore, the program given in this report is intended for use in studies of three-dimensional ground-water flow.

Rocks in the vicinity of an in situ retort are altered due to induced fracturing. As a result fracture patterns in the retort chamber are significantly different than regional fracture patterns. The values and degree of anisotropy of hydraulic conductivity within a retort chamber also differ from regional estimates. Nevertheless the fracture density usually is high, compared to the dimensions of the retort chamber, and standard porous-media techniques can be used to simulate ground-water flow in the immediate vicinity of the retort chamber.
Solute Transport

The extension of solute-transport theory to dual-porosity media has attracted considerable attention in water-resources literature. Much of the literature has been directed toward studies of radionuclide migration through individual fractures and as such is not directly applicable to field problems where mapping of individual fractures is impractical. Grisak and Pickens (1980) modeled fractured media by using separate finite elements to represent fractures and adjacent low permeable rock. Finite elements used to represent the fractures were modeled with material properties that differed from adjacent low-permeability elements. This approach was extended by Noorishad and Mehran (1982), who also introduced the use of an "upstream-weighting" technique to simulate more accurately the essentially advective transport that occurs within the fractures.

Bibby (1981) took a different approach to modeling solute movement through dual-porosity media. Molecular diffusion between fractures and the primarily static water in the shale matrix was incorporated in the model as a source-sink term utilizing an appropriate analytical solution. To apply this two-dimensional model the user needs to know average spacing, aperture diameter, and direction of fractures but does not need to map individual fractures. This approach is analogous to the method of flow analysis discussed by Snow (1969). Although no upstream-weighting technique was used, Bibby (1981) reported no difficulty in applying the model to a field problem in a limestone aquifer.
Rasmuson and others (1982) presented a model for simulating three-dimensional solute transport in fractured rocks that is based on an integrated finite-difference approach. The model produces excellent results if solute transport is dominated by hydrodynamic dispersion. Because advection dominates most solute-transport problems in oil-shale strata (Robson and Saulnier, 1981), the approach of Rasmuson and others (1982) is not considered practical for use with oil shale.

The approach to modeling solute transport presented in this report is basically the model described by Bibby (1981) and extended to three dimensions. This approach has been selected because it strikes a balance between theoretical accuracy and practical applicability. Accurate mapping of fractures is not needed to use the model, although some knowledge of the fracture system is required. The ease with which boundary conditions can be applied also supports this approach. One disadvantage of the approach is the difficulty of extending the analytical solution for diffusion between fractures and the shale matrix to problems of multiple-species transport.

A model that can be extended to problems of multiple-species transport is described by Huyakorn and others (1983). Unfortunately, fracture locations must be accurately mapped to use the model successfully. Therefore the model of Huyakorn and others (1983), although theoretically superior to the model of Bibby (1981), cannot be applied in most practical field problems.
APPLICATION OF THE FINITE-ELEMENT METHOD

Ground-Water Flow

The basic governing equation for three-dimensional flow, when Cartesian coordinate axes are aligned with the principal components of the hydraulic-conductivity tensor, is as follows:

\[
\frac{\partial}{\partial x_i} (K_i \frac{\partial h}{\partial x_i}) + W = S_s \frac{\partial h}{\partial t} \quad i = 1, 2, 3 \tag{1}
\]

where \(K_i\) = the hydraulic conductivity tensor \([LT^{-1}]\);
\(W\) = the source-sink function (positive for a source) \([T^{-1}]\);
\(S_s\) = specific storage \([L^{-1}]\);
\(h\) = the hydraulic head \([L]\);
\(x_i\) = Cartesian coordinate \([L]\), and use of a repeated subscript indicates summation on that subscript; and
\(t\) = time \([T]\).

The source-sink term may be distributed areally or may represent a well. Boundary conditions that may be applied on the periphery of the problem area include known specific discharge normal to the boundary or known hydraulic head. Parameters \(K_i\), \(W\), and \(S_s\) are approximated by subdividing the region of interest into discrete zones. Parameters are assumed to be constant within each zone which gives rise to internal boundary conditions at zonal discontinuities. Along these internal boundaries both hydraulic head and normal specific discharge must remain unchanged as the boundary is crossed.
Equation 1 may be solved by using the finite-element method based on the Galerkin criteria. Details of this method are described in Zienkiewicz (1971) and Pinder and Gray (1977). Within this report, first-order basis functions are used to describe each cubic element. While use of these basis functions requires more elements than if higher-order functions were used, the reduced oscillatory behavior and integration time associated with linear functions make this simpler approach preferable.

The matrix equation resulting from the finite-element discretization of equation 1 is as follows:

\[
\left( \frac{1}{\Delta t_m} \bar{c} + \theta \bar{K} \right) \bar{h}^m = \bar{q} + \left( \frac{1}{\Delta t_m} \bar{c} - (1-\theta)\bar{K} \right) \bar{h}^{m-1}
\]  

(2)

where \( \bar{c} \) = a coefficient matrix involving specific storage \( S_s \) and calculated for a single finite element as \( \iiint_V S_s \bar{n} (\tilde{n})^t dV \);

\( \bar{K} \) = a coefficient matrix, with off-diagonal components equal to zero, involving hydraulic conductivity and calculated for a single finite element as

\[ \iiint_V (K_i \frac{\partial \tilde{n}}{\partial x_i} \frac{\partial \bar{n}}{\partial x_i})^t dV, \quad i = 1,2,3; \]

\( h^m \) = the vector of hydraulic head at time \( m \);

\( \bar{q} \) = the known vector involving source-sink terms and specified flux boundary conditions;

\( \Delta t_m \) = the length of the time step;

\( \theta \) = a number ranging from 0 for an explicit solution to 1 for an implicit solution;

\( V \) = the volume of the finite element;

\( \tilde{n} \) = the vector of finite-element shape functions; and

\( (\ )^t \) = the transpose of the enclosed vector.
Equation 2 is solved by Gaussian elimination for banded symmetric matrices. Although other direct-solution techniques, such as Cholesky decomposition, can be used, the procedure used in this report has proven adequate. Gupta and Tanji (1976) has suggested the use of matrix solvers that take full advantage of the sparse nature of coefficient matrices in attempts to reduce core storage requirements. The trade-offs in these matrix solvers are increased disk access and increased computational time. With the introduction of virtual-memory operating systems used by most computers, such detailed attention to minimizing core storage is not required.
Solute Transport

The transport of a conservative solute in ground water is described by the following equation:

\[ \frac{\partial}{\partial x_i} (D_{ij} \frac{\partial c}{\partial x_j}) - \frac{\partial}{\partial x_i} (c q_i) = \phi \frac{\partial c}{\partial t} - W c^* \quad i,j = 1,2,3 \]

(3)

where \( D_{ij} \) = the hydrodynamic-dispersion coefficient \([L^2 T^{-1}]\);
\( c \) = solute concentration \([ML^{-3}]\); and
\( \phi \) = porosity [dimensionless];
\( q_i = -k_i \frac{\partial h}{\partial x_i} \) = the Darcian fluid velocity \([LT^{-1}]\);
\( W \) = a source-sink function \([T^{-1}]\);
\( c^* \) = solute concentration in a fluid source \([ML^{-3}]\).

When applied to dual-porosity media such as oil shale, the terms are defined relative to the joint or fracture system, with the shale matrix considered impermeable. The hydrodynamic-dispersion coefficient \( D_{ij} \) is related to Darcian fluid velocity in the fracture system by

\[ D_{ij} = a_{ijmn} \frac{q_m q_n}{|q|} + D^* \quad i,j,m,n = 1,2,3 \]

where \( a_{ijmn} \) = dispersivity of the fractured media \([L]\),
\( q_m \) and \( q_n \) = Darcian fluid velocity \([LT^{-1}]\),
\( |q| \) = the magnitude of the Darcian velocity vector \([LT^{-1}]\), and
\( D^* \) = the molecular-diffusion coefficient \([L^2 T^{-1}]\).

for isotropic media,
\( a_{i} = \alpha_L \) = the longitudinal dispersivity for \( i = 1,2,3 \); and
\( a_{ij} = \alpha_T \) = the transverse dispersivity for \( i,j = 1,2,3 \); and
\( a_{ij} = \frac{1}{2} (\alpha_L - \alpha_T) \) for \( i,j = 1,2,3 \).

There is no corresponding theory describing hydrodynamic dispersion in anisotropic media.
The form of the transport equation used in this report also is used by Pinder and Gray (1977), and Bibby (1981). Konikow and Bredehoeft (1978) and most studies of solute transport done by the U.S. Geological Survey use a form of the equation that is obtained by dividing equation 3 by porosity. The hydrodynamic-dispersion coefficient then is defined in terms of seepage velocity. Either form of the equation can be used successfully. However, when comparing results of studies using different forms of the transport equation, it should be recognized that the dispersion coefficients will differ by the magnitude of porosity.
Galerkin's method of weighted residuals, when applied to equation 3 with isoparametric finite elements, gives

\[
\left( \frac{1}{\Delta t_m} \bar{P} + \theta \bar{D} \right) \bar{c}^m = q_c^* + \left( \frac{1}{\Delta t_m} \bar{P} - (1-\theta) \bar{D} \right) \bar{c}^{m-1} \tag{4}
\]

where \( \bar{P} \) = a coefficient matrix involving porosity and is calculated for a single finite element as

\[
\iint_V \phi \bar{n} (\bar{n})^t \, dv;
\]

\( \bar{D} \) = a coefficient matrix involving hydrodynamic dispersion and advection and is calculated for a single finite element as

\[
\iint_V (D_{ij} \frac{\partial \bar{n}}{\partial x_i} \frac{\partial \bar{n}}{\partial x_j})^t - q_i \frac{\partial \bar{n}}{\partial x_i} (\bar{n})^t \, dv \quad i, j, = 1, 2, 3;
\]

\( \bar{c}^m \) = the vector of solute concentration in fractures at time \( m \); and

\( q_c^* \) = a known vector involving specified flux boundary conditions and source-sink terms (W), solute concentration in fluid sources (\( c^* \)), and diffusion between fractures and the rock.

