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Review of Ground-Water Flow and Transport Models in the Unsaturated Zone

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Operated by
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Commission

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SUMMARY

Models of partially saturated flow and transport in porous media have application in the analysis of existing as well as future low-level radioactive waste facilities located above the water table. An extensive literature search along with telephone and mail correspondence with recognized leading experts in the field, was conducted to identify computer models suitable for studies of low-level radioactive waste facilities located in the unsaturated zone. Fifty-five existing models were identified as potentially useful. Ten of these models were selected for further examination.

This report contains a statement of the ground-water flow-contaminant transport problem, a discussion of those methods used to reduce the physical problem to a computer model, a brief discussion about the data requirements of these models. The procedure used to select the ten codes for further discussion is given, along with a list of these models.

Finally, the Appendices contain the data about the fifty-five codes examined. Specifically Appendix D contains the detailed discussion of each of the ten selected codes. Included in each discussion are such items which a potential user requires in determining whether the code is suitable for his applications. Appendix E contains brief summary information about each of the fifty-five codes. Included in the summaries are identification data, authors, pertinent references, and model type.

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REVIEW OF GROUND-WATER FLOW AND TRANSPORT MODELS IN THE UNSATURATED ZONE

INTRODUCTION

The advantages of disposing low-level radioactive wastes in the unsaturated zone above the fluctuations of the water table have been recognized for some time. Indeed several of the existing low-level waste disposal facilities are sited and designed to dispose of the low-level waste in unsaturated media. In addition, proposed regulations for near-surface disposal of low-level wastes (10 CFR 61) would require disposal in the unsaturated zone above the fluctuations of the water table unless it can be conclusively demonstrated that the site characteristics will result in diffusion being the predominant mechanism of transport. In all cases except the diffusion-dominated system, migration of radionuclides which may be leached from the low-level waste would be through unsaturated media. Hence, the analysis of potential releases of radionuclides from the disposal units must include flow and transport in partially-saturated media. Although not relying solely on modeling to determine the suitability of a proposed or existing site, modeling can be nevertheless a valuable tool with which to calculate potential migration of radionuclides from the disposal site.

Modeling is also useful when designing a disposal facility. Covers and disposal units must be designed to minimize infiltration and contact of water with the wastes. Again, modeling of the movement of moisture and solute in partially-saturated media can be a valuable tool with which to evaluate the effectiveness of design features such as cover systems, specially-selected vegetative covers, or granular backfill.

But what computer codes should be used? Which natural processes and physical properties should be incorporated, and which can reasonably be ignored, in the models? What are the limitations on the existing computer codes and how do they affect their usefulness at this time? How do these computer codes mate with saturated flow and transport codes? Does adequate documentation exist for the codes? What data requirements are imposed by the selection of the codes? Can the data requirements be reasonably met in the field? Have the codes been verified against field studies?

The Low-Level Waste Licensing Branch (WMLL) of the U.S. Nuclear Regulatory Commission has an immediate need to evaluate potential releases of radionuclides and the effectiveness of design features at both existing and future low-level waste disposal sites. To meet this need, WMLL must proceed based on computer codes currently available, while improving this capability as refinements or new developments permit. WMLL has therefore committed to a program of developing an in-house modeling capability and sharing this capability through prequalification of a group of prospective computer codes for partially-saturated and saturated flow and transport (Siefken 1982).

This report contains the results of examining some 55 different models for flow and transport in variably saturated media. The main text contains discussions in general terms of the modeling problem, how the theoretical problem is approximated, data requirements and general comments. Of the 55 models examined, 10 have been selected for further study. An additional 16 were not included on the selected list because documentation was inadequate. An extensive individual discussion for each of the selected codes appears in Appendix D.

This study was confined to the examination of information written about each code. No attempt was made to actually run on a computer, any of the codes discussed in this report.

Appendix E contains a short summary for each of the models examined. Each of the 55 models has been assigned an identification number, i.e., an integer from 1 to 55. The models are listed by sequence number in Appendix E and in most other tables. In addition each model has a name assigned to it. This name is the name used in the literature if the originator(s) used one in his (their) writings. If no name is apparent from the literature a name is assigned, using the primary author's name with a suffix to assure uniqueness of model name. Appendix A contains lists of models indexed by model name to the Appendix E list. Thus given a model name one can go to Appendix A, obtain the model number and locate the associated short summary in Appendix E. Appendix B lists by code name the major properties of each code in Appendix E. Appendix C contains the code evaluation form used to determine the selected codes. Appendix D contains the detailed individual discussion for each of the selected codes.

REVIEW OF THEORY

Hydraulic systems are usually classified according to the zones in which the ground water appears. These zones are known as the saturated, partially saturated and tension-saturated zones. Freeze and Cherry (1979) summarize the properties of each zone as follows:

Saturated Zone:

1. It occurs below the water table.
2. The soil pores are filled with water, and the volumetric moisture content equals the porosity.
3. The fluid pressure is greater than atmospheric, so the pressure head (measured as gage pressure) is greater than zero.
4. The hydraulic head must be measured with a piezometer.
5. The hydraulic conductivity is a constant; it is not a function of the pressure head.

Partially Saturated Zone:

1. It occurs above the water table and above the capillary fringe.
2. The soil pores are only partially filled with water; the volumetric moisture content is less than the porosity.
3. The fluid pressure is less than atmospheric; the pressure head is less than zero.
4. The hydraulic head must be measured with a tensiometer.
5. The hydraulic conductivity and the moisture content are both functions of the pressure head.

Tension-Saturated Zone:

1. It occurs between the saturated and unsaturated zones.
2. The soil pores are filled with water.
3. The fluid pressure is less than atmospheric.

The unsaturated or partially saturated zone is also called the zone of aeration or the vadose zone. The tension-saturated zone is sometimes called the capillary fringe region.

Some authors do not distinguish between the tension-saturated zone and the saturated zone since both are saturated. Since our primary interest is in the unsaturated zone, we will not be particularly concerned with the tension-saturated zone. An excellent discussion of the three zones is given by de Laat (1980).

Ground-water models are generally based on one or more partial differential equations. These equations are derived by combining mathematical statements for the conservation of mass and energy with constitutive equations relating these statements to measureable quantities such as pressure, temperature and concentration. These partial differential equations are the basic equations of ground-water flow and transport. Ground-water flow involves the three space variables and the time variable.

In the general case a set of partial differential equations are used to describe subsurface movement under partially saturated conditions. The equations of interest here are usually labeled the flow, transport and the energy equations. We now consider the general two-phase flow equations. In what follows the subscripts m , a and w denote matrix, air and water, respectively. It is also convenient to let α denote one of m , a or w .

The flow equations have the form

$$\left. \begin{aligned} \frac{\partial}{\partial t} \left(\frac{\phi s_w}{B_w} \right) &= \nabla \cdot \lambda_w \nabla \phi_w - q_w \\ \frac{\partial}{\partial t} \left(\phi \left[\frac{s_a}{B_a} + R \frac{s_w}{B_w} \right] \right) &= \nabla \cdot \lambda_a \nabla \phi_a + \nabla \cdot R \lambda_w \nabla \phi_w - q_a \end{aligned} \right\} (1)$$

where $\lambda_\alpha = (kk_{r\alpha})/(B_\alpha \mu_\alpha)$. In the above equations ϕ is the porosity, Φ is the potential, s is the saturation ($s_a + s_w = 1$), B is a media volume factor (B_w is the ratio of the volume of water with air dissolved in it in situ, to the volume of water at standard conditions; B_a is the ratio of the volume of air in situ, to the volume of the same gas at standard conditions), R is the ratio of the volume of air dissolved in water to the volume of water, both at standard conditions, k is the intrinsic permeability at saturation, $k_{r\alpha}$ is the relative permeability ($0 \leq k_{r\alpha} \leq 1$), μ is viscosity, and q is a source/sink term.

There is one composition or transport equation for each constituent. They have the form

$$\begin{aligned} & \frac{\partial}{\partial t} [(1 - \phi) \rho_m C_m] + \frac{\partial}{\partial t} [\phi s_a \rho_a C_a] + \frac{\partial}{\partial t} [\phi s_w \rho_w C_w] \\ &= \nabla \cdot (D_a \nabla C_a) + \nabla \cdot (D_w \nabla C_w) - \nabla \cdot (\rho_a C_a V_a) - \nabla \cdot (\rho_w C_w V_w) \end{aligned} \quad (2)$$

In the above equation ρ is the density, C is the constituent concentration, D is the dispersion coefficient, and V is the velocity in the appropriate phase.

The energy equation has the following form

$$\begin{aligned} & \frac{\partial}{\partial t} (\rho_m s_m U_m) + \frac{\partial}{\partial t} (\rho_a s_a U_a) + \frac{\partial}{\partial t} (\rho_w s_w U_w) \\ &= \nabla \cdot \lambda_a H_a \nabla p + \nabla \cdot \lambda_w H_w \nabla p + \nabla \cdot T_c \nabla T - q_T \end{aligned} \quad (3)$$

where U is internal energy, H is enthalpy, T_c is heat conduction transmissibility, T is temperature, and q_T is a heat source/sink term.

One frequently finds the saturation of water s_w , replaced with the moisture content θ , defined as

$$\theta = \phi S_w \quad (4)$$

in the above equations.

It should be noted that k , k_r and θ are functions of position, time and water pressure when in the partially saturated zone. Hence Equations (1), (2) and (3) are nonlinear.

In the completely general case, the Equations (1), (2) and (3) are coupled and must be solved simultaneously. However, in many situations the coupling may be neglected permitting the equations to be solved separately. For example, if the temperature change is unimportant, one may consider an isothermal system and thus eliminate the energy equation entirely. Another example frequently seen involves the flow equations. If the air is static and remains at atmospheric pressure and if one ignores any air dissolved in the water then the second equation of (1) drops out and the first equation becomes Richard's equation for partially saturated flow. Oden (1982) presents an excellent review of fluid flow in porous media as applied by the petroleum industry. This paper is reasonably complete and yet is presented in an elementary straight forward manner.

Most of the codes examined here are based on isothermal assumptions and use only the first equation of (1). In the general classification used here, those codes which solve the flow Equations (1) only are called *flow* codes. Those which solve only the composition Equations (2) are called *transport* codes, and those solving both the flow and composition equations are called *flow-transport* codes.

NUMERICAL APPROXIMATIONS AND FORMULATIONS

Various methods are used to replace the partial differential Equations (1), (2) and (3) with equations which are tractible by computational methods. The most popular methods can be classified into one of three categories, finite differences, integrated finite differences and finite elements. In each case, the partial differential equations are replaced with a system of algebraic equations which are then solved by a variety of techniques.

It is not intended that this section provide a complete discussion of the various numerical methods used in ground-water modeling. Only a broad discussion will be given here. A number of excellent papers exist in the literature and are available to the interested reader. Faust and Mercer (1980) give an excellent discussion of the methods used to deal with the partial differential equations of ground-water flow. Other excellent expositions are given by Narasimhan and Witherspoon (1977a, 1977b).

The discussion below is largely confined to the two-dimensional geometry. The treatment of boundary conditions is generally ignored. For illustrative purposes consider a special case of the flow equation

$$\nabla \cdot K \nabla h = c \frac{\partial h}{\partial t} \quad (5)$$

where K is the hydraulic conductivity, h is the hydraulic head, and c is the specific storage or specific fluid capacity.

The basic goal of numerical methods is to discretize the region of interest into appropriately small subregions then apply the same conservation principles to each subregion. One source of error in the numerical process is this discretization procedure. To minimize this error, one chooses the subregions sufficiently small so that the various descriptive properties associated with the subregion do not vary significantly over the subregion.

A number of methods are available for defining the shape and size of this subregion and its relationship to the flow region. Figure 1 shows an arbitrary flow region (a) and three methods for numerically treating it. The three methods shown are (b) finite differences, (c) integrated finite differences, and (d) finite elements. The classical finite difference method (FDM) constructs the subregions such that bounding surfaces are perpendicular to the coordinate axes and located midway between nodes as shown in Figure 1(b). For this method, the problem of mass conservation is one of equivalent velocity gradients assuming linear velocity variations within the subregion.

In applying the FDM to the required equation, a finite difference grid is imposed on the region of interest and the nodes identified. At each node, one replaces the derivatives in the partial differential equation with appropriate finite difference quotients. The end result is a difference equation which relates the unknown or variable sought at a specific node to each of its neighbors. One such equation is obtained for each node where the unknown is to be determined.

The integrated finite difference method (IFDM) utilizes a somewhat less regular grid. The region of interest is divided into smaller areas. Thomas (1973) calls these areas nodal areas, since they each contain a node which is connected to its neighbors by appropriate difference equations. Generally, the properties throughout the nodal area are taken to be those of the node itself.

In applying the IFDM to a partial differential equation, the discretizing grid is imposed on the region of interest and the nodes (and nodal areas) identified. The IFDM is not applied directly to the partial differential equation. It is applied to an integral equation obtained by spatially integrating over a conveniently small finite subregion Γ , the divergence theorems permits the replacement of the area integral by a line integral over the boundary $\partial\Gamma$ of Γ . Thus from (5) one has

$$c A \frac{\partial h}{\partial t} = \int_{\partial\Gamma} K \nabla h \cdot \vec{n} ds \quad (6)$$

(a) THEORETICAL FLOW REGION

(b) FINITE DIFFERENCE

(c) INTEGRATED FINITE DIFFERENCES

(d) FINITE ELEMENTS

FIGURE 1. Relationships Between Various Discretizations and Approximations Used in Numerical Models

where A is the area of Γ and $\vec{n}$ is a unit vector directed to the outside of Γ and perpendicular to the boundary of Γ .

The region Γ in (6) is taken to be an arbitrary nodal area produced by the grid. The central idea here is to discretize the total flow domain into conveniently small subdomains or nodal areas and perform a mass balance on each small area as required.

The nodal locations are chosen such that the lines joining adjacent nodes are perpendicular to the intervening boundary interface. See Figure 1(c). Thus, the normal gradient at the boundary interface may be replaced with finite differences and the line integral in (6) evaluated. Replacing the time derivative with a finite difference produces a difference equation similar to that obtained by the FDM, relating the node to each of its neighbors.

The IFDM enables one to treat problems with complicated boundaries. The main drawback of the method is that, since it is designed around the normal gradients, it does not directly allow for the evaluation of tangential gradients at the interfaces.

Like the IFDM, the finite element method (FEM) utilizes an arbitrary grid, and is applied to an integral equation rather than a differential equation. The FEM equations are sometimes developed from variational principles but we shall confine the discussion here to the method of weighted residuals in general and more specifically to the Galerkin method using triangular elements where a linear approximations is used.

In the Galerkin method, the partial differential equation is first multiplied by an appropriate weighting function and then integrated over the specified region. The weighting functions are also used to approximate the dependent variables in that they are interpolation functions, i.e., basis functions.

The region of interest is discretized into a system of triangles as shown in Figure 1(d). More general shapes may be used but for this discussion we consider only triangles. The triangles are called elements, the vertices of the elements are called nodes. The nodes are then numbered in some order. We approximate the dependent variable, the hydraulic head in our example, by an interpolation function

$$h(x,t) \approx \sum_m \xi_m(x) h(x_m,t) \quad (7)$$

where the sum is over all nodes m . The variable x represents a two component vector. The functions $h(x_m,t)$ represent the as yet undetermined head values at node m which are dependent on time t . The interpolation functions $\xi_m(x_m) = 1$ and $\xi_m(x_n) = 0$ for $n \neq m$. The basis function ξ_m varies linearly over the

elements which have node m as a vertex. Usually $\xi_m(x)$ is defined as zero for any point x which is not in an element having the node m as a vertex.