Detailed information on formulating this equation can be obtained from Bibby (1981) or Pinder and Gray (1977, p. 144-148). Equation 4 is solved by the Gauss-Doolittle method for banded, nonsymmetric matrices.
Diffusion within the Oil-Shale Matrix

The exchange of solute between water in a system of parallel fractures and the essentially static water in the adjacent oil-shale matrix can occur by molecular diffusion and can be simulated by the addition of a source-sink term to equation 4. Bibby (1981) gives this source-sink term as a convolution integral that is expressed here in discrete form at time $t_m$.

$$\dot{W}_c = -\frac{\phi_B b}{A(t)(f+b)} [c_B(t_m) - c_B(t_{m-1})]$$

where $\dot{W}_c$ = the mass flux of solute entering the fracture [$M/L^3/T$];
$\phi_B$ = the porosity of the oil-shale matrix [dimensionless];
b = the average distance between parallel fractures [L];
$A(t_m) = [t_m - t_{m-1}]$, the length of the time step [T];
f = the average fracture width [L];
c_B = the average solute concentration in the oil-shale matrix [$M/L^3$];

$$c_B(t_m) = c(t_0) \left[1 - \frac{3}{\pi^2} \sum_{n=0}^{\infty} \frac{1}{E_n} \exp \left(-B_n t_m\right) \right] + \sum_{i=1}^{m} \left[ c(t_m) - c(t_{i-1}) \right] \left[1 - \frac{3}{\pi^2} \sum_{n=0}^{\infty} \frac{1}{E_n} \exp \left(-B_n (t_m - t_i)\right) \right]$$

c(t_0) = the solute concentration in the fracture at the beginning of the simulation [$M/L^3$];
n = an index of summation [dimensionless];

$$E_n = (2n - 1)^2;$$
$$B_n = D_d (2n+1) \pi^2/b^2;$$
c(t_i) = the solute concentration in the fracture at time $t_i$ [$M/L^3$]; and
$$D_d = \text{molecular diffusion of solute within the oil-shale matrix} [L^2/T].$$
The only unknown variable in equation 5 is $c(t_m)$. Therefore, the coefficient associated with $c(t_m)$ is placed on the main diagonal of the $D$ matrix in equation 4, while the remainder of the expression is placed in the right-hand vector of known values. Equation 5 involves summation over the entire period of the simulation. Fortunately, little truncation error is introduced by retaining only a small number of terms in the summations. The optimum number of terms to retain depends on the values of $D_d$, $b$ and $\Delta t_m$; however, from information presented by Bibby (1981), it is apparent that between five and ten terms are adequate for most applications.

Several aquifer properties must be determined to use equation 5 successfully. These properties include molecular diffusion within the oil-shale matrix ($D_d$), average distance between parallel fractures ($b$), average fracture width ($f$), and can be obtained for each of these properties, model calibration usually must be used to improve upon the estimates. Therefore equation 5 generally is useful only in studies with well distributed and frequent measurements of solute concentration in wells.
Sources of Solute Within the Retort Chamber

Mechanisms for creating and leaching chemicals from burned shale within an in situ retort chamber to the formation water are poorly understood. Knowledge of conditions during the retort process is needed to determine the chemicals that are created, while an understanding of dissolution controls is needed to predict how the created chemicals are transferred from the burned shale to the formation water.

The retort temperature, total time of retorting, permeability of the retort chamber, and initial mineralogy affect the type and amount of chemicals created during a burn. During combustion of a retort chamber, a "flame front" or zone of combustion moves through the fractured oil-shale bed. Hot gases from this combustion move ahead of the flame front and provide energy for pyrolysis of kerogen. In the process, a number of chemical by-products are created. A discussion of how these by-products are created is outside the scope of this report. However, it is important to recognize that the resulting chemicals will vary from retort chamber to retort chamber. In large chambers, the distribution of chemical by-products within the chamber also may be important. Coring of an abandoned retort chamber before it resaturates and lab analysis of the cores by long-term leaching studies can provide some understanding of the chemicals that are created during retorting.
After the retort operation ceases, the chamber resaturates and chemicals created during the burn are leached into the water. During the time that it takes to resaturate the retort chamber a rapid increase in the concentration of solute occurs. For many studies of solute transport, an equation to describe the initial dissolution is not needed because migration of solute from the retort chamber is unlikely until the formation resaturates.

After the retort chamber resaturates, Hall (1982) proposed that diffusion between the pores of the oil-shale matrix and fractures acts as a dominant mechanism for introducing solute to a ground-water system. This mechanism is simulated by equation 5. As discussed previously, equation 5 describes diffusion between the oil-shale matrix and a system of parallel fractures. Fracturing within a retort chamber is much more irregular but can be conceptualized as two systems of parallel fractures, one vertical and one horizontal, resulting in cubes of oil-shale. Matrix diffusion within the retort chamber can be simulated by applying equation 5 once for each fracture orientation.

In addition to rock and fracture characteristics discussed previously, the use of equation 5 to simulate a source of solute requires an estimate for the initial solute concentration in the pores of the oil-shale matrix \(C_B\). Water-quality sampling as the retort chamber resaturates will provide a measure of solute concentration in fractures but not of solute concentration in the shale-matrix pores. In cases where solute migration outside the chamber does not occur until some time after the initial resaturation the initial solute concentration with the shale-matrix pores may be approximated by the initial solute concentration within fractures. Study by the author and the Department of Energy in situ oil-shale retort near Rock Springs, Wyo. indicate that this approximation may be reasonable in many cases.
In situ retort chambers are sources of solute for extended periods of time after retorting stops. This characteristic has been observed by the author at the U.S. Department of Energy, experimental, in situ, oil-shale retort near Rock Springs, Wyoming and by Hall (1982) in laboratory experiments. The source of solute cannot be explained solely by diffusion from burned shale into fractures.

Hall (1982) has proposed a mechanism to explain the long-term source of solute that is based on the slow dissolution of the mineral matrix from pore walls. Although he was unable to provide a good theoretical basis for this slow dissolution, he proposed the use of an empirical expression to simulate the mechanism. The expression is

\[ K^* A (c_e - c) \]

where

\[ K^* = \text{the mass transfer coefficient} \quad [L^{-2}T^{-1}], \]
\[ A = \text{the interfacial area} \quad [L^2], \]
\[ c_e = \text{the equilibrium concentration of fluid in contact with shale blocks} \quad [ML^{-3}], \text{ and} \]
\[ c = \text{the solute concentration} \quad [ML^{-3}]. \]

This equation acts as a source-sink term to the solute-transport equation and simulates the dominant mechanism for leaching of burned shale after the passage of two to three pore volumes of water.
Application of the proposed leaching mechanism to a field problem requires that $K^*, A$, and $c_e$ in equation 6 be determined. While Hall (1982) determined values of the product $K^*A$ for organic solute from column experiments, the applicability of these values to field problems is unknown. Therefore $K^*A$ is effectively a parameter that must be estimated during model calibration. The equilibrium concentration, $c_e$, can be estimated from long-term leaching tests of burned shale. Unfortunately, these tests have been performed for very few of the chemical species found in oil-shale retort water.

The use of empirical equation 6 to describe mass transfer essentially provides an infinite source of solute to the medium where, in reality, such a source is finite. Therefore the use of equation 6 will overestimate solute concentrations in the trailing part of a plume. The use of equation 6 is justified in studies of solute transport in oil shale where the distribution of solute in the trailing part of the plume is not considered, or in studies where an estimate of maximum probable concentration of solute in the trailing part of a plume is needed.
MODEL CALIBRATION AND SENSITIVITY

The approach to ground-water flow and solute transport used in this report along with the three-dimensional nature of flow through oil shale, introduces an unusually large number of calibration parameters. Considering the amount and distribution of water-level and solute-concentration data that are available in most field studies, it is possible to reach a point where additional detail in the simulation procedure does not significantly improve the model fit. Therefore, it is important to assess the uncertainty associated with the various calibration parameters if the model is to remain a practical one for use in field problems.

Cooley (1977) presents a method for evaluating the reliability of a model within the framework of steady-state flow of ground water in two dimensions. This technique has been extended to three dimensions and is described in a later section. Before presenting the technique, the relationship between measured data in wells and model-calculated hydraulic head is discussed. Observation wells that have been installed in oil-shale strata rarely are piezometers.
Relationship of Measured Data and Calculated Results

Hydraulic Head

The relationship between hydraulic head in the formation and the water level measured in a well open to part or all of the formation is governed by aquifer properties, well-bore characteristics and the vertical-head gradient within the formation. An accurate treatment of the relationship would involve solving the three-dimensional equation of ground-water flow in the close vicinity of the well bore using model estimates of aquifer properties and a boundary condition of uniform head along the well bore. The computed head in the well could be compared to measured water-level data. This approach is not practical in most field problems. Instead, a relationship is used in the model that is based on the steady-state conservation of water within the well bore and Darcy's law. The result is a simple weighted average of hydraulic head.

\[
\frac{\int_{z_1}^{z_2} K_{ii} h dz}{\int_{z_1}^{z_2} K_{ii} dz} = \frac{h_{int}}{i = 1,2}
\]

where \( h_{int} \) = the depth-integrated head in the well [L],
\( h \) = hydraulic head obtained from the solution to equation 2 [L],
\( z_2 \) = the altitude of the top of the well bore open to the formation [L],
\( z_1 \) = the altitude of the bottom of the well bore open to the formation [L], and
\( K_{ii} \) = hydraulic conductivity [LT^{-1}].
Equation 7 is derived by writing Darcy's law for radial flow and integrating along the open interval of the well. Applying Darcy's law for radial flow from a circular boundary with no drawdown due to well-bore effects and assuming a well radius of 1 foot gives

\[ q = \frac{2\pi K (h_b - h_{int})}{\ln(r)} \]

where \( q \) = the Darcian flux per unit length of well bore \([LT^{-1}]\),

\( K \) = the hydraulic conductivity \([LT^{-1}]\),

\( h_b \) = the head at the boundary \([L]\),

\( h_{int} \) = the head in the well \([L]\), and

\( r \) = the distance to the boundary \([L]\).

The distance \( r \) may be thought of as the radius of influence by the well bore. By assuming steady-state flow along the well bore, the amount of water entering the well along part of the open interval must equal the amount leaving along the remainder of the open section. The integral expression for this conservation of mass is

\[ \int_{z_1}^{z_2} q \, dz = 0. \]

Substitution of Darcy's law for radial flow into the expression for conservation of mass gives

\[ \int_{z_1}^{z_2} \frac{K}{\ln(r)} h_b \, dz = h_{int} \int_{z_1}^{z_2} \frac{K}{\ln(r)} \, dz. \]

Treating distance to the boundary as a constant, \( \ln(r) \), may be moved outside the integral and equation 7 obtained.

The model in this report uses information on the open intervals of wells, estimates of hydraulic conductivity and calculated hydraulic head to determine the depth-integrated head at each observation well. The result may be compared to measured water-level data as a guide during model calibration when piezometers are not available.
Solute Concentration

The relationship between solute concentration in the formation and that in a well is governed by the three-dimensional equation of solute transport. As with hydraulic head, it is not practical to solve this problem at each well bore. By assuming steady-state conservation of solute and using Darcy's law, one can obtain an expression similar to equation 7.

\[
\frac{\int_{z_3}^{z_4} c q_i \, dz}{\int_{z_3}^{z_4} q_i \, dz} = \frac{\int_{z_3}^{z_4} c q_i \, dz}{\int_{z_3}^{z_4} q_i \, dz}
\]

where \( c_{\text{int}} \) = the depth-integrated solute concentration \([M/L^3]\),
\( c \) = solute concentration obtained from the solution to equation 4 \([M/L^3]\),
\( z_3 \) to \( z_4 \) = the part of the well bore where water enters \([L]\), and
\( q_i = K_{ii}(h-h_{\text{int}}) \).