Substituting (7) for h in (5), multiplying both sides of the resulting equation by $\xi_n(x)$ and integrating over the entire region of interest yields one equation. This equation is further modified by mathematical transformations to yield a first-order differential equation in time, which is linear in the $h(x_m, t)$ where the node m is a neighbor of node n , i.e., the elements m share the node n as a vertex. The coefficients of the $h(x_m, t)$ are evaluated either analytically or numerically. This procedure is repeated for all nodes n which, when boundary conditions are included yield a system of first-order differential equations in time. The time derivations are then replaced by finite differences to produce a system of algebraic equations.

The end-product of each method, FDM, IFDM and FEM is a system of algebraic equations where the unknowns are the hydraulic head at the node points. A discussion of the pros and cons of these methods appear in Faust and Mercer (198D).

Referring back to Item 5 of the list of properties characterizing the unsaturated zone given above, the hydraulic conductivity K , and the water content θ , are functions of the pressure head ψ . This means that in the unsaturated zone the flow and composition equations are non-linear. This also means that the approximating algebraic equations are non-linear. The usual method of dealing with this complication is to make further approximation by linearizing the algebraic system and/or iterating to a solution.

To complicate matters even more the functional relationships between the hydraulic conductivity K , and the capillary pressure ψ , and the moisture content θ are not uniquely defined. In fact, there is considerable evidence that K is a unique result of θ , but θ and ψ may not be uniquely related. Empirical results show that during the wetting part of the wetting-drying cycle seen in the unsaturated zone the relationship of ψ and θ is uniquely defined. Similarly, the relationship is unique for the drying part of the cycle. The usual treatment is to tabulate ψ as a function of θ for each part of the cycle. The function values are then obtained by interpolation techniques.

Another source of non-linearity is the source/sink term q of Equations (1), (2) and (3). The processes of evapotranspiration are introduced through this term. These processes include plant growth and the atmospheric-soil interface and are also sometimes included through empirical functions.

Stochastic models of ground-water systems have appeared recently (Narasimhan and Witherspoon 1977b). Two such models are included in this study. These models are based on assumptions from probability theory. In a stochastic model one begins with a partial differential equation where certain parameters and/or boundary and initial conditions are assumed to have uncertainties associated with them. The solution to such an equation is not one single solution but rather a distribution of solutions. This distribution is generally difficult to obtain and so the usual procedure is to settle for one or two moments of

the distribution. That is one obtains the average or mean solution and, if possible, a variance which measures how closely the distribution of solutions clusters around the average solution.

The stochastic differential equation is approximated by another differential equation which accounts for all such second order variations (that is the approximation is second order). This approximate differential equation is obtained subject to the original differential equation satisfying a certain "smallness" criterion, that is "the differential operator must be small in norm" (Gibbs 1980).

The approximate differential equation is then replaced with an expectation equation that the solution must satisfy. The mean solution of the expectation equation is then found by standard numerical methods. Finite difference methods are preferred because of the simple form of the approximating algebraic equations, though this is not a requirement (Oster and Gibbs 1981). In addition, the final relationship for the mean solution may require that deviations from the mean be relatively small. See for example Gibbs (1980).

DATA REQUIREMENTS

The data required for each code depends on the assumptions upon which the model is based. In general, the input data must include some or all of the following values, functions, etc.

- Program control parameters
 1. Identification data
 2. Auxiliary data file options
 3. Output media options
 4. Print out frequency
 5. Interrupt-restart options
 6. Solution method selection options
- Geometry parameters for discretization grid definition
- Initial distribution values for:
 1. Pressure head
 2. Solute concentrations
 3. Moisture content
 4. Temperature/energy/enthalpy
- Boundary conditions as functions of space and time for:
 1. Pressure head
 2. Ground water and solute flux
 3. Temperature/energy/enthalpy

- Media properties as functions of space
 1. Permeabilities
 2. Hydraulic conductivity (tensor)
 3. Moisture capacity
 4. Porosity
 5. Thermal conductivity
- Fluid properties as functions of space
 1. Viscosity
 2. Density
 3. Mass capacity
- Source/sink functional relationships in both space and time:
 1. Plant root and leaf growth models
 2. Recharging functions, e.g., rainfall, irrigation
 3. Evaporation models
 4. Geothermal and solar sources

If the model is for the solute transport problem only, one also requires a pore velocity field description as input. The usual method is to obtain this field of data by calculating it with a code to solve Equation (1).

In addition to the data required by the deterministic codes, the stochastic models require additional data about uncertainty in any stochastic parameters. This uncertainty is usually in the form of covariance functions. Such functions may be generated by the use of kriging techniques (DeVary and Doctor 1981).

PRACTICALITIES

The ground-water modeler is confronted by problems which have been well described by Bellman (1957) as "To predict quantitatively, one must have a ... mathematical model. It seems reasonable to suppose that the more realistic this mathematical model, the more accurate the prediction.

"There is, however, a point of diminishing returns. The actual world is extremely complicated... If we attempt to include too many features of reality in our mathematical model, we find ourselves engulfed by complicated equations containing unknown parameters and unknown functions. The determination of these functions leads to even more complicated equations with even more unknown parameters and functions, and so on."

At one extreme, the modeler might use the one-dimensional Richard's equation (Freeze and Cherry 1979) and at the other he might use one of the very general three-dimensional codes which have much greater data demands. The user must decide whether his available data justify the cost and effort of using a sophisticated model. One is reminded of Hamming's statement, "The purpose of computing is insight, not numbers" (Hamming 1962).

In practice, one might use a simple model, involving little expense, to gain sufficient insight to narrow the scope of the problem to a point when a more expensive model can be used. It is entirely possible that the simple model will yield all the results required.

Another problem frequently faced is the question of reliability of the output. There are a number of ways to obtain the sensitivity of output to changes in the input parameters. One might, for example, make many computer runs varying different input parameters to obtain insight into the bounds on the output. Another alternative is to use one of the stochastic codes to produce in one calculation the mean solution and its variance. The decision of which course to follow will be made based on many input factors including availability of initial data.

The three popular methods FDM, IFDM and FEM are not without their problems. With conventional versions of these methods one finds solutions which show numerical dispersion and numerical oscillation. Numerical dispersion produces results which are blurred or smeared while oscillatory solutions can contain such results as large negative concentrations etc. Usually the numerical dispersion is associated with the finite difference methods while numerical oscillation is associated with the finite element method, however, depending upon the approximation used for the convection term, both methods can yield solutions exhibiting either type of behavior.

The method of characteristics (MOC) has been used as a means of avoiding the above stated problems. This method is not without its problems as well. The MOC is usually used in conjunction with a finite difference method though this is not a requirement. In applying the MOC one replaces the transport equation with an equivalent system of ordinary differential equations. The curves in space along which this system of ordinary differential equations hold are known as the characteristic curves, hence the name, method of characteristics.

The MOC is particularly useful when hydrodynamic dispersion is negligible as this method has minimal numerical dispersion. However the determination of points along the characteristic curves and iterating to include the dispersive parts of the transport equation can be fairly expensive (Faust and Mercer 1980).

COMPILING THE LIST OF CODES

Starting with the list of unsaturated flow and transport models given by Bachmat et al. (1980), and conducting an extensive literature search along with telephone and mail correspondence with recognized leading individuals in the field produced most of the models studied here. Finally some important items were derived from the Symposium on Unsaturated Flow and Transport Modeling held in Seattle on March 23-24, 1982. The proceedings of this symposium appear in Nelson et al. (1982).

A short summary for each code investigated is contained in Appendix E. These codes are listed there according to an assigned sequence number. Each

of these codes has a name associated with it. Appendix A contains a cross index by code name to Appendix E. That is given a code name, one obtains the sequence number from Appendix A to locate the short summary page in Appendix E.

PREFERRED CODES

The models listed in Appendix E have been ranked so as to determine which are potentially more useful than others. The ranking procedure is based on:

- Documentation
- Applications
- Code Availability.

Documentation is considered in three forms. First, there is a description of the model which includes both the physical principles used and the resulting mathematical statement of the process being modeled. The second form of documentation is one or more publications describing applications of the model to actual problems. The third form of documentation is a user's manual. Included within the user's manual are detailed instructions on data requirements and data preparation, and a listing of the code along with some sample problems with the solutions. In several cases, all three forms appear under the same cover.

Some models have been applied to laboratory experiments only. Others have been applied to field data on various occasions. In general, the more times a model has been applied the higher ranking it should receive. Unfortunately, there is no sure way of knowing how many times a code had been successfully applied. Appendix C contains the form, Table C.1, used to rank the codes. In determining the entries in Table C.1, an X was placed in the appropriate applications column if the author claimed it had been applied to experimental or field data, with no question of how many times the application may have been made. In general, a model for which a code was available either in the form of computer listings, punched cards or magnetic tape was ranked higher than those for which no code is available. Any code known to be proprietary and for which additional information is lacking was considered as though the code was not available.

By this ranking procedure, several models have been identified as candidates for further study. This further study would entail such things as application to benchmark problems. The codes selected here are given in Table 1. Appendix D contains an extensive description for each code listed in this table.

An examination of Table 1 and Table C.1 reveals the existence of models not included in Table 1 but having as many X's as those so listed. Some of these models are listed in Table 2 and are discussed in the next section. The other codes were not selected for a number of reasons. In some cases the only information available is given by Bachmat et al. (1980). Data for the Bachmat report was collected prior to 1978. When the current information consisted of only this dated material it was assumed that the code was preliminary and hence was not included in the selected set. This was the case for Code Nos. 7,

TABLE 1. Codes Selected for Further Study

<u>Code Number</u>	<u>Code Name</u>	<u>Type</u>	<u>Principal Contact</u>
4	TRUST	Flow	Narasimhan
9	SEGOL	Flow/Transport	Segol
10	UNSAT1D	Flow	Bond
11	SUMATRA-1	Flow/Transport	van Genuchten
18	TARGET	Flow/Transport	Sharma
24	FEMWATER	Flow	Yeh
25	FEMWASTE	Transport	Yeh
26	UNSAT2	Flow	Neuman
45	VS2D	Flow	Lappala
54	MLTRAN	Transport	Reisenauer

TABLE 2. Codes of Potential Interest But Which Lack Documentation

<u>Code Number</u>	<u>Code Name</u>	<u>Type</u>	<u>Principal Contact</u>
5	FLUMP	Flow	Narasimhan, Neuman
8	VERGE	Flow	Verge, Frind
20	MCCANN	Flow/Transport	McCann, Wiles
21	ALPURS	Flow	Bansal, Harper, McDonald
29	COOK	Flow	Cook
31	GPSIM	Flow	Exxon
32	TS&E	Flow	Technical Software and Engineering
37	AMOCO	Flow	AMOCO
38	CMG	Flow	CMG
40	BETAIL	Flow	Intercorp.
41	SCC	Flow	SCC
42	SHELL	flow	Shell Oil Company
43	SHAMTU	Flow/Transport	Vauclin
49	PORES	Flow	UKAEA
50	WAFE	Flow	Travis
55	TRACR3D	Flow	Travis

15, and 47. Though not included in the Bachmat report, Code No. 27 was not selected for similar reasons. Code No. 11 contains Code No. 28 as the flow calculation module, hence No. 28 was not included in either Table 1 or 2.

OTHER CODES OF POTENTIAL INTEREST

There are several other codes which might well have been included in Table 1 but were excluded because of one or more reasons. The primary reason is lack of published information about the code. In some cases the only information available is listed by Bachmat et al. (1980). Other codes with little published information are the proprietary codes. In all cases the proprietary nature of a code results in minimal disclosure of details to the public. Only one code listed in Table 1 claims the ability to solve the energy Equation (3). That code is TARGET. The nature of codes held by the petroleum industry may well have this capability too (Oden 1982).

Table 2 lists those codes from Tables B.1, B.2 and B.3 which might have been listed in Table 1 had more documentation been available. It is interesting that only two codes listed in Table 2 have both flow and transport capabilities.

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APPENDIX A

PARTIALLY SATURATED AND MULTIPHASE CODES INVENTORIED,
INDEXED BY CODE NAME AND TYPE

TABLE A.1. Index by Code Name

Code Name	Code Number	Code	Principal Contact(s)
ALPURS	21	Flow	Bansal, Harper, McDonald
AMOCO	37	Flow	AMOCO
BACHMAT	6	Transport	Bachmat, Chetboun
BETAI1	40	Flow	Intercomp
BRUTSAERT1	33	Flow	Brutsaert
BRUTSAERT2	39	Flow	Brutsaert
CMG	38	Flow	CMG
COOK	29	Flow	Cook, Jacoby, Ramesh
DELAAT	48	Flow	de Laat, van der Akker
DUGUID-REEVES	19	Transport	Duguid, Reeves
FECTRA	17	Transport	Baca, Lu, Yee
FEMWASTE	25	Transport	Yeh, Ward
FEMWATER	24	Flow	Yeh, Ward
FLUMP	5	Flow	Narasimhan, Neuman
GANDALF	30	Flow	Morrison
GPSIM	31	Flow	Spillette, Hillestad, Stone
HANKS	1	Flow/transport	Hanks, Childs
MARINO	53	Flow/transport	Marino
MCCANN	20	Flow/transport	McCann, Wiles
MLTRAN	54	Transport	Reisenauer, Nelson, Newbill
MMT-DPRW	44	Transport	Foote, Serne
MOBIDIC	14	Flow/transport	Couchat, Le Cardinal, Moutonnet
MOMOLS	52	Flow	Rojstaczer
NMODEL	15	Flow/transport	Selim, Davidson
PORES	49	Flow	UKARA
REEVES-DUGUID	22	Flow	Reeves, Duguid
SCAT1D(a)	35	Transport	Oster
SCAT2D(a)	36	Transport	Oster
SEGOL	9	Flow/transport	Segol
STAMTU	43	Flow/Transport	Vauclin, Haverkamp, Hamon
SHELL	42	Flow	Shell Oil Company
SCC	41	Flow	SCC
STGWT/MOGWT	27	Flow	de Smedt, van der Beken
SUM-2	46	Flow	de Laat, van der Akker
SUMATRA-1	11	Flow/Transport	van Genuchten
SUPERMOCK	47	Flow	Reed, Bedinger, Terry
TARGET	18	Flow/Transport	Dames & Moore
TRACR3D	55	Flow	Travis
TRANS	23	Flow/Transport	Walker, Sabey, Hampton
TRANSONE	12	Flow/Transport	Van Genuchten

(a) Stochastic code.