Equation 7 is used in the model to infer sections of the well bore where water enters. The derivation of equation 8 essentially is identical to the derivation of equation 7 and will not be given here.
Estimating Parameters for Models of Steady-State Ground-Water Flow

Direct measurement of all hydrogeologic parameters needed to construct models of ground-water flow and solute transport is rarely possible. As a result, values of unmeasured parameters usually are adjusted until measured and calculated water levels and solute concentrations match in some acceptable manner. Cooley (1977) proposed a regression method for estimating an optimal set of hydrogeologic parameters and assessing parameter reliability within the framework of two-dimensional steady-state flow. An extension of this method to three dimensions is included in the model described in this report.

The following method is used to estimate parameters and assess reliability for a three-dimensional model of steady-state ground-water flow. Throughout the following development, deviations from the two-dimensional development of Cooley (1977) are noted. The method is an iterative technique that minimizes the squared difference between measured and calculated water levels in wells. To set up the iterative technique it is necessary to linearize the finite-element form of the equation of ground-water flow with respect to unknown model parameters, differentiate the linearized equation with respect to these parameters, and, setting each derivative equal to zero, solve the system of equations.
The derivatives of unknown model parameters are obtained in the following manner. A truncated Taylor series expansion of equation 2 is written for $(\Delta t)^{-1}$ equal to zero and $\theta$ equal to one. The resulting iterative equation is identical to the one given by Cooley (1977). Solving this Taylor series for hydraulic head gives

$$\tilde{h}^{r+1} = \tilde{h}^r + \tilde{\Delta}_r + \tilde{S}_r \tilde{b}^{r+1}$$

(9)

where $\tilde{h}^{r+1}$ = the vector of hydraulic head at the r+1 iteration;
$\tilde{h}$ = the vector of hydraulic head at the r iteration,
$\tilde{\Delta}_r$ = $-(\tilde{K}_r)^{-1} \tilde{f}_r$;
$\tilde{K}_r$ = the matrix involving estimates of hydraulic conductivity used in equation 2 at the r iteration;
$\tilde{f}_r$ = the functional representation of equation 2 at the r iteration,
$\tilde{S}_r$ = $-(\tilde{K}_r)^{-1}(\partial \tilde{G}_r / \partial \tilde{a}_r)$;
$\tilde{a}_r$ = the vector of model-parameter estimates at the r iteration, and
$\tilde{b}^{r+1}$ = $\tilde{a}^{r+1} - \tilde{a}_r$.

This equation is identical to the one used by Cooley (1977) to calculate hydraulic heads for each new iteration. The definitions of the variables are given in three dimensions instead of two.
Hydraulic head calculated by equation 9 cannot be compared directly to water-level measurements in wells unless the wells are constructed as piezometers. Because wells usually are open to some interval of aquifer, water levels represent a depth-integrated value of hydraulic head. Therefore, the least squares criterion that must be satisfied differs slightly from the criterion used by Cooley (1977), where vertical-head variations were not considered.

\[
\frac{\partial}{\partial b^{r+1}} \{ \tilde{w}(\tilde{h}_m - \tilde{h}_{\text{int}}^{r+1})^2 \} = 0
\]  

(10)

where \( \tilde{w} \) = a vector of weights between 0 and 1 describing the reliability of \( \tilde{h}_m \),

\( \tilde{h}_m \) = the measured head, and

\( \tilde{h}_{\text{int}}^{r+1} \) = the vector of depth-integrated head at the \( r+1 \) iteration.

Depth-integrated head is calculated by using the finite-element approximation to equation 7 in conjunction with equation 9. Substitution of the result in equation 10 gives the following:

\[
\tilde{w}(\tilde{N}_r \tilde{r})^T \tilde{N}_r \tilde{r} b^{r+1} = (\tilde{N}_r \tilde{r})^T \tilde{w}(\tilde{h}_m - \tilde{h}_r^{r+1} + \tilde{A}_r^{r+1})
\]  

(11)

where \( \tilde{N}_r \) = the matrix of finite-element approximations of equation 7 involving estimated hydraulic conductivity at the \( r \) iteration, and,

\( (\quad)^T \) = the matrix-transpose operation.

With the exception of the \( \tilde{N}_r \) term, equation 11 is identical to the least squares equation used by Cooley (1977). Equation 11 can be solved for \( \tilde{b}^{r+1} \) which in turn can be used to calculate estimates of model parameters. Because the Taylor series expansion used to linearize the equations of ground-water flow is an approximation, the solution of equation 11 may not give global optimum values of \( \tilde{b}^{r+1} \) unless \( \tilde{r}_{r}^{r+1} = \tilde{r}_r \) and \( \tilde{A}_{r}^{r+1} = \tilde{A}_r \) are small. Therefore iteration must be used.
The iteration procedure is identical to the one used by Cooley (1977). An initial estimate of aquifer properties and other unknown model parameters is used to solve equation 2 for hydraulic head. The coefficients $\frac{\partial f}{\partial a^r}$ are calculated and equation 11 is used to solve for $b^{r+1}$ and new estimates of model parameters. The iteration number is advanced by one and the Taylor series expansion of equation 2 is used to compute $f^r$. An iterative cycle is begun by resolving equation 2 with the latest estimates of aquifer properties and boundary flux rates until values for $f^{r+1}$ are less than some acceptable error.
Sensitivity Analysis of Transient Ground-Water Flow and Solute Transport

Development of a statistical procedure for estimating model parameters under transient conditions is more difficult than under steady-state conditions. Several approaches to solving this problem may be possible, but all have proven overly expensive in terms of disc storage, core storage or computational time. Therefore, calibration of transient ground-water flow and solute-transport models remains a trial-and-error process in this report.

A review of the differential equation of solute transport (eq. 3) shows that ground-water velocity acts as a calibration parameter. Therefore, it usually is necessary to develop a ground-water flow model concurrently with the development of a solute-transport model. Darcy's law is used to compute velocity from estimates of hydraulic conductivity and model-calculated head. The linkage between ground-water flow and solute transport often forces the hydrologist to iterate between the flow and transport models until a distribution of hydraulic conductivity is obtained that reproduces both historical water-level and solute-concentration data. Bibby (1981) observed that the solute-transport model can have a strong influence in determining optimal estimates of hydraulic conductivity.
EVALUATION OF MODEL

A number of tests of the model have been made including comparisons of model results to analytical solutions and to one field application. Because analytical solutions rarely exist for three-dimensional problems, tests have been designed to verify the accuracy of the model in one and two dimensions. Repeated applications of the test problems in each of the three directions were used to isolate any programming or logic errors. Comparisons of model results with analytical solutions are discussed below. Application of the model to a field problem, solute transport from an in situ oil-shale retort near Rock Springs, Wyo., will be discussed in a later report (K. C. Glover, U.S. Geological Survey, written commun., 1985).

Ground-Water Flow

An evaluation of the basic model of ground-water flow (eq. 2) has not uncovered any unusual characteristics. For problems with relatively regular boundaries, the evaluation showed that the finite-element method did not improve upon head distribution calculated by finite-difference methods. In problems with complex and irregular aquifer geometry, the finite-element method can be used to model the flow system with fewer nodes.
Model results were compared to Theis's analytical solution for drawdown in the vicinity of a pumping well (Lohman, 1979). The Theis solution is for a fully penetrating well in an infinite confined aquifer with no vertical movement of water. These conditions were simulated in the flow model by using variable node spacing, a zero-drawdown boundary 20,000 ft from the well, and uniform aquifer properties. The aquifer was assumed to be 100 ft thick with a hydraulic conductivity of 12.5 ft/d and specific storage of $10^{-6}$ ft$^{-1}$. Well discharge, distributed uniformly along the well bore, was simulated at a rate of 2.0 ft$^3$/sec. Model results and the analytical solution are plotted in figure 2 for three distances from the pumping well.
Figure 2.--Comparison of flow-model results with Theis's analytical solution.
The remainder of this section is a discussion of the regression technique for estimating aquifer properties and boundary-flow rates in steady-state systems. Most of the major conclusions of Cooley (1977 and 1979) seem to be appropriate for flow in three as well as two dimensions. Specific points of interest to three-dimensional problems are discussed below.

The number of aquifer properties and flux rates that are treated as regression parameters can have a strong influence on the convergence characteristics of the model. The vertical anisotropy that is common in most three-dimensional systems increases the number of regression parameters and can cause convergence problems more easily than in two-dimensional flow. The number of regression parameters in three dimensions also increases because horizontal hydraulic conductivity often varies with depth. With the large number of parameters that can occur in three-dimensional models it may be difficult to obtain adequate water-level data for all strata and convergence can be very slow. In cases where the number of regression parameters approaches the number of measured water levels, no solution may be possible. These characteristics can limit the use of the regression technique in three-dimensional problems.
Boundary-flux rates usually are measured with greatest accuracy when the flow occurs at or near the land surface. This fact has a number of implications in using the regression technique. If significant recharge and discharge occurs at depth as underflow and the hydraulic conductivity is not known exactly, the least-squares matrix usually is ill-conditioned and no solution is possible. On the other hand, if boundaries are identified at depth such that no flow occurs across them, a solution may be possible. However, the standard errors of estimate for hydraulic conductivity usually will be very large. Large standard errors can be common especially if measured water-level data do not accurately describe vertical head gradients throughout the study area.

Cooley (1977) found that models of ground-water flow are characterized by having large standard errors for the parameters. These errors are caused by anomalous measured water levels as well as errors in specified boundary conditions. If errors that usually occur in boundary-flux estimates are not considered during model applications, the resulting standard errors for the parameters usually will be artificially small. Test problems using the three-dimensional regression procedure supported these conclusions.
The regression model in this respect can be used to assess reliability of computed parameters and predicted values of head if the model is approximately linear with respect to the parameters. Cooley (1979) provides a test for linearity that also is applicable to three dimensions. Because the model is nonlinear with respect to hydraulic conductivity, the large number of hydraulic-conductivity parameters in most three-dimensional systems makes it more difficult to pass this test of linearity. Therefore, the use of confidence regions and test of hypothesis may not be appropriate for many three-dimensional problems. Additional testing of the regression method in three dimensions is needed to evaluate this conclusion.
Solute Transport

An analytical solution for one-dimensional solute transport from a specified concentration boundary into a fractured aquifer of uniform thickness is given by Bibby (1981, p. 1078). Fractures are assumed to be horizontal and separated by sufficient impermeable strata to be considered of infinite extent. The solute is considered to be non-reactive. The analytical solution was obtained by analogy to a corresponding solution for conduction and convection of heat into an aquifer.