TABLE A.1. (contd)

<u>Code Name</u>	<u>Code Number</u>	<u>Code</u>	<u>Principal Contact(s)</u>
TRANSTWO	13	Flow/transport	Shapiro
TRIPM	51	Flow	Gureghian
TRIMDL	2	Transport	Av-Ron
TRUST	4	Flow	Narasimhan
TS&E	32	Flow	Technical Software and Engineering
UNFLW	3	Flow/Transport	Kapuler
UNFLOW	7	Flow	Pickens
UNSAT1	28	Flow	van Genuchten
UNSAT2	26	Flow	Neuman, Feddes, Bresler
UNSAT1D	10	Flow	Bond, Gupta
VERGE	8	Flow	Verge, Frind
VS2D	45	Flow	Lappala
WAFE	50	Flow	Travis
WATSOL	16	Flow/transport	Gaudet, Haverkamp
WHC	34	Flow/transport	Crooks, Yeh

TABLE A.2. Flow Codes Indexed By Code Name

Code Name	Code Number	Principal Contact
ALPURS	21	Bansal, Harper, McDonald
AMOCO	37	AMOCO
BETAI	40	Intercomp
BRUTSAERT1	33	Brutsaert
BRUTSAERT2	39	Brutsaert
CMG	38	CMG
COOK	29	COOK, Jacoby, Ramesh
DELATT	48	de Laat, van der Akker
FEMWATER	24	Yeh, Ward
FLUMP	5	Narashimhan, Neuman
GANDALF	30	Morrison
GPSIM	31	Spillette, Hillestad, Stone
MOMOLS	52	Rojstoczer
PORES	49	UKARA
REEVES-DUGUID	22	Reeves, Duguid
SHELL	42	Shell Oil Company
SSC	41	SSC
STGWT/MOGWT	27	de Smedt, van der Beken
SUM2	46	de Laat, van der Akker
SUPERMOCK	47	Reed, Bedinger, Terry
TRACR3D	55	Travis
TRIPM	51	Gureghian
TRUST	4	Narasimhan
TS&E	32	Technical Software and Engineering
UNFLOW	7	Pickens
UNSAT1	28	van Genuchten
UNSAT2	26	Neuman, Feddes, Bresler
UNSAT1D	10	Bond, Gupta
VERGE	8	Verge, Frind
VS2D	45	Lappala
WAFE	50	Travis

TABLE A.3. Transport Codes Indexed by Code Name

<u>Code Name</u>	<u>Code Number</u>	<u>Principal Contact</u>
BACHMAT	6	Bachmat, Chetboun
DUGUID-REEVES	19	Duguid, Reeves
FECTRA	17	Baca, Lu, Yee
FEMWASTE	25	Yeh, Ward
MLTRAN	54	Reisenauer, Nelson, Newbill
MMT-DPRW	44	Foote, Serne
SCAT1D(a)	35	Oster
SCAT2D(a)	36	Oster
TRNMDL	2	AV-Ron

(a) Stochastic code.

TABLE A.4. Flow/Transport Codes Indexed by Code Name

<u>Code Name</u>	<u>Code Number</u>	<u>Principal Contact</u>
HANKS	1	Hanks, Childs
MARINO	53	Marino
MCCANN	20	McCann, Wiles
MOBIDIC	14	Couchat, Le Cardinal, Moutonnet
NMODEL	15	Selim, Davidson
SEGOL	9	Segol
SHAMTU	43	Vaucelin, Haverkamp, Hamon
SUMATRA-1	11	van Genuchten
TARGET	18	Dames & Moore
TRANS	23	Walker, Sabey, Hampton
TRANSONE	12	van Genuchten
TRANSTWO	13	Shapiro
UNFLW	3	Kapuler
WATSOL	6	Gaudet, Haverkamp
WHC	34	Crooks, Yeh

APPENDIX B

SUMMARY CHARTS OF INVENTORIED CODES

TABLE B.1. Flow Code Summary

Code		Spatial Characteristics							Special Features	Past Applications	Principal Contact	Comments
Name	No.	Dimensions			Discretization Method							
		1	2	3	FDM	IFDM	FEM	Other				
AMOCO	37			X	X				Three-phase oil, water, gas	Oil reservoir	AMOCO	Proprietary Code
ALPURS	21			X	X						Mobil Corp.	Proprietary Code
BETA-II	40			X	X					Oil reservoir	Intercomp.	Proprietary Code
BRUTSAERT1	33		X		X				Experimental/Laboratory	Brutsaert		
BRUTSAERT2	39		X		X					Brutsaert		
CMG	38			X	X					Oil reservoir	CMG	Proprietary Code
COOK	29		X						Two-phase oil & gas	Oil reservoir	Cook	Proprietary Code
DELAAT	48		X				X		Roots, evapotranspiration	Ground-water extraction crop production	De Laat	European Code
FEMWATER	24		X				X				Yeh	
FLUMP	5		X				X				Narasimhan	
GRANDALF	30		X		X					Underground nuclear explosions	Morrison	
GPSIM	31			X	X						Exxon	Proprietary Code
MOMOLS	52	X			X					Experimental	Rojstoczer	
PORES	49			X	X					Oil reservoir	UKAEA	European Code
REEVES-DUGUID	22		X				X		Radioactive decay		Reeves	
SHELL	42			X	X					Oil reservoir	Shell Oil Co.	Proprietary Code
SSC	41			X						Oil reservoir	SSC	Proprietary Code
STGWT/MOGWT	27	X			X						de Smedt	European Code
SUM2	46		X				X		Roots, evapotranspiration	Ground-water extraction	De Laat	European Code
SUPERMOCK	47		X		X				Roots	Ground-water extraction	Reed	
TRACR3D	55			X		X			1- or 2-phase flow with tracer in either phase (air or water)	Tracer flow in unsat. conditions, Radionuclide transport, Tracer flow in fractured system	Travis	Can operate in 1, 2 or 3 dimensions
									Freundlich, Langmuir sorption, radioactive decay, capillary effects			
TRIPM	51		X				X		3-member decay chain	Radioactive waste disposal	Gureghian	
TRUST	4			X			X				Narasimham	
TS&E	32			X						Oil reservoir	Tech. Soft. & Eng.	Proprietary Code
UNFLOW	7		X				X			Radioactive waste disposal	Pickens	
UNSAT1	28	X					X		Roots, evapotranspiration Roots		van Genuchten	
UNSAT1D	10	X			X					Crop studies	Bond	
UNSAT2	26		X				X			Engineering design	Neuman	
VERGE	8			X			X			Radioactive waste storage	Verge	
VS2D	45		X		X				Roots, evapotranspiration		Lappala	
WAFE	50		X			X			Coupled heat & 2-phase mass transport (air vapor & liquid) Accurate treatment of H ₂ O Separate velocity field phase	Confined underground radioactive waste disposal, In-situ fossil energy recovery studies, 2-phase flow and tracer studies	Travis	Can operate in 1 or 2 dimensions

KEY: FDM = finite difference method.
 IFDM = integrated finite difference method.
 FEM = finite element method.

TABLE B.2. Transport Code Summary

Code Name	No.	Spatial Characteristics Dimensions			Discretization Method				Special Features	Past Applications	Principal Contact	Comments
		1	2	3	FDM	IFDM	FEM	Other				
BACHMAT	6	X			X				Surface/ground water		Backmat	Middle-east Code
DUGUID-REEVES	19		X				X		Absorption & decay		Duguid	Compatible with Code No. 22
PECTRA	17		X				X		1st-order decay, sorption		Baca	
FEMWASTE	25		X				X				Yeh	Compatible with Code No. 22
MLTRAN	54		X				X				Reisenauer	Compatible with Code No. 44
MMT-DPRW	44		X					X		Ground-water studies	Simmons	Discrete Parcel Random Walk
SCAT1D	35	X			X				Stochastic velocity field		Oster	Stochastic Code
SCAT2D	30		X		X				Stochastic velocity field		Oster	Stochastic Code
TRNMDL	2	X			X						Av-Ron	Middle-east Code

KEY: FDM = finite difference method.
 IFDM = integrated finite difference method.
 FEM = finite element method.

TABLE B.3. Flow-Transport Code Summary

Code		Spatial Characteristics							Special Features	Past Applications	Principal Contact	Comments
Name	No.	Dimensions			Discretization Method							
		1	2	3	FDM	IFDM	FEM	Other				
HANKS	1	X			X				Roots	Crop production studies	Hanks	
MARINO	53			X			X		1st-order reactions		Marino	
MCCANN	20		X		X				Heat transfer		McCann	
MOBIDIC	14		X		X				Roots		Couchat	European Code
NMODEL		X			X						Selim	
SEGOL	9			X			X				Segol	
SHAMTU	43	X			X					Water loss by evaporation	Vauclin	European Code
SUMATRA-1	11	X					X		0- & 1st-order decay		van Genuchten	
TARGET	18			X		X			Heat transfer, elegant numerical solution. 0- & 1st-order decay. Variable saturation. Radio-active decay products	Tailings and chemical waste disposal, radio-active waste disposal	Dames & Moore	Proprietary Code
TRANS	23		X				X				Walker	
TRANSONE	12	X					X				van Genuchten	
TRANS TWO	13		X		X						Shapiro	
UNFLW	3	X			X						Kapuler	
WATSOL	16	X			X					Salinity studies	Gaudet	European Code
WHC	34			X				X			Crooks	Integrated Compartment Method

KEY: FDM = finite difference method.
 IFDM = integrated finite difference method.
 FEM = finite element method.

APPENDIX C

CODE EVALUATIONS

TABLE C.1. Code Evaluations

No.	Code Name	Documentation		User's Manual	Applications		Code Availability	
		Model Description	Published Applications		Laboratory Data	Field Data	Available	Proprietary
1	HANKS	X	X		X		X	
2	TRNMDL	X			X			
3	UNFLW	X			X	X		
4	TRUST	X	X	X		X	X	
5	FLUMP	X	X	X		X	X	
6	BACHMAT						X	
7	UNFLDW	X	X			X	X	
8	VERGE	X	X	X		X	X	
9	SEGOL	X	X	X		X	X	
10	UNSAT1D	X	X	X		X	X	
11	SUMATRA-1	X	X	X		X	X	
12	TRANSONE							
13	TRANSWO							
14	MOBIDIC	X				X		
15	NMODEL						X	
16	WATSOL	X	X		X		X	
17	PECTRA	X		X			X	
18	TARGET	X				X		X
19	DUGUID-REEVES	X	X				X	
20	MCCANN	X				X	X	
21	ALPURS	X						X
22	REEVES-DUGUID	X		X			X	
23	TRANS	X			X		X	
24	FEMWATER	X	X	X		X	X	
25	FEMWASTE	X	X	X		X	X	
26	UNSAT2	X	X	X		X	X	
27	STGWT/MOGWT	X		X	X			X
28	UNSAT1	X	X	X			X	
29	COOK	X						X
30	GANDALF	X					X	
31	GPSIM	X						X
32	TS&E	X						X
33	BRUTSAERT1	X					X	
34	WHC	X		X			X	
35	SCAT1D	X					X	
36	SCAT2D	X					X	
37	AMOCO							X
38	CMG							X
39	BRUTSAERT2				X		X	
40	BETA II							X
41	SSC							X
42	SHELL							X
43	SHAMTU	X	X	X		X	X	
44	MMT-DPRW	X				X	X	
45	VS2D	X		X		X	X	
46	SUM-2		X				X	
47	SUPERMOCK	X		X		X	X	
48	DELAAT		X			X		
49	PORES					X		
50	WAFE					X		
51	TRIPM	X	X			X		
52	MOMOLS	X					X	
53	MARINO	X						
54	MLTRAN	X	X	X		X	X	
55	TRACR3D					X		

APPENDIX D

SUMMARY OF SELECTED CODES

Model Name: TRUST

Code No. 4
Type: Flow

I. Summary of Code

Purpose and Scope--TRUST was developed to study fluid flow problems arising in variably saturated porous media with complicated geometry. The fluid mass conservation equations used are based on elemental volumes that have a constant volume of solid. Nonelastic deformation of the skeleton is permitted, permeability and compressibility coefficients may be nonlinearly related to effective stress, relationships between permeability and saturation with pore water pressure in the unsaturated zone may include hysteresis.

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Code Functions--TRUST provides a versatile tool to solve a wide spectrum of fluid flow problems arising in variably saturated deformable porous media. The governing equations express the conservation of fluid mass in an elemental volume that has a constant volume of solid. Deformation of the skeleton may be nonelastic. Permeability and compressibility coefficients may be nonlinearly related to effective stress. Relationships between permeability and saturation with pore water pressure in the unsaturated zone may include hysteresis.

The code grew out of the original TRUMP code written by Edwards (1968). The code uses an integrated finite difference algorithm for numerically solving the governing equation. Marching in time is performed by a mixed explicit-implicit numerical procedure in which the time step is internally controlled. The time step control and related feature in the TRUST code provide an effective control of the potential numerical instabilities that can arise in the course of solving this difficult class of nonlinear boundary value problem.

Potential Usage--TRUST has the capabilities for treating the wetting-drying front problem which appears in arid regions where many potential low level waste repository sites occur. In addition, the following list enumerates some of the problems which have been solved in the past using TRUST: settlement and consolidation in soft-clay systems under constant or variable loads; deformation of organic soils undergoing drainage and desaturation; simulation of drainage and infiltration in variably saturated columns, ditches and sand boxes; slug tests, constant rate or constant drawdown well-tests in porous media with single or multiple-fractures; internal drainage into mines expanding with time; response of an aquifer-well system of earthquakes or earth tides.

Relation to NRC Issues--Not applicable as no list of issues currently exists for low level radioactive waste treatment.

Restrictions on Use--TRUST is in the public domain and is listed in Reisenauer, et al. (1982).

Compatibility with Other NRC Codes--TRUST is written in FORTRAN IV, using no special equipment. The code does use some statements which are specific for some but not all computers. These are identified in Reisenauer, et al. (1982) so that conversion should be readily accomplished.

II. Summary of Findings

General Critique--The TRUST code grew out of the original TRUMP code for thermal modeling. The TRUMP model was written by Edwards (1968) of the Lawrence Livermore Laboratory.

The basic motivation in developing the original TRUST algorithm was to have a fairly general computational tool to implement the mass conservation equation over complex, multidimensional flow regions occupied by porous materials under conditions of variable saturation and deformation. The simple, one-dimensional deformation assumption of Terzaghi has helped dispense with the need to solve an additional set of stress-strain equation, while still enabling the consideration of matrix deformation in so far as it affects fluid flow. Viewed in this phenomenological context, the TRUST approach provides a powerful, versatile tool to solve a wide spectrum of fluid flow problems arising in disciplines such as hydrogeology, soil mechanics, soil physics, rock-mechanics, and related subjects.

In order that the versatility of the tool be preserved, it is necessary that the data-input structure be kept flexible and general. For this reason, it is important to make special note of the following two special features of TRUST: a) the computational model considers pressure-dependent density variations of water and conserves the mass of water, and b) the physical parameters in the governing equation are used in their primitive forms. Although options are available to employ familiar forms rather than primitive forms of the parameters, it is felt that a greater inter-disciplinary flexibility is afforded by the latter. Thus, intrinsic permeability, fluid viscosity, fluid density and gravitational constants are separately input rather than hydraulic conductivity; so also, fluid mass capacity, assembled from deformation and desaturation parameters is physically more realistic than the traditional concept of specific storage. In addition, the organization of the input of the geometric data in the TRUST approach is such that the algorithm does not intrinsically differentiate between a one-, two-, or three-dimensional problem. In a sense this enables one to have the invariant physics in focus while using TRUST.

Applicability to Medium--TRUST is designed to simulate fluid flow in variably saturated porous deformable media. The simulation can be carried out in one-, two- or three-dimensions.