Model results were compared to this analytical solution using representative values for aquifer characteristics. Seepage velocity of water in the fissures was set equal to 0.5 ft/d. Longitudinal and transverse dispersivities were set to 100 ft/d, and the diffusion coefficient of solute in water in the unfractured formation blocks was $5 \times 10^{-5}$ ft$^2$/d. The block porosity was set to unity to permit comparison with the analytical solution thickness of the blocks made sufficiently large so as not to violate assumptions in the analytical solution. Several simulations with various block dimensions were made to insure the assumptions were reproduced.

Model and analytical results after 100 days of solute transport are presented in figure 3. The close comparison verifies the model theory and program logic. The model slightly overestimates solute concentrations in the leading part of the profile and slightly underestimates concentrations in the trailing part. This characteristic probably is due to the effects of numerical dispersion associated with nodal spacing.
Figure 3.--Comparison of results from solute-transport model with analytical solution at 100 days.
Additional simulations were made with the dual-porosity equation to evaluate the sensitivity of the model to variations in the dual-porosity coefficients. The coefficients that had the greatest effect on the distribution of solute appeared to be shale-matrix porosity and fracture width. The matrix-diffusion coefficient and fracture density also were important in determining the distribution of solute. These observations are in agreement with those of Grisak and Pickens (1980) and show that in fractured rock, matrix diffusion can be an important mechanism for solute transport. Factors reducing the need to consider matrix diffusion are small matrix porosities and large fracture width and density.

A review of the dual-porosity equation (eq. 5) shows that a large number of coefficients must be known even for relatively simple fracture geometries. Because in most studies these coefficients must be estimated during model calibration, the amount of water-quality data needed is far greater than the amount needed to use a continuum model. Within the framework of a three-dimensional system, sufficient data may be available only for a preliminary calibration of the model. Nevertheless in rock where matrix diffusion is dominant, a scarcity of data is not sole justification for ignoring the more complex model.
A listing of the FORTRAN program that solves the three-dimensional equations of flow and solute transport in dual-porosity media is given in table 1 (at end of report). Data-input formats are described in table 2 (at end of report). Although data entry into a finite-element program typically is more cumbersome than for finite-difference programs, the increased data-entry time usually is compensated by increased flexibility in locating nodes. With a finite-element model, nodes can be accurately located at observation or pumping wells. In general, fewer nodes are needed to accurately model aquifer geometry when using a finite-element model.

Data entry into a finite-element program is more cumbersome because of the need to identify the relationships among all nodes and elements. As a result, all nodes and elements must be numbered, the Cartesian coordinates of all nodes must be coded, and the nodes associated with each element must be designated.

The system used to number aquifer nodes and elements has a significant impact on the efficiency and size of the computer program. The global coefficient matrices developed in equations 2 and 4 represent the largest block of computer storage used by the program. The solution technique is more efficient, in terms of time and storage requirements, if the size of the global coefficient matrices is minimized. Storage requirements of the global coefficient matrices are directly related to the largest difference between two node numbers in an aquifer element. Therefore, efficient nodal ordering minimizes this difference and improves the efficiency of the solution. The program calculates and prints the band width. If the dimensions of arrays are not sufficient, the simulation will stop.
SAMPLE SIMULATION

Use of the model is illustrated by simulating solute transport from a buried source in a three-layer aquifer system. The bottom layer represents an aquifer where horizontal joints are common within relatively thick impermeable rock. The middle layer represents an aquifer where vertical fractures are common. The top layer represents a homogeneous isotropic sandstone. Boundary conditions and nodal locations are shown horizontally in figure 4 and vertically in figure 5. Aquifer properties for each layer are given in table 3. Pumping by two wells, one from the bottom layer and one from the top, also is simulated. Steady-state flow conditions are assumed.

The input data used in the model run and results for one time step are listed in tables 4 and 5 (at end of report). Results present total time into the simulation, and the hydraulic head and solute concentration for each node in the finite-element grid. Principal components of Darcian velocity and dispersion coefficient also are printed for each element.
Figure 4.--Boundary conditions and node locations along the bottom of the aquifer system used in the sample simulation.
Figure 5.--Boundary conditions and node locations along a vertical section of the aquifer system used in the sample simulation.
<table>
<thead>
<tr>
<th>Aquifer property</th>
<th>Bottom layer</th>
<th>Middle layer</th>
<th>Top layer</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hydraulic conductivity</td>
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<td></td>
<td></td>
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<td>x-direction (feet/day)</td>
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<td>40.0</td>
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<tr>
<td>Hydraulic conductivity</td>
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<td></td>
<td></td>
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<td>z-direction (feet/day)</td>
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<td>.2</td>
<td>.4</td>
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<td>Specified-head boundary (feet)</td>
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<td>Solute-concentration boundary</td>
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<tr>
<td>(milligrams per liter)</td>
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</table>
SUMMARY

The model described in this report can simulate three-dimensional ground-water flow and solute transport in oil shale and associated hydrogeologic units. The model treats oil shale as a dual-porosity medium by simulating flow and transport within fractures using conventional finite-element methods. Diffusion of solute between fractures and the essentially static water of the shale matrix is simulated by including an analytical solution that acts as a source-sink term to the differential equation of solute transport. While knowledge of fracture orientation and spacing is needed to effectively use the model, it is not necessary to map the locations of individual fractures.

The computer program listed in the report incorporates many of the features of previous dual-porosity models while retaining a practical approach to solving field problems. As a result the report does not extend the theory of solute transport in any appreciable way. The emphasis in the report is on bringing together various aspects of solute-transport theory in a manner that is particularly suited to the unusual ground-water flow and solute-transport characteristics of oil-shale systems.

Methods for quantifying the uncertainty in parameter estimates that occur during model development are given in this report. The quasilinear regression method described by Cooley (1977) for estimating parameters and assessing reliability for two-dimensional models of steady-state ground-water flow has been extended to three dimensions. Because the number of model parameters in three-dimensional simulations generally is larger than in two-dimensional simulations, adequate water-level data may not be available for evaluating parameter reliability. When it is possible to evaluate parameter reliability, standard errors for hydraulic-conductivity estimates of buried strata generally are large.
A large number of aquifer properties must be evaluated when simulating solute transport through dual-porosity media. Because properties such as the matrix-diffusion coefficient, matrix porosity, and fracture width and density often are estimated during model calibration, a large amount of water-quality data is needed. Within the framework of a three-dimensional system, sufficient data may be available only for a preliminary calibration of the model. Nevertheless, matrix diffusion can be an important mechanism for solute transport in fractured rock.
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Table 1.—Computer-program listing

- A finite element program for the solution of
- Three-dimensional transient ground-water flow and solute
- Transport in fractured material
- Observations may be values of head and concentration in wells
- Elements are isoparametric cubes with linear sides.
- Guidelines for array dimensions -- if not solving transport problem
- The dimensions of transport arrays may be reduced to 1
- Let NVarH=NParH+NQPar+NPPar
- Set IDim.GE.NUHNP, JDIMH.GE.IBH, JDIMC.GE.IBC, KDIM.GE.NUHNP
- CURRENTLY DIMENSIONS ARE FOR A MAXIMUM OF
- NUHNP= 490 NUMEL=300 NTIME=52 IBH= 90 IBC=180 NPER=52 NTO=1
- NTRE= 0 NWT= 0 NOBMAX=30 NPBC= 0 NTB=0
- NParH= 8 NQPar= 0 NUMAT=7 NTFRAC=9 ITFRAC= 10 NLayer= 3
- MAIN ARRAYS
  - XTXH(NVarH,NVarH),BH(4*NVarH)
  - PH(NVarH),RKH(NVarH),HINT(NTO*NOBMAX)
  - ZSPACE(NLAYER-1),CINT(NTO*NOBMAX),TITLE(20),HP1(NUMNP*2), CP1(NUMNP*2),CO(NTO*NOBMAX), NXTO(NTO+1),NXTW(NTW+1),NXTS(NTS+1),NXTB(NTB+1)
  - DIMENSION XTXH(8,8),BH(32), PH(8),RKH(8),HINT(30),CINT(30), ZSPACE(3),TITLE(20), CO(30),NXTO(1), NXTW(1),NXTS(2),NXTB(1)
- COFBLK ARRAYS
  - H(NUMNP*2),C(NUMNP*2),QHMP(NUMNP),WELL(NUMNP*(NTW+1)), CFRAC(NUMNP*NTW+1),CINIT(NUMNP), WNODE(NUMNP),SFOBSH(NUMNP+NOBMAX),SFOBSC(NUMNP+NOBMAX), WPRH(NUMNP),CINIT(NUMAT),RX(NUMAT),RY(NUMAT),RZ(NUMAT), HO(NUMNP*NOBMAX),RC(NUMNP),RPR(NUMNP),DL(NUMAT),DT(NUMAT), IPH(NUMNP),HAT(NUMAT),NBP(NUMNP),RMT(NUMAT)
  - COMMON/COFBLK/CFRAC(10, 490),QHMP( 490),CINIT( 490), H( 980),C( 980),WELL( 490),WELLC( 490), RX( 7),RY( 7),RZ( 7), RFPR( 7),DFSPH( 520),DFSPSC( 520),WINOD( 490), DL( 7),DT( 7),THETA1,TIME,TIMFAC,TIMEH,CEQUI,DFW,
  - XORD(NUMNP),YORD(NUMNP),ZORD(NUMNP),QS(NUMNP*(NTS+1)),CS(NUMNP)
  - COMMON/SINBLK/QEH(8),QEC(8),XORD( 490),YORD( 490),ZORD( 490), $ QH( 980),CS( 980),CF( 1),NP(300,8),IPRHM(3,7),NAT(300),NBP( 490),IELHR
  - COMMON/SINBLK/QEH,QEC
- SENBLK ARRAY
  - WH(NUMNP*NOBMAX),WC(NUMNP*NOBMAX),NPBC(NUMNP,NTB+1),NODOBS(NUMNP)
  - COMMON/SENBLK/WH( 30), $ WC( 30),THETA1,NPBC( 490, 1),NODOBS( 490)
- LDUBLK --
Table 1.--Computer-program listing--Continued