Sensitivity Analysis--No sensitivity analysis has been published.

Code Validation and Field Verification--TRUST has been used in many applications. See Potential Usage above. A particularly good field study is given by Nelson, et al. (1980). This study involved using TRUST to analyse seepage from a buried uranium mill tailings site. The analysis involved the combined partially saturated and saturated modeling of four tailings management alternatives. The site being in the arid west involved severely desiccated soils with sharp advancing wetting fronts.

III. General Description

Operating Characteristics--TRUST as listed in Reisenauer, et al. (1982) has been made operational on UNIVAC and VAX-II computers. It is also available on the CDC 6400/6600/7000 system at LBL. The UNIVAC and CDC versions of TRUST are card oriented, the VAX version is not. Also, there are single and double precision variants on the VAX system.

Inputs--Inputs for TRUST include:

- Grid geometry
- Initial heads
- Prescribed head and flux boundary conditions
- Intrinsic permeabilities
- Fluid viscosity
- Fluid density
- Gravitational constant
- Fluid mass capacity

Outputs--The TRUST code output can be controlled by a print frequency input parameter. The input data are printed always and at specified points in time the following variables are printed for each node:

- Pressure heads
- Fluid potential
- Change in pressure head
- Volumetric fluid generation rate
- Quantity of fluid
- Fluid mass added up to print time
- Total mass flow into node up to print time
- Fluid properties

Available Documentation--TRUST is documented in Reisenauer, et al. (1982) which contains the equations, theory, user's manual, sample input and sample output.

IV. Review of Theory

Equations--The fundamental equation of transient groundwater motion is an equation of mass conservation and can be expressed as

$$G + \int_{\Gamma} \rho_w \frac{k \rho_w g}{\mu} \nabla(z + \psi) \cdot \vec{n} d\Gamma = \frac{d}{d\psi} (\rho_w V n S) \frac{D\psi}{Dt} \quad (1)$$

where

G = source term

Γ = closed surface of the domain of interest in the flow region

ρ_w = mass density of water

k = permeability

g = gravitational constant

μ = coefficient of viscosity

z = elevation

ψ = pressure head

$\vec{n}$ = unit outer normal to $d\Gamma$

V = bulk volume

S = saturation

$\frac{D}{Dt}$ = total derivative

Equation (1) is derived from the mass conservation equation in an integral form for a flow region which deforms with time. Assumptions were made that $Dz/Dt = 0$, implying that z is fixed during the time interval and that if ρ_w , V , n and S are functions only of ψ , then $\theta = nS$.

The right-hand side of (1) can be expressed as

$$\begin{aligned} M_c &= \frac{d}{d\psi} (\rho_w V n S) \\ &= V_s \rho_{wo} \left(S e \rho_{wo} \beta g + \frac{S Y_w X^1 C_c}{2.303 \sigma^1} + e \frac{dS}{d\psi} \right) \end{aligned} \quad (2)$$

where

V_s = volume of solids

ρ_{wo} = density of water at atmospheric pressure

e = void ratio

β = coefficient of compressibility of water

γ_w = specific weight of water

χ' = parameter correlating change in effective stress and change in pore pressure

C_c = compression index

σ' = effective stress

The parameter M_c in Equation (2) represents the mass of fluid which the volume V can absorb due to a unit change in the average value of ψ over V . The three terms on the right-hand side represents the compressibility of water, deformability of soil skeleton and desaturability of pores. The derivation of (2) is given in Reisenauer et al. (1982).

Note that in (2) the quantities ρ_w , S , and e are all functions of ψ and change continuously with time. The parameter χ' is also a function of ψ , since S is related to ψ .

Numerical Approximations--Equations (1) and (2) are solved by an integrated finite difference method (IFDM) in which physical quantities such as potential, density, void ratio and saturation, are properly defined averages over defined subdomains. In addition to this integral basis, the IFDM employs finite difference gradients for implementing Darcy's Law.

Finally, TRUST uses a mixed explicit-implicit approach, in setting up the final matrix equations. The mixed explicit-implicit approach recognizes the fact that in a flow region with volume elements having widely varying time constants (stable time steps), isolation groups of elements with relatively small time constants are only weakly coupled to each other through other elements with larger time constants. A practical consequence of this recognition is, that over a time step of a given Δt , it is necessary to solve simultaneous equations only for the isolated groups of elements with time constants less than Δt . In other words, the large matrix of the entire flow region is partitioned into one or more submatrices for purposes of matrix solution, leading to efficiency of computation. Currently, TRUST uses a Point-Jacobi type iterative scheme with an acceleration factor for solving the implicit equations.

Consider an appropriately small subregion of the flow region (Figure 1) over which the variation of ψ is not rapid, and let the average properties of this volume element be associated with a representative nodal point ℓ . Furthermore, let the volume element be so chosen that the lines joining the nodal point ℓ to its neighbors be normal to the interfaces between the respective elements. It is assumed that the average properties, such as the ψ associated with each

nodal point, are functions only of time, while the spatial variation of these average properties between adjacent nodal points can be represented by a simple linear relation which is independent of time. Then, applying (1) to the element in Figure 1, we can write

$$G_{\ell} + \sum_m \rho_w \frac{k \rho_w g}{\mu} \left[\frac{(z_m + \psi_m) - (z_{\ell} + \psi_{\ell})}{d_{\ell,m} + d_{m,\ell}} \Gamma_{\ell,m} \right] = M_{c,\ell} \frac{\Delta \psi_{\ell}}{\Delta t} \quad (3)$$

Note that the quantity within the summation sign in (3) represents the flux across the interface between elements ℓ and m . The quantities k and ρ_w in (3) are evaluated at the interface $\Gamma_{\ell,m}$ between the elements. When there is material heterogeneity and elements ℓ and m are composed of different materials, a harmonic mean permeability is used in order to preserve continuity of flux at the interface.

Let $U_{\ell,m}$ denote the flux across the interface ℓ,m due to a unit difference between $(z_m + \psi_m)$ and $(z_{\ell} + \psi_{\ell})$. It is shown in Reisenauer et al. (1982) that (3) can be solved explicitly for $\Delta \psi_{\ell}$. For an element ℓ whose boundary surface

FIGURE 1. Volume Element Associated with Nodal Point ℓ

may partly coincide with portions of the boundary of the overall flow region, the equation for $\Delta\psi_\ell$ is

$$\Delta\psi_{\ell,\text{exp}} = \frac{\Delta t}{M_{c,\ell}} \left\{ G_\ell + \sum_b U_{\ell,b} \left[(z_b + \bar{\psi}_b) - (z_\ell + \psi_\ell^0) \right] + \sum_m U_{\ell,m} \left[(z_m + \psi_m^0) - (z_\ell + \psi_\ell^0) \right] \right\} \quad (4)$$

where the subscript exp denotes explicit nature of the equation and where the subscript b denotes boundary values.

To permit reasonably large time steps to be used in the numerical solution the interpolation (stability) parameter λ is introduced, which permits one to write $\Delta\psi_\ell$ as the sum of an explicit component and an implicit component

$$\Delta\psi_\ell = \Delta\psi_{\ell,\text{exp}} + \frac{\lambda \Delta t}{M_{c,\ell}} \left\{ - \sum_b U_{\ell,b} \Delta\phi_\ell + \sum_m U_{\ell,m} (\Delta\psi_m - \Delta\psi_\ell) \right\} \quad (5)$$

Note that for $\lambda = 0$, (5) reduces to (4). The three cases, $\lambda = 0$, $\lambda = 0.5$, and $\lambda = 1.0$, are known as forward differencing, central differencing, and backward differencing procedures, respectively.

The local nature of stability and the form of (5) suggest that in order to carry out the solution process over the whole flow domain, one could first compute $\Delta\psi_{\ell,\text{exp}}$ for all the nodal points in the flow region and compute the implicit correction only for those elements whose stability limit is exceeded by Δt .

Probabilistic or Statistical Aspects--None.

Assumptions and Simplifications--The main assumptions are:

Darcy's Law is valid and hydraulic-head gradients are the only significant driving mechanisms for fluid flow.

Structure and Level of Detail--TRUST provides the user with a method using discretization cells which are quite general. Where detail is required the user simply defines smaller cells, where the detail is not needed larger cells may be used. Similarly the treatment of one-, two- or three-spatial dimensions is readily accomplished.

Applicability, Limitations, Validity and Completeness--This code is applicable to both saturated and unsaturated flow in porous, deformable media. The code has been successfully used on a wide variety of problems, many related to the earth sciences.

References--

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- Reisenauer, A. E., K. T. Key, T. N. Narasimhan, and R. W. Nelson. 1982. "TRUST: A Computer Program for Variably Saturated Flow in Multidimensional, Deformable Media," NUREG/CR-2360, PNL-3975, prepared for Division of Health, Siting and Waste Management, Office of Nuclear Regulatory Research, U.S. Nuclear Regulatory Commission by Pacific Northwest Laboratory, Richland, Washington.

Acceptance and Adequacy--TRUST is based on state-of-the-art research and is generally accepted by the research community as being as good as is possible at the current level of understanding.

Model Name: SEGOL

Code No. 9
Type: Flow/Transport

I. Summary of Code

Purpose and Scope--SEGOL was developed to simulate in two- or three-dimensions, mass transport in variably saturated flow systems.

Author--SEGOL was developed by Dr. Genevieve Segol. Her current address is:

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The primary contact for SEGOL is:

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Department of Earth Sciences
University of Waterloo
Waterloo, Ontario
N2L 3G1

Code Functions--SEGOL is a three-dimensional model for the analysis of mass transport in variably saturated flow systems. The Galerkin-finite element method is used to obtain the approximate sets of governing equations. Advantage is taken of the banded nature of the arrays in using out-of-core equation solvers to reduce the computer storage requirements. A two-dimensional model is also available, which is identical in all respects to the three-dimensional one except that the third dimension is discarded and that the solution is performed entirely in core.

Potential Usage--SEGOL can be used to investigate three-dimensional mass transport problems. The flow region may have any complex shape and may consist of different soil types arranged in arbitrary patterns. The following boundary conditions can be imposed; prescribed pressure head, prescribed flux normal to the boundary and seepage faces. The two-dimensional model may be used to check, if necessary, the results obtained with the three-dimensional code on a case where the third dimension may be irrelevant; it also provides the user with a means to quantify the importance of the three-dimensional nature of a particular problem and to decide whether or not the more expensive three-dimensional analysis is justified.

Relation to NRC Issues--Not applicable as no list of issues currently exists for low level radioactive waste treatment.

Restrictions on Use--This code is in the public domain and is listed in Segol (1976a).

Compatibility with Other NRC Codes--SEGOL is written in FORTRAN IV using no special equipment, hence it is compatible with other FORTRAN codes.

II. Summary of Findings

General Critique--The SEGOL code may be useful to the NRC for the analysis of contaminant concentration distributions in a three-dimensional saturated or unsaturated aquifer system. The two-dimensional version of the code, being more efficient computationally, may be used to quantify the importance of the three-dimensional nature of a particular problem and hence determine whether or not a more expensive three-dimensional analysis is justified. Hysteresis has not been included in the code, thus restricting its usage to either a single wetting or drying cycle.

Sensitivity Analysis--No sensitivity analyses have been published.

Code Validation and Field Verification--Simulation of a one-dimensional infiltration experiment reported by Warrick, et al. (1971) was used to check the accuracy of the three- and two-dimensional models. The comparison of this simulation is briefly given in Segol (1976a) and more fully in Segol (1976b). Good agreement was obtained in this check.

III. General Description

Operating Characteristics--SEGOL is written in FORTRAN IV and is operational on an IBM 360/75. It consists of 19 subprograms. Nine scratch files are used by the three-dimensional code and four scratch files are used by the two-dimensional program.

Inputs--Input quantities for SEGOL include:

- Basic program control parameters
- Grid geometry (node coordinates and incidences)
- Source and sink fluid and mass fluxes
- Initial pressure and concentration data
- Elemental parameters:
 - Hydraulic conductivity (anisotropic)
 - Longitudinal and transverse dispersivity
 - Porosity, elastic constants
 - Retardation coefficients and decay constants
- Dirichlet boundary conditions for flow and concentration
- Neumann boundary nodes for flow and concentration
- Initial position of seepage faces
- Unsaturated flow properties

Outputs--All output is to a line printer. This output includes the input information and the pressure head and concentration in both space and time.

Available Documentation--Segol (1976a) is a user's manual and includes a code listing for both the three-dimensional and the two-dimensional programs.

IV. Review of Theory

Equations--The equation governing water movement in a saturated-unsaturated zone has the form

$$L_{\psi} = \left(\kappa + \frac{\theta}{\epsilon} S_s \right) \frac{\partial \psi}{\partial t} - \sum_{\alpha=1}^3 \sum_{\beta=1}^3 \frac{\partial}{\partial x_{\alpha}} \left(K_r K_{\alpha\beta}^s \frac{\partial \psi}{\partial x_{\beta}} + K_r K_{\alpha\beta}^s \right) - Q = 0 \quad (1)$$

with

$$\begin{aligned} \kappa &= \frac{\partial \theta}{\partial \psi}, \text{ moisture capacity (L}^{-1}\text{)} \\ K_r &, \text{ relative hydraulic conductivity} \\ K_{\alpha\beta}^s &, \text{ hydraulic conductivity at saturation (LT}^{-1}\text{)} \\ Q &= A_w(x_{w\alpha}) \delta(x_{\alpha} - x_{w\alpha}), \text{ strength of source or sink function (T}^{-1}\text{)} \\ Q_w &, \text{ well discharge (L}^3\text{T}^{-1}\text{)} \\ S_s &, \text{ specific storage (L}^{-1}\text{)} \\ x_{w\alpha} &, \text{ coordinate of discharge or recharge point (L)} \\ \epsilon &, \text{ porosity} \\ \theta &, \text{ moisture} \\ \psi &, \text{ pressure head (L)} \end{aligned}$$

In the unsaturated zone Equation (1) is nonlinear since moisture content and hydraulic conductivity are functions of the pressure head. Hysteresis is not considered in the present analysis and consequently the relationships $K(\psi)$ and $\phi(\psi)$ are uniquely defined.

The initial and boundary conditions of the problem take the form

$$\psi(x_{\alpha}, 0) = \psi_0 \text{ in } \Omega \quad (2)$$

$$\psi(x_{\alpha}, t) = \bar{\psi} \text{ on } \Gamma_1 \quad (3)$$

$$K_r \sum_{\alpha=1}^3 \left[K_{\alpha 3}^s + \sum_{\beta=1}^3 K_{\alpha \beta}^s \frac{\partial \Psi}{\partial x_{\beta}} \right] = -V \text{ on } \Gamma_2 \quad (4)$$

where Ω is a three-dimensional domain bounded by a surface $\Gamma = \Gamma_1 + \Gamma_2$.

Along those boundaries where infiltration or evaporation take place, the exact boundary conditions cannot in general be predicted a priori. A solution is sought by maximizing the absolute value of the flux subject to the requirements.

$$\left| K_r \sum_{\alpha=1}^3 \left[K_{\alpha 3}^s + \sum_{\beta=1}^3 K_{\alpha \beta}^s \frac{\partial \Psi}{\partial x_{\beta}} \right] \right| \leq |E_s| \quad (5)$$

$$\left. \begin{array}{ll} \Psi_L \leq \Psi \leq 0 & \text{for infiltration} \\ \Psi \geq \Psi_L & \text{for evaporation} \end{array} \right\} \quad (6)$$

where E_s is the maximum possible surface flux and where Ψ_L is the minimum allowed pressure head at the soil surface.