C** CPKH(IDIN,IBH),SH(NVARH,NUNNP),QH(NUNNP) 540
C** CPKC(IDIM,IBC),QC(IBC) 550
COMMON/LDKBLK/CPKC(490,180),CPKH(490,90),SH(8,490), 560
$ QC(490),QH(490),IBC,IBH 570
REAL*8 CPKC,CPKH,SH,QC,QH 580
C** SHAZLKSURBLK AND LINBLK -- ALL DIMENSIONS CONSTANT 590
COMMON/SHABLK/SF(4,8,8),WF(4,8),WT(8),NUHPT 600
COMMON/SURBLK/AF(3,4),AWT,NQPAR 610
COMMON/LINBLK/RLF(2,2),RLWT,LINOD(4,2) 620
DOUBLE PRECISION SF,WT,WF,AF,AWT 630
C** SET # RECORDS IN FILE 8 TO (NTIME/NTPER+1), # WORDS TO NUNNP 640
C** SET # RECORDS IN FILE 9 TO (NTIME+1), # WORDS TO NUNNP 650
OPEN (UNIT=8,FILE='HEADS',ACCESS='DIRECT',FORM='UNFORMATTED', 660
$ RECL=816) 670
OPEN (UNIT=9,FILE='CONCN',ACCESS='DIRECT',FORM='UNFORMATTED', 680
$ RECL=816) 690
OPEN (UNIT=5,FILE='SAMPLE.INPUT',STATUS='OLD') 700
OPEN (UNIT=6,FILE='SOLUTION.PRT') 710
IDIM=490 720
JDIMH=90 730
KDIN=300 740
NVH=8 750
LDIMH=NVH*4 760
JDINC=180 770
DO 105 I=1,3 780
READ(5,1) TITLE(J),J=1,20 790
WRITE (6,2) (TITLE(J),J=1,20) 800
105 CONTINUE 810
WRITE (6,3) 820
READ (5,4) NUMEL,NUNNP,NUNMAT,NTIME,NTPER,NTB,NTO,NOMAX,NTW, 830
$ NTS,NPARH,NQPAR,NBPAR 840
WRITE (6,5) NUMEL,NUNNP,NUNMAT,NTIME,NTPER,NTB,NTO,NOMAX,NTW, 850
$ NTS,NPARH,NQPAR,NBPAR 860
READ (5,4) NPLAYR,NEPLAY 870
WRITE (6,68) NPLAYR,NEPLAY 880
READ (5,4) ITHMAX,IVELPR,IFRAC,NTFRAC,NIFRAC,NLAYER,IBEALE 890
WRITE (6,6) ITHMAX,IVELPR,IFRAC,NTFRAC,NIFRAC,NLAYER,IBEALE 900
WRITE (6,7) 910
READ (5,8) NTPRT,IP,O,P,R,P,RP,RE,CE 920
WRITE (6,8) NTPRT,IP,O,P,R,P,RP,RE,CE 930
READ (5,9) DTIME,TINFAC,THETAH,THETAC,DFW,CEQUI 940
WRITE (6,10) DTIME,TINFAC,THETAH,THETAC,DFW,CEQUI 950
READ (5,9) ALFAX,ALSAX,ALFAY,ALFZ 960
WRITE (6,11) ALFAX,ALSAX,ALFAY,ALFZ 970
C** INITIALIZE 980
TIMBGN=DTIME 990
DO 110 I=1,NUNNP 1000
H(I)=0.0 1010
NPBI(I)=0 1020
NPBC(I,1)=0 1030
NODOS(I)=0 1040
110 CONTINUE 1050
IF (THETAC.LT.0.0) GO TO 130 1060
Table 1.--Computer-program listing--Continued

DO 120 I=1,NUMNP
   C(I)=0.0
DO 120 J=1,NTFRAC
   CFRAC(J,I)=0.0
120 CONTINUE

130 N=NOBMAX*NTO
   NXTO(1)=999999
   IF (N.LE.0) GO TO 150
   DO 140 I=1,N
      HO(I)=0.0
      WH(I)=0.0
   CONTINUE
   IF (THETAC.LT.0.0) GO TO 140
   CO(I)=0.0
   WC(I)=0.0
140 CONTINUE

150 N=NUMNP*(NTW+1)
   NXTW(1)=999999
   DO 156 I=1,N
      WELL(I)=0.0
   CONTINUE
   IF (THETAC.GE.0.0) WELLC(I)=0.0
156 CONTINUE

150 N=NUMNP*(NTS+1)
   NXTS(1)=999999
   DO 158 I=1,N
      QS(I)=0.0
   CONTINUE
   IF (THETAC.GE.0.0) CS(I)=0.0
158 CONTINUE

160 CONTINUE
   NUMH=NUMNP-NLAYER+1
   NLAY2=NLAYER-2
   NLAY1=NLAYER-1
   DO 162 I=1,NH
      NH(I)=N-1
   CONTINUE
   DO 162 J=1,NH
      XORD(I+J)=XORD(I)
      YORD(I+J)=YORD(I)
      ZORD(I+J)=ZORD(I)+ZSPACE(J)
   CONTINUE
   WRITE(5,13) N

162 CONTINUE
   READ (5,13) N
   WRITE (6,13) (ZSPACE(I),I=1,NLAY1)
   WRITE (6,14) (ZSPACE(I),I=1,NLAY2)
   DO 164 J=1,NPBC(I,1)
      WRITE (6,15) (I,NPBC(I,1),NODOBS(I),WINOD(I),H(I),WELL(I),QS(I),
   $   ZORD(I),I=1,N)
   WRITE (6,16) (I,NPBC(I,1),NODOBS(I),WINOD(I),H(I),WELL(I),QS(I),
   $   ZORD(I),I=1,N,NUMNP)
   IF (THETAC.LT.0.0) GO TO 164
<table>
<thead>
<tr>
<th>Line</th>
<th>Code</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>160</td>
<td>WRITE (6,16)</td>
<td></td>
</tr>
<tr>
<td>161</td>
<td>READ (5,17) N</td>
<td></td>
</tr>
<tr>
<td>162</td>
<td>READ (5,17)(I,C(I),WELLC(I),CS(I),II=1,N)</td>
<td></td>
</tr>
<tr>
<td>163</td>
<td>WRITE(6,67)(I,C(I),WELLC(I),CS(I),I=1,NUMNP)</td>
<td></td>
</tr>
<tr>
<td>164</td>
<td>DO 163 I=1,NUMNP</td>
<td></td>
</tr>
<tr>
<td>165</td>
<td>CINIT(I)=C(I)</td>
<td></td>
</tr>
<tr>
<td>166</td>
<td>IBH=0</td>
<td></td>
</tr>
<tr>
<td>167</td>
<td>WRITE(6,18)</td>
<td></td>
</tr>
<tr>
<td>168</td>
<td>DO 170 I=1,NEPLAY</td>
<td></td>
</tr>
<tr>
<td>169</td>
<td>READ (5,19) I,N,(NP(I,J),J=1,4)</td>
<td></td>
</tr>
<tr>
<td>170</td>
<td>NM1=N-1</td>
<td></td>
</tr>
<tr>
<td>171</td>
<td>MAT(I)=1</td>
<td></td>
</tr>
<tr>
<td>172</td>
<td>DO 166 J=5,8</td>
<td></td>
</tr>
<tr>
<td>173</td>
<td>NP(I,J)=NP(I,J-4)+1</td>
<td></td>
</tr>
<tr>
<td>174</td>
<td>IF (NM1.LE.2) GO TO 170</td>
<td></td>
</tr>
<tr>
<td>175</td>
<td>DO 168 K=1,NM1</td>
<td></td>
</tr>
<tr>
<td>176</td>
<td>MAT(I+K)=K+1</td>
<td></td>
</tr>
<tr>
<td>177</td>
<td>NP(I+K,J)=NP(I,J)+K</td>
<td></td>
</tr>
<tr>
<td>178</td>
<td>CONTINUE</td>
<td></td>
</tr>
<tr>
<td>179</td>
<td>IF (J1.GT.IBH) IBH=J1</td>
<td></td>
</tr>
<tr>
<td>180</td>
<td>DO 174 I=1,NUMEL</td>
<td></td>
</tr>
<tr>
<td>181</td>
<td>WRITE (6,20) I,(NP(I,J),J=1,8)</td>
<td></td>
</tr>
<tr>
<td>182</td>
<td>DO 172 J=1,8</td>
<td></td>
</tr>
<tr>
<td>183</td>
<td>DO 172 K=1,8</td>
<td></td>
</tr>
<tr>
<td>184</td>
<td>J1=IABS(NP(I,J)-NP(I,K))</td>
<td></td>
</tr>
<tr>
<td>185</td>
<td>IF (J1.GT.IBH) IBH=J1</td>
<td></td>
</tr>
<tr>
<td>186</td>
<td>CONTINUE</td>
<td></td>
</tr>
<tr>
<td>187</td>
<td>IF (NUHNP.GT.IDIX) STOP</td>
<td></td>
</tr>
<tr>
<td>188</td>
<td>IBPRM(I)=0</td>
<td></td>
</tr>
<tr>
<td>189</td>
<td>READ (5,26) RX(I),RY(I),RZ(I),RC(I),II=1,NMAT</td>
<td></td>
</tr>
<tr>
<td>190</td>
<td>DO 190 I=1,NMAT</td>
<td></td>
</tr>
<tr>
<td>191</td>
<td>IF (RC(I).NE.0.0) ISTEDY=0</td>
<td></td>
</tr>
</tbody>
</table>

Table 1.--Computer-program listing--Continued
Table 1.--Computer-program listing--Continued

READ (5,27) (DL(I),DT(I),DM(I),RPR(I),FP(I),FQ(I),RMT(I),
RPBR(I),I=1,NMAT) 2130
WRITE (6,29) (I,DL(I),DT(I),DM(I),RPR(I),FP(I),FQ(I),RMT(I)
RPBR(I),I=1,NMAT) 2140
IF (IFRAC.NE.1) GO TO 196 2150
WRITE (6,32) 2160
READ (5,27) (CBINIT(I),I=1,NMAT) 2170
WRITE (6,33) (CBINIT(I),I=1,NMAT) 2180
IF (NPARH.LT.1) GO TO 206 2190
DO 198 I=1,NPARH 2200
RKH(I)=0.0 2210
196 CONTINUE 2220
WRITE (6,34) 2230
READ (5,35) (I,IPRMH(1,I),IPRM(2,I),IPRMH(3,I),I=1,NMAT) 2240
WRITE (6,35) (I,IPRMH(1,I),IPRM(2,I),IPRMH(3,I),I=1,NMAT) 2250
IXTRFL=0 2260
DO 200 I=1,NMAT 2270
IF (IPRMH(1,I).GT.0) IXTRFL=1 2280
IF (IPRMH(2,I).GT.0) IXTRFL=1 2290
IF (IPRMH(3,I).GT.0) IXTRFL=1 2300
200 CONTINUE 2310
WRITE (6,36) 2320
READ (5,37) (I,RKH(I),I=1,NPARH) 2330
WRITE (6,37) (I,RKH(I),I=1,NPARH) 2340
IF (NQPAR.LE.0) GO TO 208 2350
WRITE (6,40) 2360
READ (5,41) (I,QF(I),RKH(I+NP),I=1,NQPAR) 2370
WRITE (6,41) (I,QF(I),RKH(I+NP),I=1,NQPAR) 2380
IXTRFL=1 2390
IF (THETAC.LT.0.0) GO TO 208 2400
WRITE (6,42) 2410
READ (5,37) (I,CF(I),I=1,NQPAR) 2420
WRITE (6,37) (I,CF(I),I=1,NQPAR) 2430
208 CONTINUE 2440
WRITE (6,44) (I,NBP(I),I=1,NUMP) 2450
WRITE (6,45) (I,NBP(I),I=1,NUMP) 2460
DO 210 I=1,NBP 2470
READ (5,43) (I,RKH(I+NPAH+NQPAR),I=1,NQPAR) 2480
WRITE (6,37) (I,RKH(I+NPAH+NQPAR),I=1,NQPAR) 2490
210 CONTINUE 2500
WRITE (6,46) (I,NTP(I),I=1,NTP) 2510
WRITE (6,47) (I,NTP(I),I=1,NTP) 2520
CONTINUE 2530
212 CONTINUE 2540
DO 216 I=1,NUMP 2550
H(I+NUMP)=H(I) 2560
IF (THETAC.LT.0.0) GO TO 216 2570
C(I+NUMP)=C(I) 2580
IF (IFRAC.EQ.0) GO TO 216 2590
DO 214 J=1,NTP 2600
214 CONTINUE 2610
216 CONTINUE 2620
C** READ TRANSIENT DATA 2630
IF (NTP.LE.0.AND.ITMAX.EQ.0) GO TO 228 2640
NXTB(1)=999999 2650
Table 1.—Computer-program listing—Continued