The equation describing the solute transport is taken in the form

$$L_c = \frac{\partial \theta c}{\partial t} - \sum_{\alpha=1}^3 \sum_{\beta=1}^3 \frac{\partial}{\partial x_{\alpha}} \left(\theta D_{\alpha \beta} \frac{\partial c}{\partial x_{\beta}} \right) - \sum_{\alpha=1}^3 \frac{\partial q_{\alpha} c}{\partial x_{\alpha}} + Q c' = 0 \quad (7)$$

with c , solute concentration (ML^{-3})

c' , concentration of the considered ion in the source of sink fluid (ML^{-3})

$D_{\alpha \beta}$, dispersion tensor (L^2T^{-1})

q_{α} , volumetric flux of water (LT^{-1})

The moisture content θ appearing in (7) is a unique function of Ψ and can therefore be evaluated from the solution of (1). The mass-transport equation is also coupled to the flow equation through the mass-average velocity q_{α} which is obtained from Darcy's Law as

$$q_{\alpha} = -K_r \left[K_{\alpha 3}^s + \sum_{\beta=1}^3 K_{\alpha\beta}^s \frac{\partial \Psi}{\partial x_{\beta}} \right]. \quad (8)$$

The coefficients $D_{\alpha\beta}$ include the effects of mechanical dispersion and molecular diffusion, and are taken in the form

$$D_{\alpha\beta} = D_{\alpha\beta}^M(V, t) + D_p(\theta, t) \delta_{\alpha\beta} \quad (9)$$

where

$$D_{\alpha\beta}^M = a_L \left| V \right| \delta_{\alpha\beta} + (a_L - a_T) \frac{V_{\beta} V_{\alpha}}{|V|} \quad (10)$$

a_L and a_T being the longitudinal and transverse dispersivities, respectively; $V_{\alpha} = q_{\alpha}/\theta$ is the component of velocity in the direction x_{α} . The soil diffusion coefficient $D_p(\theta, t)$ is assumed to be an exponential function of moisture content. Thus,

$$D_p(\theta, t) = D_0 a e^{b\theta} \quad (11)$$

a and b being empirical constants characteristic of the soil, and D_0 being the equivalent diffusion coefficient in a free-water system.

The initial conditions required to solve (7) are expressed in a manner analogous to (2) in the form

$$c(x_{\alpha}, 0) = c_0 \text{ in } \Omega \quad (12)$$

Dirichlet, Neumann or mixed boundary conditions are specified in the form

$$c(x_{\alpha}, t) = \bar{c} \text{ on } \Gamma_1' \quad (13)$$

$$n_{\alpha} \frac{\partial c}{\partial x_{\beta}} = 0 \text{ on } \Gamma_2' \quad (14)$$

$$\left(-D_{\alpha\beta} \frac{\partial c}{\partial x_\beta} + q_\beta c \right) n_\alpha = q_\beta n_\alpha C_0(t) \text{ on } \Gamma_3' \quad (15)$$

where $\Gamma = \Gamma_1' + \Gamma_2' + \Gamma_3'$

where $C_0(t)$ is the concentration of solute in the influx water, and n_α is a component of the outward normal unit vector.

In many practical problems, the flow can be assumed to be two-dimensional and only a vertical cross-section of the three-dimensional space need to be considered. The flow and solute movements referred to the $x_1 - x_2$ plane are still described by Equations (1) and (7), respectively, where the indices α and β take on values equal to 1 and 2.

Numerical Approximations--The nonlinear set of Equations (1) and (7) are solved by using the Galerkin finite element method. In this approach, one seeks the solution of a partial differential equation

$$L(\phi) = 0 \quad (16)$$

by assuming that the unknown variable $\phi(x_\alpha, t)$ can be represented by a series expansion of the form

$$\phi(x_\alpha, t) \approx \hat{\phi}(x_\alpha, t) = \sum_{i=1}^N Y_i(t) w_i(x_\alpha) \quad (17)$$

where $w_i(x_\alpha)$ are known functions of space, or basis functions. The functions $w_i(x_\alpha)$ are linearly independent, satisfy the boundary conditions imposed on (16) and constitute a complete set. The $Y_i(t)$ are unknown time-dependent coefficients which correspond to the approximate solution of (16) at specified points within the domain of interest.

Since only a finite number $n < N$ of the basis functions can be taken into account, $L[\hat{\phi}(x_\alpha, t)]$ is equal to a certain non-zero residual. This residual is minimized by requiring that $L[\hat{\phi}(x_\alpha, t)]$ be orthogonal to each basis function, that is

$$\int_{\Omega} L[\hat{\phi}(x_\alpha, t)] w_i(x_\alpha) d\Omega = \int_{\Omega} L \left[\sum_{j=1}^n Y_j(t) w_j(x_\alpha) \right] w_i(x_\alpha) d\Omega = 0 \quad (18)$$

$$i = 1, 1, \dots, n$$

Equation (18) represents a set of n equations which will be solved for the n unknown coefficients $Y_j(t)$. Such a system can be conveniently expressed in the matrix form

$$[A] \{Y\} = \{B\} \quad (19)$$

where the arrays $[A]$ and $\{B\}$ are functions of the space coordinates and can be evaluated by performing the relevant integrations, and where $\{Y\}$ is a vector containing the unknown, time-dependent coefficients.

The region of interest is subdivided into a network of isoparametric hexahedral elements. A number is assigned to each element and to each node of the discretized domain. The choice of a node numbering scheme is important because it affects the bandwidth of the final system of algebraic equations and, consequently, the size of the coefficient matrices.

Let the variables ψ and c be approximated by series expansions of the form:

$$\psi(x_\alpha, t) \approx \hat{\psi}(x_\alpha, t) = \sum_{j=1}^n P_j(t) \omega_j(x_\alpha) \quad (20)$$

$$c(x_\alpha, t) \approx \hat{c}(x_\alpha, t) = \sum_{j=1}^n C_j(t) \gamma_j(x_\alpha) \quad (21)$$

Upon substituting (20) and (21) into (1) and (7) and applying the orthogonality theorem (18) one obtains

$$[S] \frac{d\{P\}}{dt} + [H] \{P\} + \{F\} = 0 \quad (22)$$

$$[M] \frac{d\{C\}}{dt} + [N] \{C\} + \{R\} = 0 \quad (23)$$

where the coefficient matrices are given by Equations (28) and (29), pages 12 to 13 of Segol (1976a).

The time derivatives appearing in (22) and (23) are treated using a finite difference scheme such that

$$\left. \frac{d\{P\}}{dt} \right|_{t+\epsilon\Delta t} = \frac{1}{\Delta t} (\{P\}_{t+\Delta t} - \{P\}_t) \quad (24)$$

$$\left. \frac{d\{C\}}{dt} \right|_{t+\epsilon\Delta t} = \frac{1}{\Delta t} (\{C\}_{t+\Delta t} - \{C\}_t) \quad (25)$$

where Δt is the time step. The parameter ϵ is equal to 1 if an implicit scheme is used and to 1/2 in a time-centered scheme. The value of $\{P\}$ and $\{C\}$ at $t+\Delta t$ are obtained from the relation

$$\{P\}_{t+\epsilon\Delta t} = \epsilon\{P\}_{t+\Delta t} + (1-\epsilon)\{P\}_t \quad (26)$$

$$\{C\}_{t+\epsilon\Delta t} = \epsilon\{C\}_{t+\Delta t} + (1-\epsilon)\{C\}_t \quad (27)$$

The solution of the mass-transport equation was found to be more stable when the backward difference algorithm is used. The present model does not allow one to use different values of ϵ in the flow and mass-transport equations. Substitution of (24) and (25) in (22) and (23), respectively, yields for $\epsilon = 1$.

$$\left(\frac{1}{\Delta t} [S] + [H] \right) \{P\}_{t+\Delta t} = -\{F\} + \frac{1}{\Delta t} [S] \{P\}_t \quad (28)$$

$$\left(\frac{1}{\Delta t} [M] + [N] \right) \{C\}_{t+\Delta t} = -\{R\} + \frac{1}{\Delta t} [M] \{C\}_t \quad (29)$$

When a Dirichlet condition is specified along a boundary, the value of the variable is kept constant at the nodes located along that boundary. As a consequence no equation in the system (28) is generated for a node where a constant pressure is specified. Similarly, no equation in the system (29) is generated for a node of constant concentration.

When a Neumann condition is specified along a boundary the normal derivative of the variable is known along that boundary. In the flow equation this condition is incorporated through the surface integral term.

$$\int_{\Gamma} K_r \left(K_{\alpha\beta}^S \sum_{m=1}^n \frac{\partial \omega_m}{\partial x_\beta} P_m + K_{\alpha\beta}^S \right) n_\alpha \omega_i \, d\Gamma = - \int_{\Gamma} V_n \omega_i \, d\Gamma \quad (30)$$

where V_n is the flux normal to the bounding surface. For a node located on a no-flow boundary $V_n = 0$ and (3) is not generated.

Similarly, Neumann boundary conditions can be specified for the mass-transport equation through the term

$$\int_{\Gamma} D_{\alpha\beta} \sum_{m=1}^n \frac{\partial \gamma_m}{\partial x_{\beta}} C_m \gamma_i d\Gamma = \int_{\Gamma} D_{\alpha\beta} \frac{\partial c}{\partial n} \Gamma_i d\Gamma \quad (31)$$

where $\partial c / \partial n$ represents the normal concentration gradient at the boundary. In the present documentation it is assumed that wherever $\partial c / \partial n$ is specified its value is zero and (31) is not generated.

Mixed boundary conditions are specified for the mass-transport equation along those parts of the boundary where infiltration or evaporation take place. Using (15) one writes, for infiltration,

$$\left(-D_{\alpha\beta} \frac{\partial c}{\partial x_{\beta}} + q_{\beta} c \right) n_{\alpha} = q_{\beta} n_{\alpha} C_0(t) \quad (32)$$

while for evaporation

$$\left(-D_{\alpha\beta} \frac{\partial c}{\partial x_{\beta}} + q_{\beta} c \right) n_{\alpha} = 0 \quad (33)$$

Atmospheric boundary conditions cannot be fixed a priori but depend on the current moisture conditions of the soil. Iteration is thus used to determine whether a Dirichlet or a Neumann condition should be applied at a node located on such a boundary. During the first iteration in each time step, the surface nodes may be treated as Neumann nodes and are then assigned an arbitrary fraction of the maximum flux. If the computed values of pressure head satisfy (6), the absolute value of the flux at each node is increased by $|\Psi_L|/|\Psi|$ in the case of evaporation, or by $|\Psi_L|/|\Psi_L - \psi|$ in the case of infiltration. If a value of Ψ does not satisfy (6) then during the subsequent iteration a Dirichlet boundary condition is specified at that node with $\Psi = 0$ for infiltration and $\Psi = \Psi_L$ for evaporation. This situation is maintained as long as Equation (5) is satisfied. Otherwise, a Neumann type boundary condition is assigned again.

A similar iterative procedure is used along a seepage face, since under transient conditions its exact extent is unknown.

It follows that for those nodes located on atmospheric boundaries or seepage faces the equations corresponding to Dirichlet nodes must nevertheless be included in the global matrix which is then modified appropriately.

For unsaturated flow, the values of permeability and moisture content must be evaluated at the beginning of each time step from an estimate of the pressure in the next time interval. Thus, before solving for the $(k + 1)^{\text{th}}$ time increment the value of ψ at $t^{k+1/2}$ is predicted by linear interpolation of the previous results from

$$\psi^{k+1/2} = \psi^k + \frac{\Delta t^k}{2\Delta t^{k-1}} (\psi^k - \psi^{k-1}) \quad (34)$$

Consequently the coefficient matrices are evaluated at half the time step, $k + 1/2$, which has a dampening effect on possible numerical oscillations.

Due to the nonlinear nature of (1) the initial estimate of pressure must be improved by an iterative procedure. Thus if ψ^{k+1} is the most recent value of pressure head at time $k + 1$, the pressure estimate during the next iteration is computed from

$$\psi^{k+1/2} = \frac{1}{2} (\psi^k + \psi^{k+1}) \quad (35)$$

The relations between permeability, moisture content and pressure head are provided in the form of tables and cubic splines are used to interpolate between the data points. It was found that the accuracy of the process can be improved by performing the spline fit on the logarithmic expressions of K and ψ . Similarly, the moisture capacity $\kappa = \partial\theta/\partial\psi$ is evaluated from

$$\kappa = \frac{1}{\psi} \frac{\partial\theta}{\partial \log\psi} \log e \quad (36)$$

where the expression $\partial\theta/\partial \log\psi$ is a quadratic polynomial corresponding to the first derivatives of the cubic spline.

The coefficient matrices appearing in (22) and (23) are evaluated for each element and are assembled using the well-known direct stiffness method. When the system of equations (22) is being processed, the coefficient matrices $[M]$ and $[N]$, are placed into secondary storage. Conversely, the arrays $[S]$ and $[H]$ are saved on scratch storage during assembly and solution of the mass-transport equation. Therefore, only two matrices need to be in high-speed core storage at the same time: the upper triangular parts of $[S]$ and $[H]$ when

dealing the the flow equation, or the upper triangular part of [M] and the banded portion of [N] when the mass-transport equation is being processed. For practical purposes, the stiffness matrices [H] and [N] are assembled in their transposed form. Finally, the left-hand sides of (28) and (29) are evaluated and stored in [S] and [N]^T, respectively.

The Cholesky algorithm is used to solve the symmetric system of equations for flow. The Gauss elimination procedure with a partial pivoting intended to reduce round-off errors is applied to the mass-transport equation in which the coefficient matrix is nonsymmetrical.

In the three-dimensional transport model, out-of-core equation solvers are used in order to decrease the storage space requirements. In this approach the matrices are assembled by blocks where a block is defined as a square sub-matrix of dimension equal to the semi-bandwidth for a symmetric matrix or to the bandwidth for a nonsymmetric matrix. When a block has been processed, it is transferred to secondary storage so that only two blocks need to be in memory at the same time. The present three-dimensional model is therefore mainly intended for systems in which the bandwidth is small compared to the total number of equations, as is often the case. The drawback of this technique is of course an increased number of I/O operations and a longer solution time.

Probabilistic or Statistical Aspects--None.

Assumptions and Simplifications--The main assumptions are:

- Darcy's Law is valid and hydraulic-head gradients are the only significant driving mechanisms for fluid flow.
- The maximum rate of transpiration is determined by atmospheric conditions alone.
- The hydraulic conductivity at each point is exposed as a symmetric tensor $K_{ij} = K^r(\theta) K_{ij}^s$, where K_{ij}^s is the conductivity at saturation and $K^r(\theta)$ is the relative conductivity ($0 \leq K^r(\theta) \leq 1$) as a function of volumetric moisture content.

Structure and Level of Detail--SEGOL models a flow system in a complete three-dimensional coordinate system. In cases where one-dimensions can be ignored, there is a two-dimensional form of the code.

Major Variables--Aside from the input parameter, the major dependent variables are pressure head and solute concentration.

Applicability, Limitations, Validity and Completeness--This code is applicable to both saturated and unsaturated flow in porous media. There is no provision for hysteresis included, thus the code's usage is restricted to either a single wetting or drying cycle.

References--

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Acceptance and Adequacy--SEGOL is based on state-of-the-art research and is generally accepted by the research community both in the United States and abroad, as being as good as is possible given the present level of understanding.

Model Name: UNSAT1D

Code No. 10
Type: Flow

I. Summary of Code

Purpose and Scope--UNSAT1D was developed to simulate one-dimensional flow through a partially-saturated flow system. UNSAT1D simulates infiltration, vertical seepage, and plant uptake by roots as a function of the hydraulic properties of a soil, soil layering, root growth characteristics, evapotranspiration rates, and frequency, rate and amount of precipitation and/or irrigation.

Authors--UNSAT1D was developed at Battelle's Pacific Northwest Laboratories by S. K. Gupta and C. S. Simmons. The primary contact for UNSAT1D is

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Phone: (509)376-8339

Code Functions--UNSAT1D is a fully implicit finite difference model of a one-dimensional flow through a partially saturated flow system. UNSAT1D simulates infiltration, vertical seepage, and plant uptake by roots as a function of the hydraulic properties of a soil, soil layering, root growth characteristics, evapotranspiration rates, and frequency, rate and amount of precipitation and/or irrigation.

Potential Usage--UNSAT1D can be used to estimate ground-water recharge; irrigation and consumptive use of water, irrigation return flows and other related areas dealing with partially-saturated and saturated soils. Other applications of interest to the NRC include aiding in the design of low-level radioactive waste repositories at shallow depths.

Relation to NRC Issues--Not applicable as no list of issues currently exists for low level radioactive waste treatment.

Restrictions--The code is in the public domain and is therefore available to the NRC.

Compatibility with Other NRC Codes--UNSAT1D is written in FLECS (Beyer 1975) which is compatible with FORTRAN. Some subroutines are written in FORTRAN IV. The code utilizes PNL graphics software and relies on graphical hardware for use in the interactive mode.

II. Summary of Findings

General Critique--The UNSAT1D model is a one-dimensional finite difference, fully implicit approach to simulating ground-water flow in the unsaturated zone. UNSAT1D simulates infiltration, vertical seepage, and plant uptake by roots as a function of the hydraulic properties of a soil, soil layering, the root growth characteristics of a given crop in a given soil profile, evapotranspiration rates, and frequency, rate, and amount of rainfall and/or irrigation. It can be used for estimation of ground-water recharge, irrigation and consumptive use of water, irrigation return flows, and other related areas dealing with unsaturated and saturated soils.

UNSAT1D is designed for use under varied field conditions. The application of water can be in the form of rain, sprinkler, or flooding. Actual evapotranspiration can be estimated as a function of moisture content and potential evapotranspiration using on-off, linear decrease, logarithmic decrease, or combination methods. The soil profile can be homogeneous, heterogeneous, or layered. The hydraulic properties can be defined as polynomials or other empirical equations. The root growth uptake has built-in options for the root suction, root-distribution or user defined mathematical model. The lower boundary conditions can be water table, dynamic, quasi-dynamic, or unit gradient.

UNSAT1D may be useful to the NRC for the analysis of infiltration with various plant populations and deep percolation in a saturated-unsaturated flow system. The capability of treating irrigation and/or rainfall and plant root uptake are often essential for analysis of shallow waste repositories.

Applicability to Medium--UNSAT1D is designed to simulate water movement in saturated or unsaturated or a combination of saturated and unsaturated flow systems which can adequately be represented by a one-dimensional model.

Sensitivity Analysis--No sensitivity studies have been published.

Code Validation and Field Verification--Bond et al. (1982) contains a detailed example based on hypothetical, but realistic, input parameters.

III. General Description

Operating Characteristics--The UNSAT1D model consists of a single computer code that makes the unsaturated flow predictions and several support codes used for preparation of input data, and for evaluating and displaying model results. The complete series of codes which formulate the unsaturated flow modeling package is known in the documentation, as the UNSAT1D Model Sequence.

The UNSAT1D code itself is written in FLECS (Beyer 1975), a structured programming language akin to FORTRAN. (The FLECS compiler acts as a preprocessor to FORTRAN producing a FORTRAN code as output). Other supporting programs in the UNSAT1D Model Sequence are written in either FORTRAN IV or FLECS. The UNSAT1D Model Sequence is operational on the DEC family of computers. The

UNSAT1D system operates in the interactive mode and requires graphical output devices for full utilization of its capabilities.

Inputs-- The amount of input data required by UNSAT1D is dependent on the given problem. In general, the input data includes soil profile description, (homogeneous, heterogeneous, or layered), hydraulic properties of each layer (package includes estimation of hydraulic conductivity for the unsaturated zone on the basis of moisture retention curve), plant characteristics (rooting depth constant or function of growth, root distribution, leaf area index, wilting point), water application (precipitation, irrigation, ponding), and potential evaporation/transpiration (package includes estimation from climatic data by Blaney Criddle, radiation, Penman, or ETPAN method).

Outputs--The output from the UNSAT1D model includes soil water potential (suction), moisture content, and soil water flux rate at each node (depth increment) for each time interval. The results can be in the form of lineprinter listings, binary files, or Calcomp plots.

Available Documentation--The analytical documentation is contained in Gupta et al. (1978). Bond et al. (1982) is a user's manual describing not only the UNSAT1D code but the several supporting codes. The described codes are all listed in an appendix.

IV. Review of Theory

Equations--The basic differential equation solved by UNSAT1D is

$$C(\theta) \frac{\partial h}{\partial t} = \frac{\partial}{\partial z} \left[K(\theta) \frac{\partial H}{\partial z} \right] - S \quad (1)$$

where

$C(\theta)$ = soil water differential capacity

θ = volumetric water content of the soil

h = pressure head

t = time

z = vertical coordinate with origin at the soil surface and positive downward

$K(\theta)$ = hydraulic conductivity of soil

H = total head

$= h - z$

S = source/sink term representating rainfall and irrigation influx or water uptake by plants

The above equation is obtained from Darcy's Law, continuity principles and Richard's transformation.

To solve the governing partial differential equations with the appropriate sink term, the following initial and boundary conditions must be determined. The initial conditions are $h_s(z,0) = h_0(z)$ [or $\theta(z,0) = \theta_0(z)$] at $0 \leq z \leq Z$ and $t = 0$, where Z is the depth of the semi-infinite depth, or the static quasi-dynamic or dynamic water table at $t = 0$, and subscript 0 denotes initial condition.

Boundary conditions are of two kinds, the upper-boundary or soil surface conditions and the lower-boundary or sub-surface conditions. At the soil surface, $z = 0$ and $t > 0$, $|q(0,t)| \leq |Q_0(t)|$, $h_d \leq h_s(0,t) \leq 0$ or $\theta_d \leq \theta(0,t) \leq \theta_s$, where $Q_0(t)$ is the prescribed maximum possible flux ($\text{cm}^3 \cdot \text{cm}^{-2} \cdot \text{s}^{-1}$) as governed by meteorological conditions, plant growth, and irrigation; and subscripts d and s respectively denote dry and saturated conditions. If irrigation is by ponding, the upper-boundary condition is $h(0,t) = P(t)$, where P is the depth of ponding (cm) at the surface.

Lower-boundary conditions considered are:

1. semi-infinite depth; under the assumption of unit gradient at base, $q(Z,t) = K[\theta(Z,t)]$
2. with static or quasi-dynamic water table, $h_0(Z,t) = 0$
3. with dynamic water table, $q(z,t) = Q_z(t)$ where $Q_z(t)$ is the prescribed flux at depth $Z(\text{cm}^3 \cdot \text{cm}^{-2} \cdot \text{s}^{-1})$.

Additional conditions are imposed on the source term S . There are pressure limits in the plant root xylem. At the soil surface, h_{x0} (water potential root xylem at the soil surface) can take values between zero (maximum) and the "wilting point" h_{xwilt} so that $h_{xwilt} \leq h_{x0} \leq 0$.

The actual rate of transpiration (T) is maximized subject to the constraints $T \leq (PET - \text{surface evaporation})$ and $h_{x0} \geq h_{xwilt}$. PET is the potential evapotranspiration.

Numerical Approximations--It is assumed that θ and h are related by a soil water characteristic curve. The UNSAT10 Model Sequence provide approximations to this relationship by interpolation or fitting low order polynomials.

The basic differential equation is replaced by the following system of finite difference equations. In the following description, h stands for h_s , omitting subscript so to simplify notation. The working numerical equation then becomes:

$$\begin{aligned}
\left[\frac{h_i^j C_i^j - h_i^{j-1} C_i^{j-1}}{\Delta t} \right] &= \frac{1}{(z_{i+1} - z_{i-1})} \left[\left(\frac{h_i^{j-1} - h_{i-1}^{j-1} + 2z_i}{2\Delta z_1} \right) K_{i-\frac{1}{2}}^{j-1} \right. \\
&\quad \left. - \left(\frac{h_{i+1}^{j-1} - h_i^{j-1} + 2z_i}{2\Delta z_2} \right) K_{i+\frac{1}{2}}^{j-1} \right] + \left[\left(\frac{h_i^j - h_{i-1}^j + 2z_i}{2\Delta z_1} \right) K_{i-\frac{1}{2}}^j \right. \\
&\quad \left. - \left(\frac{h_{i+1}^j - h_i^j + 2z_i}{2\Delta z_2} \right) K_{i+\frac{1}{2}}^j \right] - \text{sink} \quad (2)
\end{aligned}$$

where

i = subscript representing the depth of a node

j = subscript representing time

$$\Delta z_1 = z_i - z_{i-1}$$

$$\Delta z_2 = z_{i+1} - z_i$$

Each nonboundary node has a finite difference Equation (2) associated with it. This collection of equations can be written as a matrix equation where the coefficient matrix is tri-diagonal. Such systems of linear equations are readily solved using Gaussian elimination. The elements of this matrix depend on C and K which depend on θ . At each time step, C^j and K^j are initially taken as C^{j-1} and K^{j-1} . The total moisture content in a given soil profile is estimated from the values of h^j and also by mass balance (initial - outflow + inflow). If option for iteration is chosen, then the iterations are carried out with estimated C^{j+1} and K^{j+1} from h^{j+1} of last iterative solution at that time step. If convergence is not achieved within 10 iterations the Δt is reduced by half and the process is repeated until convergence is satisfactory. If Δt is less than the lower limit provided by the user, the program prints a message and proceeds without further iterations, to provide some data for review by the user.

Probabilistic or Statistical Aspects--None.

Assumptions and Simplifications--The primary assumptions are:

1. Richard's equation holds
2. Sufficient symmetry exists so that a one-dimensional model is adequate.

Structure and Level of Detail--UNSAT1D is a one-dimensional model for simulating ground-water flow in the unsaturated zone. UNSAT1D simulates infiltration, vertical seepage, and plant uptake by roots as a function of the hydraulic properties of a soil, soil layering, the root growth characteristics of given crop in a given soil profile, evapotranspiration rates, and frequency, rate, and amount of rainfall and/or irrigation. UNSAT1D is designed for use under varied field conditions. The application of water can be in the form of rain, sprinkler, or flooding. Actual evapotranspiration can be estimated as a function of moisture content and potential evapotranspiration using on-off, linear decrease, logarithmic decrease, or combination methods. The soil profile can be homogeneous, heterogeneous, or layered. The hydraulic properties can be defined as polynomials or user mathematical equations. The root growth uptake has built-in options for the root suction, root-distribution or user defined mathematical model. The lower boundary conditions can be water table, dynamic, quasi-dynamic, or unit gradient.

Major Variables--Aside from the input variables, the major variables are the soil water potential (head or suction), moisture content, and flux at each node in the one-dimensional column.

Applicability, Limitations, Validity and Completeness--This code can be used in situations where a one-dimensional model is adequate. It is useful to predict the amount and rate of water entering and moving through a partially-saturated flow system.

References--

- Beyer, T. 1975. "Flecs User's Manual." Department of Computer Science, University of Oregon, Eugene, Oregon.
- Bond, F. W., C. R. Cole and P. J. Gutknecht. 1982. "Unsaturated Flow Model (UNSAT1D) Computer Code Manual." To be published by EPRI. Research Project 1406-1.
- Gupta, S. S., K. Tanju, D. Nielsen, J. Biggar, C. Simmons, and J. MacIntyre. 1978. "Field Simulation of Soil-Water Movement with Crop Water Extraction." Water Science and Engineering Paper No. 4D13. Department of Land, Air and Water Resources, University of California, Davis, California.

Acceptance and Adequacy--UNSAT1D is based on state-of-the-art research and is generally accepted by the research community both in the United States and abroad, as being as good as is possible given the present level of understanding.

Model Name: SUMATRA-1

Code No. 11

Type: Flow/Transport

I. Summary of Code

Purpose and Scope--SUMATRA-1 was written to simulate the simultaneous flow of water and solutes transport in a one-dimensional (vertical) soil profile under transient saturated-unsaturated conditions.

Author--SUMATRA-1 was written by

Dr. M. Th. van Genuchten
U.S. Salinity Laboratory
4500 Glenwood Drive
Riverside, CA 92501

Code Functions-- SUMATRA-1 is based upon a Hermitian (cubic) finite element solution of the governing transport equations. The model includes such processes as linear equilibrium adsorption and zero- and first-order decay.

Potential Usage--This model is capable of performing a one-dimensional (vertical) simulation of a subsurface flow region. This flow system may have regions of saturated or unsaturated porous media. Hysteresis is not considered which restricts the usage to only one side of the wetting-drying front cycle.

Relation to NRC Issues--Not applicable as no list of issues currently exists for low-level radioactive waste treatment.

Restrictions--The code is in the public domain and is therefore available to the NRC.

Compatibility with Other NRC Codes--SUMATRA-1 is written in FORTRAN IV, using no special equipment, and is compatible with other FORTRAN codes.

II. Summary of Findings

General Critique--SUMATRA-1 is a one-dimensional code based on Hermitian (cubic) finite elements. van Genuchten (1978a) shows that this scheme produced excellent solutions though sometimes requiring more computing time than other methods.

SUMATRA-1 may be used to study water and solute movement in one-dimensional variably saturated non-homogeneous soil profile. The model considers both abrupt layering and smoothly changing soil properties.

Applicability to Medium--SUMATRA-1 is designed to simulate the simultaneous flow of water and solutes in a one-dimensional (vertical) soil profile

under transient saturated-unsaturated conditions. The model is based upon a Hermitian (cubic) finite element solution of the governing transport equations, and includes such processes as linear equilibrium adsorption and zero- and first-order decay. Since hysteresis is not considered the usage of the model is restricted to only one side of the wetting-drying front cycle.

Sensitivity Analysis--SUMATRA-1 is based on Hermitian (cubic) finite elements (HFE). van Genuchten (1978a) contains a comparison obtained by solving the same problem using (HFE), finite differences (FD) linear finite elements with mass-lumping (MFE) and linear finite elements without mass-lumping (LFE).

The HFE-scheme always generated the most accurate solutions of both the moisture and solute fronts when simulating the infiltration of water and chloride in a 125-cm deep soil profile, but this occurred at the expense of somewhat more computation time. It is concluded that the FD- and MFE-schemes are preferred when infiltration in extremely dry soil needs to be simulated. The HFE-scheme seems more attractive for less extreme cases.