<table>
<thead>
<tr>
<th>Line</th>
<th>Code</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 IBCTN=1</td>
<td>2660</td>
<td></td>
</tr>
<tr>
<td>2 IHR=1</td>
<td>2670</td>
<td></td>
</tr>
<tr>
<td>3 ICR=1</td>
<td>2680</td>
<td></td>
</tr>
<tr>
<td>4 WRITE (8'IHR) (H(J),J=1,NUMNP)</td>
<td>2690</td>
<td></td>
</tr>
<tr>
<td>5 WRITE (9'ICR) (C(J),J=1,NUMNP)</td>
<td>2700</td>
<td></td>
</tr>
<tr>
<td>6 IHR=IHR+1</td>
<td>2710</td>
<td></td>
</tr>
<tr>
<td>7 ICR=ICR+1</td>
<td>2720</td>
<td></td>
</tr>
<tr>
<td>8 NTM=NTIME/NTPER</td>
<td>2730</td>
<td></td>
</tr>
<tr>
<td>9 IF (NTB.GT.0) READ(5,46) I1,I2</td>
<td>2740</td>
<td></td>
</tr>
<tr>
<td>10 DO 226 I=1,NTM</td>
<td>2750</td>
<td></td>
</tr>
<tr>
<td>11 IF (NTB.LE.0) GO TO 222</td>
<td>2760</td>
<td></td>
</tr>
<tr>
<td>12 IF (((I-1)*NTPER.LT.I1)) GO TO 222</td>
<td>2770</td>
<td></td>
</tr>
<tr>
<td>13 IBM=IBCTN</td>
<td>2780</td>
<td></td>
</tr>
<tr>
<td>14 IBCTN=IBCTN+1</td>
<td>2790</td>
<td></td>
</tr>
<tr>
<td>15 NXTB(IBM)=I1</td>
<td>2800</td>
<td></td>
</tr>
<tr>
<td>16 DO 218 J=1,NUMNP</td>
<td>2810</td>
<td></td>
</tr>
<tr>
<td>17 NPBC(J,IBCTN)=NPBC(J,IBM)</td>
<td>2820</td>
<td></td>
</tr>
<tr>
<td>18 CONTINUE</td>
<td>2830</td>
<td></td>
</tr>
<tr>
<td>19 WRITE (6,47) I1</td>
<td>2840</td>
<td></td>
</tr>
<tr>
<td>20 DO 220 K=1,IBM</td>
<td>2850</td>
<td></td>
</tr>
<tr>
<td>21 READ (5,48) J,NPBC(J,IBCTN),H(J),XI</td>
<td>2860</td>
<td></td>
</tr>
<tr>
<td>22 IF (THETAC.GE.0.0) C(J)=XI</td>
<td>2870</td>
<td></td>
</tr>
<tr>
<td>23 CONTINUE</td>
<td>2880</td>
<td></td>
</tr>
<tr>
<td>24 I1=999999</td>
<td>2890</td>
<td></td>
</tr>
<tr>
<td>25 IF (IBM.LT.NTB) READ (5,46) I1,I2</td>
<td>2900</td>
<td></td>
</tr>
<tr>
<td>26 WRITE (8'IHR) (H(J),J=1,NUMNP)</td>
<td>2910</td>
<td></td>
</tr>
<tr>
<td>27 IHR=IHR+1</td>
<td>2920</td>
<td></td>
</tr>
<tr>
<td>28 IF (THETAC.LT.0.0) GO TO 226</td>
<td>2930</td>
<td></td>
</tr>
<tr>
<td>29 DO 224 K=1,NTPER</td>
<td>2940</td>
<td></td>
</tr>
<tr>
<td>30 WRITE (9'ICR) (C(J),J=1,NUMNP)</td>
<td>2950</td>
<td></td>
</tr>
<tr>
<td>31 ICR=ICR+1</td>
<td>2960</td>
<td></td>
</tr>
<tr>
<td>32 CONTINUE</td>
<td>2970</td>
<td></td>
</tr>
<tr>
<td>33 NXTB(NTB+1)=999999</td>
<td>2980</td>
<td></td>
</tr>
<tr>
<td>34 IF (NTO.LE.0) GO TO 236</td>
<td>2990</td>
<td></td>
</tr>
<tr>
<td>35 N=NTO*NOBMAX</td>
<td>3000</td>
<td></td>
</tr>
<tr>
<td>36 DO 230 I=1,N</td>
<td>3010</td>
<td></td>
</tr>
<tr>
<td>37 HINT(I)=0.0</td>
<td>3020</td>
<td></td>
</tr>
<tr>
<td>38 IF (THETAC.GE.0.0) CINT(I)=0.0</td>
<td>3030</td>
<td></td>
</tr>
<tr>
<td>39 CONTINUE</td>
<td>3040</td>
<td></td>
</tr>
<tr>
<td>40 WRITE (6,49)</td>
<td>3050</td>
<td></td>
</tr>
<tr>
<td>41 DO 234 I=1,NTO</td>
<td>3060</td>
<td></td>
</tr>
<tr>
<td>42 READ (5, 50) I1</td>
<td>3070</td>
<td></td>
</tr>
<tr>
<td>43 WRITE (6, 51) I1</td>
<td>3080</td>
<td></td>
</tr>
<tr>
<td>44 NTO(I)=I1</td>
<td>3090</td>
<td></td>
</tr>
<tr>
<td>45 DO 234 J=1,NOBMAX</td>
<td>3100</td>
<td></td>
</tr>
<tr>
<td>46 READ (5, 52) K,X1,X2,X3,X4</td>
<td>3110</td>
<td></td>
</tr>
<tr>
<td>47 WRITE(6, 52) K,X1,X2,X3,X4</td>
<td>3120</td>
<td></td>
</tr>
<tr>
<td>48 L=NOBMAX*(I-1)+K</td>
<td>3130</td>
<td></td>
</tr>
<tr>
<td>49 HO(L)=X1</td>
<td>3140</td>
<td></td>
</tr>
<tr>
<td>50 WH(L)=X2</td>
<td>3150</td>
<td></td>
</tr>
<tr>
<td>51 IF (THETAC.LT.0.0) GO TO 234</td>
<td>3160</td>
<td></td>
</tr>
<tr>
<td>52 CO(L)=X3</td>
<td>3170</td>
<td></td>
</tr>
<tr>
<td>53</td>
<td>3180</td>
<td></td>
</tr>
</tbody>
</table>
Table 1.--Computer-program listing--Continued