Code Verification--An example problem compares results obtained with the Hermitian finite element scheme with those generated with a newly developed analytical solution for solute movement under steady-state flow conditions. The example was used to check the programming accuracy of the various decay terms in the transport equation.

Field Verification--None.

III. General Description

Operating Characteristics--SUMATRA-1 is written in FORTRAN IV. It consists of the main program and nine subprograms. The program listings are contained in van Genuchten (1978a).

Inputs--Input includes possibly making changes to one or more of the function subprograms BC, SPR and SPS. BC supplies the transient data for the boundary conditions at the soil surface. SPR defines the hydraulic functions

$\theta(h)$ = moisture content
 $K(h)$ = hydraulic conductivity
 $C(h)$ = moisture capacity
 $h(\theta)$ = pressure head

for each soil type. The function SPS specifies the soil physical and chemical parameters.

ρ = bulk density
 $D_0\tau$ = diffusion coefficient multiplied by tortuosity factor
 λ = dispersivity
 k = adsorption constant
 α = first-order liquid phase decay constant

β = first-order solid phase decay constant
 γ = zero-order liquid phase decay constant

for each soil type.

In addition, the following data is required:

Program control parameters
Grid definition
Soil type specifications
Initial pressure head or moisture content
Initial pressure gradients or moisture gradient
Initial concentration
Initial concentration gradient

Outputs--SUMATRA-1 output is entirely to the line printer and consists of the initial input data and for specified points in time the pressure head, moisture content and solute concentrations are printed for every node.

Available Documentation--SUMATRA-1 is documented in van Genuchten (1978a). van Genuchten (1978b) reports the solution of the flow equation and van Genuchten (1978a) discusses primarily solution of the transport equation. SUMATRA-1 is listed in van Genuchten (1978a) which also contains input preparation instructions.

IV. Review of Theory

Equations--The partial differential equation governing the one-dimensional vertical flow of water in a saturated-unsaturated medium is given by:

$$L_w(h) \equiv \frac{\partial}{\partial x} \left(K \frac{\partial h}{\partial x} - K \right) - C^* \frac{\partial h}{\partial t} = 0 \quad (1)$$

where

C^* is the specific soil moisture capacity (L^{-1}),
 h is the pressure head (L),
 K is the hydraulic conductivity (LT^{-1}),
 x is the vertical distance (positive down) (L), and
 t is the time (T).

The initial condition of the system is given by

$$h(x,0) = h_i(x) \quad . \quad (2)$$

One of the following two boundary conditions may be specified at the soil surface ($x = 0$)

$$h(0,t) = h_0(t) \quad (3)$$

$$\left(-K \frac{\partial h}{\partial x} + K \right) \Big|_{x=0} = q_0(t) \quad (4)$$

where $q_0(t)$ represents the actual (net) flux at the soil surface (precipitation + irrigation - evaporation). Similar boundary conditions may also be applied to the lower boundary of the soil profile ($x = \ell$), i.e.,

$$h(\ell,t) = h_\ell(t) \quad (5)$$

or

$$\left(-K \frac{\partial h}{\partial x} + K \right) \Big|_{x=\ell} = q_\ell(t) \quad (6)$$

where $q_\ell(t)$ represents the imposed drainage flux. For a free draining profile $q_\ell(t)$ equals K at $x = \ell$, and (6) reduces to

$$\frac{\partial h}{\partial x} \Big|_{x=\ell} = 0 \quad (7)$$

The solution of the chemical transport equation requires an expression relating the adsorbed concentration (S) with the solution concentration (c). Assuming only single-ion equilibrium transport and the general adsorption isotherm to be of the form

$$S = k c$$

where

k is an empirical constant ($M^{-1}L^3$) gives

$$L_s(c) = \frac{\partial}{\partial x} \left(\theta D \frac{\partial c}{\partial x} - qc \right) - \frac{\partial}{\partial t} (\theta R c) + (\alpha \theta + \beta \rho k) c + \gamma \theta \quad (8)$$

where the retardation factor R is defined as

$$R = 1 + \frac{\rho k}{\theta} \quad (9)$$

and where

- c is the solution concentration (ML^{-3}),
- D is the dispersion coefficient (L^2T^{-1}),
- S is the adsorbed concentration,
- q is the volumetric flux (LT^{-1}),
- α is a first-order rate constant (liquid phase) (T^{-1}),
- β is a first-order rate constant (solid phase) (T^{-1}),
- γ is a zero-order rate constant (liquid phase) ($ML^{-3}T^{-1}$),
- θ is the volumetric moisture content (L^3),
- ρ is the bulk density (ML^{-3}).

Equation (8) is the chemical transport equation solved in SUMATRA-1.

The initial condition for the concentration is given by

$$c(x,0) = c_i(x) \quad (10)$$

The following mixed (or third-type) boundary condition may be specified at the soil surface

$$\left(-\theta D \frac{\partial c}{\partial x} + qc \right) \Big|_{x=0} = \begin{cases} q_0(t) c_0(t) & \text{if } q_0(t) > 0 \\ 0 & \text{if } q_0(t) \leq 0 \end{cases} \quad (11)$$

where $q_0(t)$ is the same as in (4), and where $c_0(t)$ is the concentration of the infiltrating water. Note that the solute flux becomes zero during periods of evaporation ($q_0 < 0$) and redistribution ($q_0 = 0$). In some cases it may be necessary to specify a first-type boundary condition at the soil surface. In that case (11) should be replaced by

$$c(0,t) = c_0(t) \quad . \quad (12)$$

The following boundary condition at $x = \ell$ may be used when a free draining profile is considered

$$\left. \frac{\partial c}{\partial x} \right|_{x=\ell} = 0 \quad . \quad (13)$$

In some cases it may be necessary to specify a first-type boundary condition at the lower boundary of the soil profile; for example when, during periods of excessive evaporation, the profile is in contact with saline ground water. In that case one has

$$c(\ell,t) = c_\ell(t) \quad (14)$$

where $c_\ell(t)$ is the concentration of the ground water. Equation (14) holds only for upward flow of water at $x = \ell$, i.e., for $q_\ell(t) < 0$.

Numerical Approximations--Galerkin-finite element techniques are used to solve the governing flow and transport equations. Only the solution procedure for the transport equation will be given here, the treatment of the flow equation is quite parallel.

In the finite element approach the dependent variable, c , is approximated by a finite series of the form

$$c(x,t) \approx \hat{c}(x,t) = \sum_{j=1}^n \phi_j(x) a_j(t) \quad (15)$$

where the $\phi_j(x)$ are the selected basis (or shape) functions, and the $a_j(t)$ unknown, time dependent coefficients which represent solutions of (8) at specified points ("nodes") within the solution domain. Because only a finite number of basis functions are used in (15), the residual $L_S(\hat{c})$, obtained by substituting (15) into (8), will not become zero but attain a certain non-zero value. The residual is minimized by making $L_S(\hat{c})$ orthogonal to the set of basis functions $\phi_j(x)$ in (15), resulting in the following set of n equations in n unknowns

$$\int_0^\ell L_S \left[\sum_{j=1}^n \phi_j(x) a_j(t) \right] \phi_i(x) dx = 0 \quad i=1, 1, \dots, n \quad (16)$$

Substitution of (8) into (16) and further simplification will lead to a set of ordinary differential equations of the form

$$[A] \{X\} + [B] \left\{ \frac{dX}{dt} \right\} = \{F\} \quad (16)$$

where the coefficients $[A]$, $[B]$ and $\{F\}$ represent arrays which are functions of the spatial coordinate, and where $\{X\}$ is a vector containing the unknown, time dependent coefficients $a_j(t)$.

The treatment of the time derivatives proceeds along a different route than is usually seen in the literature. Equation (8) is replaced by a similar equation where the time derivatives have been replaced with finite differences and where the dispersion coefficients altered. The new equation is

$$\begin{aligned} L_S(c) \equiv & \frac{(\theta R c)^{t+\Delta t} - (\theta R c)^t}{\Delta t} \\ & - \frac{1}{2} \left[\frac{\partial}{\partial x} \left(\theta D^- \frac{\partial c}{\partial x} - qc \right) + (\alpha \theta + \beta \rho k) c + \gamma \theta \right]^{t+\Delta t} \\ & - \frac{1}{2} \left[\frac{\partial}{\partial x} \left(\theta D^+ \frac{\partial c}{\partial x} - qc \right) + (\alpha \theta + \beta \rho k) c + \gamma \theta \right]^t = 0 \end{aligned} \quad (18)$$

where

$$D^- = D - \frac{q^2 \Delta t}{6\theta^2 R} \quad (19)$$

$$D^+ = D + \frac{q^2 \Delta t}{6\theta^2 R} \quad (20)$$

Equation (18) is essentially a centered-in-time, Crank-Nicolson type scheme with correction factors applied to the dispersion coefficients. Note that the correction factors are different for the old and new time levels.

The finite element analysis, starting with (18) instead of (9), proceeds along familiar lines. Substitution of (18) into (16) and integrating by parts the spatial derivatives yields the following matrix equation

$$[P]^{t+\Delta t} \{X\}^{t+\Delta t} = [Q]^t \{X\}^t + \{S\} . \quad (21)$$

The coefficient matrices $[P]$, $[Q]$ and the vector $\{S\}$ are given on pages 12 and 13 of van Genuchten (1978a). The unknown vector $\{X\}^t$ has $a_i(t)$ for the i^{th} component. Once $\{X\}^{t+\Delta t}$ is obtained by solving (21) the approximate solution $\hat{c}(x, t+\Delta t)$ is obtained by substitution of $\{X\}^{t+\Delta t}$ into (15).

The flow equation is approximately solved by applying the above method to (1) to yield $\hat{h}(x, t+\Delta t)$.

The basis functions used in SUMATRA-1 are based on Hermitian polynomials and permit the user to not only solve for the values of the function but also solve for the values of the spatial derivatives. A discussion of these basis functions appear in van Genuchten (1978a).

Probabilistic or Statistical Aspects--None.

Assumptions and Simplifications--The main assumptions are:

- Darcy's Law is valid
- Only single-ion equilibrium transport occurs
- The general adsorption isotherm is linear
- The one-dimensional geometry is adequate

Structure and Level of Detail--SUMATRA-1 models the flow system as a soil column in one-dimension.

Major Variables--Aside from the input parameter, the major variables are the hydraulic heads, moisture contents, and solute concentrations.

Applicability, Limitations, Validity and Completeness--This code is applicable to both saturated and unsaturated flow and solute transport in a porous medium. The application must be restricted to those problems where a one-dimensional model is adequate. For those problems where SUMATRA-1 can be applied, it should be economical to use.

References--

van Genuchten, M. Th. 1978a. "Mass Transport in Saturated-Unsaturated Media: One-Dimensional Solutions" Research Report 78-WR-11, Water Resources Program, Department of Civil Engineering, Princeton University, Princeton, New Jersey.

van Genuchten, M. Th. 1978b. "Numerical Solutions of the One-Dimensional Saturated-Unsaturated Flow Equation" Research Report 78-WR-9, Water Resources Program, Department of Civil Engineering, Princeton University, Princeton, New Jersey.

Acceptance and Adequacy--SUMATRA-1 is based on state-of-the-art research and is generally accepted by the research community as being about as good as is possible given the present level of understanding.

Model Name: TARGET

Code No. 18
Type: Flow/Transport

I. Summary of Code

Purpose and Scope--TARGET was developed at Dames & Moore for prediction of coupled hydrodynamics, heat transfer and chemical-species transport in saturated and unsaturated porous media.

Authors--TARGET was developed at Dames & Moore by

Dr. Devraj Sharma
Manager, Advanced Technology Center
Dames & Moore
1626 Cole Boulevard
Golden, CO 80401

Code Functions--TARGET is an integrated finite difference model of ground-water flow and effluent transport under transient conditions. The model permits zero and first order decay of reacting chemical species being transported by the ground water. Provisions are also made for heat transfer, a useful feature for radioactive waste studies. The numerical procedure used to solve the differential equations is computationally economical.

Potential Usage--TARGET should be of interest to the NRC because of its heat transfer and chemical species transport features. The model is capable of performing three-dimensional simulations of transient ground-water flow through variably saturated multilayered soils.

Relation to NRC Issues--Not applicable as no list of issues currently exists for low-level radioactive waste treatment.

Restrictions--This code is proprietary, owned by Dames & Moore.

Compatibility with Other NRC Codes--TARGET is written in FORTRAN IV, using no special equipment and is compatible with other NRC codes.

II. Summary of Findings

General Critique--The code is not available directly for use by the NRC since it is owned by Dames & Moore. This proprietary nature results in few open literature publications about the code. The code is quite flexible permitting its application to many different types of problems. The code has the capability to treat heat transfer problems.

Applicability to Medium--TARGET was designed to simulate transient ground-water flow through variably saturated soils. It has the capability to deal

with both chemical species transport and heat transfer. These later two features are not available in many models. The simulation can also be carried out in one-, two- or three-dimensions.

Sensitivity Analysis--No extensive data have been published. Dames & Moore (1980) contains results of some one-dimensional tests comparing TARGET results with results obtained by using another model and laboratory experiments. The comparison shows good agreement.

Code Verification--The code was verified by using a one-dimensional experiment of steady infiltration into a uniform sand column assumed to be uniformly unsaturated initially. Similarly the sand column was assumed to be uniformly saturated initially, the top surface maintained as impermeable while the column was drained.

Field Validation--None reported.

III. General Description

Operating Characteristics--TARGET is written in FORTRAN IV and is operational on a CDC 6600 computer.

Inputs--Input to TARGET includes:

- Grid geometry
- Initial pressure heads
- Initial moisture contents
- Initial concentrations of any chemical species being transported
- Initial temperatures
- Boundary specifications
- Boundary flow specifications
- Soil properties

Outputs--Output includes

- All input data initially
- Pressure heads
- Velocities
- Concentrations of chemical species
- Temperature

Available Documentation--Since TARGET is a proprietary code the documentation is quite limited. Dames & Moore (1980) contains some sketchy information.

IV. Review of Theory

Equations--The partial differential equation governing the distribution of "pressure head" in unsaturated-saturated regions within undeformable soils is

$$\left[\frac{\partial (n S_+)}{\partial t} \right] \frac{\partial \psi}{\partial t} = \sum_{i=1}^3 \sum_{j=1}^3 \frac{\partial}{\partial x_i} \left\{ K_+ K_{ij} \left(\frac{\partial \psi}{\partial x_j} + \frac{\partial z}{\partial x_j} \right) \right\} + S^\phi \quad (1)$$

where

- ψ is pressure head
- n is porosity
- S_+ is saturation
- t is time
- x_i is spatial coordinate
- K_+ is relative hydraulic conductivity of unsaturated media
- K_{ij} is tensorial form of saturated hydraulic conductivity
- z is vertical spatial coordinate
- S^ϕ is source (and/or sink) term for ϕ .