234 CONTINUE 3190
236 NXT0(NT0+1)=999999 3200
IF (NTW.LE.0) GO TO 242 3210
WRITE (6,53) 3220
DO 240 I=1,NTW 3230
DO 238 J=1,NUMNP 3240
J1=NUMNP*I+J 3250
WELL(J1)=WELL(J1-1)+NUMNP 3260
IF (THETAC.GE.0.0) WELLC(J1)=WELLC(J1-1)+NUMNP 3270
238 CONTINUE 3280
READ (5, 50) I1, I2 3290
WRITE (6, 54) I1 3300
NXTW(I)=I1 3310
ITMP=MOD(I1,NTPER) 3320
I1=NUMNP*(I) 3330
IF (ITMP.NE.1) GO TO 248 3340
DO 240 J=1,I2 3350
READ (5,52) K, X1, X2 3360
WRITE (6,52) K, X1, X2 3370
L=I1+K 3380
IF (ITMP.EQ.1) WELL(L)=X1 3390
IF (THETAC.GE.0.0) WELLC(L)=X2 3400
240 CONTINUE 3410
242 NXTW(NTW+1)=999999 3420
IF (NTS.LE.0) GO TO 250 3430
WRITE (6,55) 3440
DO 246 I=1,NTS 3450
DO 244 J=1,NUMNP 3460
J1=NUMNP*I+J 3470
QS(J1)=QS(J1-1) 3480
IF (THETAC.GE.0.0) CS(J1)=CS(J1-1) 3490
244 CONTINUE 3500
READ (5, 50) I1, I2 3510
WRITE (6, 56) I1 3520
NXTS(I)=I1 3530
ITMP=MOD(I1,NTPER) 3540
I1=NUMNP*(I) 3550
IF (ITMP.NE.1) GO TO 248 3560
DO 246 J=1,I2 3570
READ (5,52) K, X1, X2 3580
WRITE (6,52) K, X1, X2 3590
L=I1+K 3600
QS(L)=X1 3610
IF (THETAC.GE.0.0) CS(I)=X2 3620
246 CONTINUE 3630
GO TO 250 3640
248 WRITE(6,80) GO TO 250 3650
STOP 3660
250 NXTS(NTS+1)=999999 3670
1 FORMAT (20A4) 3680
2 FORMAT (1X,20A4) 3690
3 FORMAT (' NUMEL NUMNP NUMAT NTIME', 3700
6.2
<table>
<thead>
<tr>
<th>FORMAT</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$'\text{ NTPER }\text{ NTB }\text{ NTO NOBMAX }\text{ NTW}'$</td>
<td>3720</td>
</tr>
<tr>
<td>$'\text{ NTS NPARH NQPAR NBPAR}'$</td>
<td>3730</td>
</tr>
<tr>
<td>(14I5)</td>
<td>3740</td>
</tr>
<tr>
<td>(14I7)</td>
<td>3750</td>
</tr>
<tr>
<td>('ODTMAX=','I5,' IVELPR=','I5,' IFRAC=','I5,' $' NTFRAC=','I5,' ITFRAC=','I5,' NAYER=','I5,' IBEALE=','I5')</td>
<td>3760</td>
</tr>
<tr>
<td>(14I5)</td>
<td>3770</td>
</tr>
<tr>
<td>(3I5,5E10.3)</td>
<td>3780</td>
</tr>
<tr>
<td>(7E10.3)</td>
<td>3790</td>
</tr>
<tr>
<td>('ODTINE = ','E12.5,' TIMFAC = ','F5.2,' THETAH = ','F5.2,' &amp; ' THETAC = ','F5.2/' DFW = ','E12.5,' $' CEQUI = ','E12.5')</td>
<td>3800</td>
</tr>
<tr>
<td>('ALFLG = ','E12.5,' ALFAX = ','E12.5,' ALFAZ = ','E12.5')</td>
<td>3810</td>
</tr>
<tr>
<td>(2I10,3E10.3)</td>
<td>3820</td>
</tr>
<tr>
<td>(12I10)</td>
<td>3830</td>
</tr>
<tr>
<td>(3I10,4E10.3)</td>
<td>3840</td>
</tr>
<tr>
<td>(3I5,7E10.3)</td>
<td>3850</td>
</tr>
<tr>
<td>('NODE C WELLC CS')</td>
<td>3860</td>
</tr>
<tr>
<td>(1I10,3E10.3)</td>
<td>3870</td>
</tr>
<tr>
<td>('ELEMENT NP ARRAY')</td>
<td>3880</td>
</tr>
<tr>
<td>(8I5)</td>
<td>3890</td>
</tr>
<tr>
<td>(15,5X,8I5)</td>
<td>3900</td>
</tr>
<tr>
<td>('ELEMENT MAT IBPRM')</td>
<td>3910</td>
</tr>
<tr>
<td>$'\text{ ELEMENT MAT IBPRM}'$</td>
<td>3920</td>
</tr>
<tr>
<td>$'\text{ ELEMENT MAT IBPRM}'$</td>
<td>3930</td>
</tr>
<tr>
<td>(1I10,3E10.3)</td>
<td>3940</td>
</tr>
<tr>
<td>(8I10)</td>
<td>3950</td>
</tr>
<tr>
<td>(3I10)</td>
<td>3960</td>
</tr>
<tr>
<td>('ZONE RX RY RZ RC')</td>
<td>3970</td>
</tr>
<tr>
<td>(8E10.3)</td>
<td>3980</td>
</tr>
<tr>
<td>('ZONE DL DT DM RP')</td>
<td>3990</td>
</tr>
<tr>
<td>(3E10.3)</td>
<td>4000</td>
</tr>
<tr>
<td>('FP FQ RMT RPBR')</td>
<td>4010</td>
</tr>
<tr>
<td>(8E10.3)</td>
<td>4020</td>
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<tr>
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<td>4030</td>
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<tr>
<td>('OCBINIT VALUES')</td>
<td>4040</td>
</tr>
<tr>
<td>(1X,8F10.3)</td>
<td>4050</td>
</tr>
<tr>
<td>('ZONE IPRMH ARRAY')</td>
<td>4060</td>
</tr>
<tr>
<td>(5I5)</td>
<td>4070</td>
</tr>
<tr>
<td>('PARAMETER RKH')</td>
<td>4080</td>
</tr>
<tr>
<td>(1I10,15I5)</td>
<td>4090</td>
</tr>
<tr>
<td>('PARAMETER QF RKH')</td>
<td>4100</td>
</tr>
<tr>
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<td>4110</td>
</tr>
<tr>
<td>('PARAMETER C')</td>
<td>4120</td>
</tr>
<tr>
<td>(1I10,2E10.3)</td>
<td>4130</td>
</tr>
<tr>
<td>('PARAMETER RKH')</td>
<td>4140</td>
</tr>
<tr>
<td>(1I10,15I5)</td>
<td>4150</td>
</tr>
<tr>
<td>('PARAMETER RKH')</td>
<td>4160</td>
</tr>
<tr>
<td>(1I10,15I5)</td>
<td>4170</td>
</tr>
<tr>
<td>('NBP ARRAY'/15I5)</td>
<td>4180</td>
</tr>
<tr>
<td>('BOUNDARY PARM RKH')</td>
<td>4190</td>
</tr>
<tr>
<td>(2I5)</td>
<td>4200</td>
</tr>
<tr>
<td>('ZONE VARYING BOUNDARY CONDITIONS -- KT = ','I5')</td>
<td>4210</td>
</tr>
<tr>
<td>$'\text{ NODE NPBC',9X,'H',9X,'C'}$</td>
<td>4220</td>
</tr>
<tr>
<td>(2I15,F10.3,F10.3)</td>
<td>4230</td>
</tr>
<tr>
<td>(2I5,F10.3,F10.3)</td>
<td>4240</td>
</tr>
</tbody>
</table>
Table 1.--Computer-program listing--Continued

49 FORMAT ('OBSERVED HEAD AND CONCENTRATION DATA') 4250
50 FORMAT (2110) 4260
51 FORMAT (' TIME STEP ',I5/, ' OBS HO WH', 4270
\& ' CO WC') 4280
52 FORMAT (110,4E10.3) 4290
53 FORMAT (' TIME VARYING POINT SOURCE-SINK DATA') 4300
54 FORMAT (' TIME STEP ',I5/, ' NODE WELL WELLC') 4310
55 FORMAT (' TIME VARYING LINE SOURCE-SINK DATA') 4320
56 FORMAT (' TIME STEP ',I5/, ' NODE QS CS') 4330
57 FORMAT (' TIME STEP ',I5/, ' TOTAL TIME OF SIMULATION',F12.2/) 4340
\$ ' NODE XORD YORD', 4350
\$ ' ZORD H C') 4360
58 FORMAT (110,5E12.5) 4370
59 FORMAT (110,3E12.5,12X,E12.5) 4380
60 FORMAT (' OBS HO HINT', 4390
\& ' CO CINT') 4400
61 FORMAT (15,4(1X,E12.5)) 4410
62 FORMAT (15,26X,2(1X,E12.5)) 4420
63 FORMAT (' STATISTICS OF INITIAL HEAD SOLUTION') 4430
64 FORMAT (' STATISTICS OF INITIAL CONCENTRATION SOLUTION') 4440
65 FORMAT (' NUMBER OF OBSERVATIONS = ',I5/, ' ESTIMATED SUM OF ', 4450
\$ 'SQUARED ERRORS FOR INITIAL SOLUTION = ',E12.5/) 4460
\$ ' ERROR VARIANCE FOR INITIAL SOLUTION = ',E12.5) 4470
66 FORMAT (' INITIAL SOLUTION') 4480
67 FORMAT (110,3E10.3,110,3E10.3,110,3E10.3) 4490
68 FORMAT (' NPLAYR=',I5,' NEPLAY=') 4500
69 FORMAT (' NODE NPBC NODOBS WTNOD XORD YORD ZORD', 4510
\$ ' H WELL QS') 4520
70 FORMAT (' FLOW PROBLEM') 4530
71 FORMAT (' SOLUTE TRANSPORT PROBLEM') 4540
72 FORMAT (' FLOW PROBLEM BAND WIDTH = ',I5/, ' TRANSPORT PROBLEM ', 4550
\$ ' BAND WIDTH = ',I5) 4560
73 FORMAT (' UPDATED PARAMETERS'/' HATI RX', 4570
\$ ' RY RZ ') 4580
74 FORMAT (15,3(1X,E11.5)) 4590
75 FORMAT (' PARAMETER QF ') 4600
76 FORMAT (110,1X,E11.5) 4610
77 FORMAT (' FLOW PARAMETER ',I5,' EFFECTIVELY ZERO') 4620
78 FORMAT (' SOLUTION FAILED TO CONVERGE IN ',I5,' ITERATIONS') 4630
79 FORMAT (' SOLUTION CONVERGED IN ',I5,' ITERATIONS') 4640
80 FORMAT (' TIME STEP IS INVALID FOR A CHANGE OF PARAMETERS'/' 4650
\$ ' TIME STEP MUST BE DIVISIBLE BY NPER WITH A REMAINDER', 4660
\$ ' OF 1') 4670
CALL SHAFAC(THETAC)
CALL SURFAC
CALL LINFAC
NVARH=NPARH+NQPAR+NBPAR
NVHX2=NVARH+NVARH
NVHX3=NVARH+NVHX2
NODS=8
C** COMPUTE AND COUNT PRIOR INFORMATION
NPRIRH=0
IF (NVARH.LT.1) GO TO 254

64
Table 1.--Computer-program listing--Continued

DO 252 I=1,NVARH
PH(I)=1.0
IF (RKH(I).LE.0.0) GO TO 252
RKH(I)=EVH/(RKH(I)*RKH(I))
NPRIRH=NPRIRH+1
252 CONTINUE

C** COMPUTE INITIAL SOLUTION
254 WRITE (6,66)
IFLOW=0
KTH=0
IOBCNT=1
IWCNT=1
ISCNT=1
IBCNT=1
SKBIG=0.0
SKBIG2=0.0
DTIME=TIMBGN/TIMFAC
TIMSUM=0.0
OBSh=0.0
YSHQ=0.0
ERVARH=0.0
OBSO=0.0
YSQO=0.0
ERVAC=0.0
IOBCNT=1
DO 294 KT=1,NTIME
DTIME=DTIME*TIMFAC
TIMSUM=TIMSUM+DTIME
LU=0
IFLOW=IFLOW+1
IF (IFLOW.GT.NTPER) IFLOW=1
IF (IFLOW.EQ.1) KTH=KTH+1
IF (KT.EQ.1) LU=1
IF (KT.GT.NXTO(IOBCNT)) IOBCNT=IOBCNT+1
IF (KT.EQ.NXTB(IBCNT)) LU=1
IF (TIMFAC.GT.1.01) LU=1
LUH=LU
LUC=LU
IF (KT.EQ.NXTW(IWCNT)) IWCNT=IWCNT+1
IF (KT.EQ.NXTS(ISCNT)) ISCNT=ISCNT+1
IF (KT.EQ.NXTB(IBCNT)) IBCNT=IBCNT+1
IF (IFLOW.GT.1) GO TO 260
IF (NTB.LE.0) GO TO 258
IHR=KTH+1
DO 256 I=1,NUMNP
J=I+NUMNP
H(I)=H(J)
256 CONTINUE
J1=NUMNP+1
J2=NUMNP*2
READ (8*IHR) (H(J),J=J1,J2)
258 CALL FLOW (IWCNT,ISCNT,IBCNT,KT,KTH,
$ NTPER,NUMNP,NVARH,NPARH,LUH,NUMEL)}
Table 1.—Computer-program listing—Continued

$ ISTEDY,0,IDIM)
  CALL UDU (NUMNP,LUH)
  ICR=KI+1
  DO 262 I=1,NUMNP
  J=I+NUMNP
  IF (IFLOW.EQ.1) H(J)=QH(I)
  IF (THETAC.LT.0.0) GO TO 262
  CJ=QJ
  262 CONTINUE
  IF (THETAC.LT.0.0) GO TO 270
  IF (NTB.LE.0) GO TO 264
  J1=NUMNP+1
  J2=NUMNP*2
  READ(9'ICR) (C(J),J=J1,J2)
  IVPTMP=0
  IF (MOD(KT,NTPR).EQ.0) IVPTMP=1
  CALL SALT (IFLOW,IWCNT,ISCNT,IBCNT,KT,KTH,$
             NTPER,NUMNP,LUC,NUMEL,ISTEDY,IVPTMP,IFRAC,1,0,$
             IDIM,ALFAX,ALFAX,ALFAZ,ALFL,NTPR,ITFRAC,ITFRAC,$
             NOBMAX,IOBCNT)
  CALL LDU (NUMNP,LUC)
  DO 268 I=1,NUMNP
   C(I)=QC(I)
  IF (IFRAC.EQ.0) GO TO 268
  DO 266 J2=NTFI
   J2=J-1
   CFRAC(J1,I)-CFRAC(J,I)
  266 CONTINUE
  CFRAC(NTFI,I)=QC(I)
  268 CONTINUE
  IHR=KTH+1
  ICR=KI+1
  J1=NUMNP+1
  J2=NUMNP*2
  IF (IFLOW.GT.1.OR.NVARH.EQ.0) GO TO 272
  WRITE (8'IHR) (H(J),J=J1,J2)
  272 IF (THETAC.LT.0.0) GO TO 274
  WRITE (9'ICR) (C(J),J=J1,J2)
  274 IF (MOD(KT,NTPR).NE.0) GO TO 280
  WRITE (6,57) KT,THSUM
  DO 278 I=1,NUMNP
   C(I)=QC(I)
  IF (THETAC.GE.0.0) GO TO 276
  IF (IFLOW.EQ.1) WRITE (6,58) I,XORD(I),YORD(I),ZORD(I),H(I2)
  276 IF (IFLOW.EQ.1) WRITE (6,58) I,XORD(I),YORD(I),ZORD(I),H(I2),C(I)
  IF (IFLOW.NE.1) WRITE (6,59) I,XORD(I),YORD(I),ZORD(I),C(I)
  278 CONTINUE
  280 IF (NOBMAX.LE.0) GO TO 294
  IF (KT.NE.NXTO(IOBCNT)) GO TO 294
  C** COMPUTE INITIAL ERROR VARIANCE

44
Table 1.--Computer-program listing--Continued

DO 286 I=1,NUNNP
  282 IF (NODOBS(I).LE.0) GO TO 286
  283 I3=NUNNP+I
  284 I2=NODOBS(I)+NOBMAX*(IOBCNT-1)
  285 IF (IFLOW.GT.1) GO TO 284
  286 HINT(I2)=HINT(I2)+SFOBSH(I)*H(I3)
  288 IF (THETAC.LT.0.0) GO TO 286
  289 CONTINUE
WRITE (6,60)
  290 DO I=1,NOBMAX
  291 I2=I+NOBMAX*(IOBCNT-1)
  292 IF (IFLOW.EQ.1.AND.THETAC.GE.0.0) WRITE (6,61) I,HO(I2),HINT(I2)
$ ,CO(I2),CINT(I2)
  293 IF (IFLOW.EQ.1.AND.THETAC.LT.0.0) WRITE (6,61) I,HO(I2),HINT(I2)
  294 IF (IFLOW.GT.1.AND.THETAC.GE.0.0) WRITE (6,62) I,CO(I2),CINT(I2)
  295 CONTINUE
  296 IF (NOBMAX.LE.0) GO TO 640
  297 ERVARH=YSQH/(OBSH-NVARH+NPRIRH)
  298 NTMP=OBSH
WRITE (6,63)
  299 WRITE (6,65) NTMP,YSQH,ERVARH
  300 IF (THETAC.LT.0.0) GO TO 296
  301 ERVARC=YSQH/(OBSC-NVARGNPRIRC)
  302 NTMP=OBSC
WRITE (6,64)
  303 WRITE (6,66) NTMP,YSQC,ERVARC
C** BEGIN ITERATIONS
  304 INDT=O
  305 ERP=1000.0
  306 IF (ITMAX.LE.0) GO TO 640
  307 IF (ISTEDY.EQ.0) GO TO 640
  308 DO 372 ITER=1,ITMAX
  309 IOBCNT=1
  310 IWCHT=1
  311 ISCNT=1
  312 IBCNT=1
  313 IFLOW=1
  314 KHI=1
  315 DTIM=TINBGN/TIMFAC
  316 TIMSUM=0.0
  317 372 CONTINUE
  318 374 CONTINUE
  319 376 CONTINUE
  320 378 CONTINUE
  321 380 CONTINUE
  322 382 CONTINUE
  323 384 CONTINUE
  324 386 CONTINUE
  325 388 CONTINUE
  326 390 CONTINUE
  327 392 CONTINUE
  328 394 CONTINUE
  329 396 CONTINUE
  330 }
Table 1.--Computer-program listing--Continued

IF (AMP.LT.-.5) GO TO 304
YSQH=0.0
DO 302 I=1,NVARH
B(H(I))=0.0
DO 302 J=1,NVARH
XTXH(I,J)=0.0
302 CONTINUE
304 IHR=1
J1=NUMNP+1
J2=NUMNF*2
READ (8'IHR) (H(J),J=J1,J2)
D TIME=D TIME*TIMFAC
TIMSUM=TIMSUM+D TIME
LU=0
DO 316 I=1,NUMNP
J=I+NUMNP
H(I)=H(J)
316 CONTINUE
J1=NUMNP+1
J2=NUMNF*2
IHR=KTH+1
READ (8'IHR)(H(J),J=J1.J2)
CALL FLOW (IWCNT,ISCNT,IBCNT,KT,KTH,
$ NTPER,NVARN,HPARH,LU,NULNM,
$ ISTEP,ITER,IDI)
CALL SENS (NVARN,NUMNP,IPOK,T,KTH,IOBCNT,
$ IXTRFL,NOBMAX,IBCNT)
DO 322 I=1,NUMNP
QHTMP(I)=QH(I)
322 CONTINUE
DO 324 I=1,NUMNP
IF (NPBC(I,IBCNT).GE.0.OR.NPBC(I,IBCNT).EQ.-2.OR.NPBC(I,IBCNT) .EQ.-4) GO TO 324
IF (NBP(I).LE.0) GO TO 324
N=NBP(I)+NPARH+NQPAR
J=NUMNP+I
SH(N,I)-H(J)*THEATAH+(1.0-THEATAH)*H(I)
330 CONTINUE
330 CONTINUE
C** FORM LEAST SQUARES MATRIX
IF (AMP.LT.-.5) GO TO 344
DO 342 I=1,NOBMAX
II=I+(IOBCNT-1)*NOBMAX
HTMP=0.0
DO 332 J=1,NUMNP
IF (NDOBBS(J).NE.I) GO TO 332
HTMP=HTMP+SFOBSSH(J)*QHMP(J)
332 CONTINUE
IF (WH(I1).LE.0.0) GO TO 342
TEMP=HO(I1)-HTMP
DO 340 K=1,NVARH
STEMP=0.0
DO 344 J=1,NUMNP

6370
6380
6390
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6890
Table 1.--Computer-program listing--Continued

IF (NODOBS(J).EQ.1) STMPT=STMPT+SFOBSH(J)*SH(K,J) 6900
CONTINUE 6910
TMP=WH(I1)*STMPT 6920
DO 338 L=1,NVARH 6930
STMPT=0.0 6940
DO 336 J=1,NUMNP 6950
IF (NODOBS(J).EQ.1) STMPT=STMPT+SFOBSH(J)*SH(L,J) 6960
336 CONTINUE 6970
338 XTXH(L,K)=XTXH(L,K)+TMP*STMPT 6980
340 BH(K+NVHX2)=BH(K+NVHX2)+TMP*TEMP 6990
YSQH=YSQH+TEMP*TEMP*WH(II) 7000
342 CONTINUE 7010
344 CONTINUE 7020
J1=NUMNP+1 7030
J2=NUMNP*2 7040
IHR=KTH+1 7050
IF (IFLOW.EQ.1) WRITE (8'IHR) (H(J),J=J1,J2) 7060
WRITE (6,70) 7070
CALL LSISQ (XTXH,BH,RKH,PH,YSQH,AP,AMP,RP,EPP,NVARH,NVHX2,NVHX3, 7080
$ IPO,INDT,ITER,NVEH,LDIMH) 7.090
IF (INDT.EQ.1) GO TO 521 7100
C** UPDATE HEAD 7110
348 DO 352 I=1,NUMNP 7120
I1=NUMNP+I 7130
SUMH=0.0 7140
IF (NVARH.LE.0) GO TO 352 7150
DO 350 J=1,NVARH 7160
SUMH=SUMH+BH(J)*SH(J,I) 7170
350 CONTINUE 7180
IF (IFLOW.EQ.1) H(I1)=QHTMP(I)+SUMH 7190
352 CONTINUE 7200
IHR=2 7210
J1=NUMNP+1 7220
J2=2*NUMNP 7230
WRITE (8'IHR) (H(J),J=J1,J2) 7240
C** UPDATE PARAMETERS 7250
354 IF (IPO.EQ.1) WRITE (6,73) 7260
DO 356 I=1,NUMAT 7270
IF (NVARH.LE.0) GO TO 356 7280
L=IPRMH(1,I) 7290
IF (L.GT.0) RX(I)=RX(I)*(BH(I)+1.0) 7300
L=IPRMH(2,I) 7310
IF (L.GT.0) RY(I)=RY(I)*(BH(I)+1.0) 7320
L=IPRMH(3,I) 7330
IF (L.GT.0) RZ(I)=RZ(I)*(BH(I)+1.0) 7340
IF (IPO.EQ.1) WRITE (6,74) I,RX(I),RY(I),RZ(I) 7350
356 CONTINUE 7360
C** UPDATE SURFACE AND POINT SOURCE-SINK PARAMETERS 7370
358 IF (NQPAR.LE.0) GO TO 360 7380
WRITE (6,75) 7390
DO 358 I=1,NQPAR 7400
QF(I)=QF(I)*(BH(I+NQPAR)+1.0) 7410
IF (IPO.EQ.1) WRITE (6,76) I,QF(I) 7420