Implicit in Equation (1) is the definition of Darcy velocity for unsaturated flows:

$$U_i = - \sum_{j=1}^3 K_T K_{ij} \left(\frac{\partial \psi}{\partial x_j} + \frac{\partial z}{\partial x_j} \right) \quad (2)$$

The equation governing the concentration of the ℓ^{th} chemical species of concern is expressed as:

$$\begin{aligned} & \frac{\partial}{\partial t} \left\{ n S_+ C_\ell \left[1 + \left(\frac{1-n}{n} \right) \left(\frac{\rho_s}{\rho} - \frac{K_{d\ell}}{S_+} \right) C_\ell^{m-1} \right] \right\} + \sum_{i=1}^3 \frac{\partial}{\partial x_i} (U_i C_\ell) \\ &= \sum_{i=1}^3 \sum_{j=1}^3 \frac{\partial}{\partial x_i} \left\{ D_{\ell,ij} \frac{\partial C_\ell}{\partial x_j} \right\} + S^\ell \end{aligned} \quad (3)$$

where

- C_ℓ is concentration of ℓ^{th} chemical species
- ρ_s is dry density of soil matrix
- ρ is density of water

$K_{d\ell}$ is distribution coefficient for species ℓ in the Freundlich equation
see (8) below

m is exponent in chemical kinetic term

$D_{i,j}^{\ell}$ is dispersion coefficient of species ℓ as a variable in coordinate
directions i and j .

The equation governing conservation of thermal energy may be expressed as:

$$\frac{\partial}{\partial t} (\bar{C}_v T) + \sum_{i=1}^3 \frac{\partial}{\partial x_i} (u_i \bar{C}_p T) = \sum_{i=1}^3 \frac{\partial}{\partial x_i} \left(\Gamma_{x_i}^T \frac{\partial T}{\partial x_i} \right) + S^T \quad (4)$$

where

$\bar{C}_v$ is average specific heat capacity at constant volume

$\bar{C}_p$ is average specific heat capacity at constant pressure

T is temperature

$\Gamma_{x_i}^{\phi}$ is effective hydraulic conductivity or dispersion coefficient for
variable ϕ , in direction x_i

The relationship between unsaturated permeability and suction pressure,
as well as that between moisture content and suction pressure, are usually
obtained empirically for each soil type. One set of such relationships is:

$$K_r = \left\{ 1 + [a_{0K} (-\psi)]^{a_{1K}} \right\}^{-a_{2K}}, \quad (5)$$

$$S_r = \frac{\theta_R}{\theta_S} + \left(1 - \frac{\theta_R}{\theta_S} \right) \left\{ 1 + [a_{0S} (-\psi)]^{a_{1S}} \right\}^{-a_{2S}}, \quad (-\infty < \psi \leq 0). \quad (6)$$

The pressure head is defined by:

$$\psi \equiv \frac{P}{\rho(g/g_c)} \quad (7)$$

The dispersion coefficient D_{ij} is obtained empirically, usually with reference to laboratory-scale experiments. The adsorbed/desorbed concentration of solute in the solid matrix is usually expressed on the assumption of a simple equilibrium reaction, thus:

$$C_{S_\ell} = K_{d\ell} C_\ell^m \quad (8)$$

This expression is called the Freundlich equation and $K_{d\ell}$ is the familiar distribution coefficient.

In order to complete the mathematical specification of a given problem, both initial and boundary conditions are required to be specified. Initial conditions, supplied over the entire domain selected for solution, must include values of:

- moisture content, θ ; and when appropriate
- concentration of species, ℓ , C_ℓ .

Boundary conditions on the boundaries of the domain must be specified with respect to:

- type of flow boundary and related flow quantities;
- nature of boundary in respect of chemical species, if appropriate; and
- sources (and/or sinks) of mass on the boundaries of or within the domain.

Numerical Approximations--The numerical algorithm adopted for the set of Equations (1) to (4) is based upon an integrated finite-difference technique designed to solve efficiently, partial differential equations of the general form:

$$A \frac{\partial Q}{\partial t} + \frac{\partial (BQ)}{\partial x_1} = \frac{\partial}{\partial x_1} \left(C \frac{\partial Q}{\partial x_1} \right) + D \quad (9)$$

Details of the technique are provided in Sharma (1979). It is emphasized here however, that the technique is particularly suited to nonlinear forms of the above equation. Specifically, coefficients A, B, C and D can be strong functions of Q itself. Hence, the twin requirements that the technique satisfies the finite-difference form of the above equation at a grid node P, i.e.,

$$\left\{ \sum_P A - SN_P \right\} Q_P = \sum_K A_K Q_K + SO_P \quad (10)$$

exactly and be iterative in order to account for the dependence of the coefficients upon the dependent variable itself, are both met. In (10) the following notation is used:

SN_P is component of linearized source term at node P

SO_P is component of linearized source terms at node P

k is the index ranging over the neighboring grid lines in space about the grid node P

The sets of simultaneous algebraic equations noted above are solved by the efficient application of an alternating-direction, heavily-implicit, line-by-line solution algorithm coupled to a plane-by-plane block correction procedure. Details are provided in Sharma (1979). This algorithm applied iteratively leads to relatively monotonic solutions for most problems with commonly-encountered boundary conditions.

Probabilistic or Statistical Aspects--None.

Assumptions and Simplifications--The assumptions imposed include:

- Darcy's law holds and pressure head gradients are the only significant driving mechanisms for fluid flow
- The source term in the describing equation may be dependent on the temperature
- The hydraulic conductivity at each point is experienced as a symmetric tensor K_{ij} where K_{ij} is the relative hydraulic conductivity of the unsaturated media and K_{ij} is the saturated hydraulic conductivity. K_{ij} ranges from 0 to 1.
- Vapor diffusion in the unsaturated zone is not considered.

Structure and Level of Detail--The integrated finite difference technique allows the user to define the discretization grid to yield much detail in some regions of interest and use large cells where details are not important.

Major Variables--The major variables used in TARGET are

Pressure head
Flow rates
Chemical species concentrations
Temperature.

Applicability, Limitations, Validity and Completeness--This model is applicable to both saturated and unsaturated flow systems where thermal energy transfer and chemical transport are of interest. The integrated finite difference method allows one to apply the same model in one-, two- or three-dimensional situations.

References--

Dames & Moore. 1980. "Detailed Seepage Investigation of Mill Waste Disposal Alternatives, West Gas Hills, Wyoming, for Federal American Partners" Volume II, Dames & Moore Job 10500-004-06, Salt Lake City, Utah.

Sharma, D. 1979. "A Comprehensive Mathematical Model Capable of Predicting Flow, Heat Transfer as Well as Chemical-Species Transport in Porous Media," Dames & Moore, Advanced Technology Group, Rep. TN-DN-42.

Acceptance and Adequacy--This model is based on state-of-the-art research and is generally accepted by the research community as being about as good as is possible given the present level of understanding.

Model Name: FEMWATER

Code No. 24
Type: Flow

I. Summary of Code

Purpose and Scope--FEMWATER (A Finite-Element Model of Water Flow through Saturated-Unsaturated Porous Media) was developed to simulate ground-water dynamics in saturated-unsaturated subsurface systems.

Authors--FEMWATER was developed at Oak Ridge National Laboratory by G. T. Yeh and D. S. Ward. It is an extension of work done by Reeves and Dugid (1976). Prime contact is:

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Code Functions--FEMWATER is a finite-element model of water flow through porous media to simulate the ground-water dynamics in saturated-unsaturated subsurface systems. The response of the ground-water basin to the rainfall, artificial withdrawal, and other recharge or discharge sources (such as lakes, reservoirs, and streams) may be included in the simulation.

The aquifer to be modeled may be given an areal description or may be cross sectional. Aquifer parameters may be distributed or zoned and the system may be anisotropic. The model considers nonlinearities by allowing the storage term and the hydraulic conductivity to be a function of the pressure head. Three types of boundary conditions are considered; they all may be functions of time. Additionally, the flow field is computed in a manner consistent with the finite element approach, thus obtaining continuity of the velocities at the nodes of the finite element mesh.

Potential Usage--This model is capable of performing a two-dimensional simulation of an aquifer system. This system may have regions of unsaturated or saturated porous media. FEMWATER produces not only a continuous pressure distribution, but also a continuous velocity field. This continuous velocity field is used as input to the companion code, FEMWASTE, which simulates the contaminant transport in such a medium.

Relation to NRC Issues--Not applicable as no list of issues currently exists for low-level radiation waste treatment.

Restrictions--The code is in the public domain and is therefore available to the NRC.

Compatibility with Other NRC Codes--FEMWATER is written in FORTRAN IV using no special equipment, hence it is compatible with other NRC codes.

II. Summary of Findings

General Critique--The code may be useful to the NRC for the analysis of the flow patterns and pressure distributions in a saturated or unsaturated aquifer system. Boundary conditions consist of specified head, specified flux or a mixture of the two (seasonal variation). The model analyzes an aquifer from a plane cross-sectional or areal viewpoint. However, radial coordinates have not been implemented; this would be a major disadvantage in the analysis of radial well flow problems.

FEMWATER is an extension of the work performed by Duguid and Reeves (1976) in which the continuity equation of water mass governing the distribution of pressure head is solved by the Galerkin finite-element method subject to appropriate boundary and initial conditions. The flow field is then computed with Darcy's Law by taking the derivatives of the calculated pressure field. Inherent in that approach, however, is the resulting discontinuity in the velocity at element boundaries and nodal points, which unfortunately leads to a violation of the conservation of mass in a local sense. When the spatial distribution of the velocity is significant in the region, inputting this discontinuous flow field to the contaminant transport computation could conceivably produce a large error. FEMWATER incorporates a technique to overcome this problem by solving Darcy's law for the velocity field at nodal points by the finite-element method rather than by taking the derivatives of the pressure field. This approach is consistent with the spirit of finite-element methods, and yields a continuous velocity over the whole region of interest, including element boundaries and nodal points.

Applicability to Medium--FEMWATER is designed to simulate saturated or unsaturated water flow subject to variable boundary or initial conditions. The code is applicable to most porous media as long as vertical or horizontal averaging is valid and a two-dimensional simulation is performed.

Sensitivity Analysis--A comparison of velocity components simulated by the original code by Duguid and Reeves (1976) to FEMWATER was performed. Unique velocity fields are obtained by the revised model, while the discontinuous velocity fields at all nodal points appear by the old model. The discontinuity ranges from several hundred percent to negligible. The overall mass loss through boundaries for the transient problem is much reduced from 23.8% to 2.2% for one case and from 29.7% to 3.6% for another case.

Code Verification--Two sample problems to which solutions had previously been obtained by other validated numerical models, namely, 1) the seepage pond problem, and 2) the Freeze transient problem, were solved. In addition, results by all six alternative numerical schemes were compared in both examples, and reported in Yeh and Ward (1979).

Field Validation--None.

III. General Description

Operating Characteristics--FEMWATER is written in FORTRAN for use on an IBM 360 machine.

Inputs--Inputs for FEMWATER include:

- Grid geometry
- Initial heads
- Prescribed head and flux boundary conditions
- Hydraulic conductivity tensor
- Modified storage coefficient
- Material properties

Outputs--Output for FEMWATER consists of the pressure distribution and velocity field at each time step.

Available Documentation--FEMWATER is documented in Yeh and Ward (1979) and in Yeh (1982).

IV. Review of Theory

Equations--The governing equations to describe the pressure field in a two-dimensional subsurface system are obtained from the principle of conservation of mass and Darcy's law. This can be written in the form

$$F \frac{\partial h}{\partial t} - \left[\frac{\partial}{\partial x} \left(K_{xx} \frac{\partial H}{\partial x} + K_{xz} \frac{\partial H}{\partial z} \right) + \frac{\partial}{\partial z} \left(K_{zx} \frac{\partial H}{\partial x} + K_{zz} \frac{\partial H}{\partial z} \right) \right] - Q = 0 \quad (1)$$

where

$$F = \frac{\theta}{\phi} \alpha' + \beta' \theta + \frac{d\theta}{dh} \quad ,$$

and

$$H = h + z \quad ,$$

in which h is the pressure head; θ is the moisture content; ϕ is the effective porosity; α' and β' are the modified coefficients of compressibility of the

medium and water, respectively; K_{xx} , K_{xz} , K_{zx} , and K_{zz} are the hydraulic conductivity tensor components; x and z are the horizontal and vertical coordinates, respectively; t is the time; Q is the artificial recharge or withdrawal.

Equation (1) is defined over a region R in the x - z plane. R is bounded by the curve $B(x,z)$ which is composed of four parts, one which is denoted as B_1 , the impervious part of the boundary. Three types of boundary conditions are considered in the program. These boundary conditions partition the remaining parts of B into B_1 , B_2 and B_3 .

In the first type (Dirichlet) boundary the pressure head is prescribed as a known function of time and (x,z) on B_1 . In the second type (Neumann) boundary the flux is prescribed as a known function of time and (x,t) on the B_2 portion of the curve B . The third type is variable in the sense that either Dirichlet or the Neumann conditions may prevail as known functions of time, and (x,z) on the B_3 portion of B .

Thus the boundary condition equations are

$$h = h_1(x,z,t) \quad (2)$$

on B_1 ,

$$- \left[\left(K_{xx} \frac{\partial h}{\partial x} + K_{xz} \frac{\partial h}{\partial z} + K_{xz} \right) \cdot n_x + \left(K_{zx} \frac{\partial h}{\partial x} + K_{zz} \frac{\partial h}{\partial z} + K_{zz} \right) \cdot n_z \right] = q_2 \quad (3)$$

on B_2 , and

$$h = h_3(x,z,t) \quad (4)$$

or

$$- \left[\left(K_{xx} \frac{\partial h}{\partial x} + K_{xz} \frac{\partial h}{\partial z} + K_{xz} \right) \cdot n_x + \left(K_{zx} \frac{\partial h}{\partial x} + K_{zz} \frac{\partial h}{\partial z} + K_{zz} \right) \cdot n_z \right] = q_3 \quad (5)$$

on B_3 . In Equations (3) and (5) n_x and n_z are the directional cosines of the outward unit vector normal to the boundary at the point of application.

Initially, Equation (5) is applied to the boundary B_3 when the exact boundary conditions cannot in general be predicted a priori. Such a case

would arise at the ground surface where either ponding (Dirichlet) or infiltration (Neumann) conditions could prevail. This can only be determined in the cyclic process of solving Equation (1).

In general, Equation (1) is nonlinear as both the soil properties, F , and hydraulic conductivity, K , are functions of the pressure head.

The initial condition of Equation (1) is assumed to be known as:

$$h = h_0(x, z) \text{ in } R, \quad (6)$$

where h_0 is a known function of spatial coordinates x and z . The function h_0 may be obtained by simulating the steady-state version of (1) with time-invariant boundary conditions.

After (1) is solved for the pressure head, h [subject to initial and boundary conditions, (2) through (6)], the velocity components are then obtained from

$$v_x = - \left(K_{xx} \frac{\partial h}{\partial x} + K_{xz} \frac{\partial h}{\partial z} + K_{xz} \right) \quad (7)$$

and

$$v_z = - \left(K_{zx} \frac{\partial h}{\partial x} + K_{zz} \frac{\partial h}{\partial z} + K_{zz} \right) \quad (8)$$

Numerical Approximations--Equations (1) through (6) are solved by the Galerkin finite-element method. The region of interest is subdivided into an assemblage of smaller subdomains called elements. The quadrilateral bilinear element is used. Following the standard procedure of the Galerkin finite-element method, an approximate formulation of the pressure head h is obtained.

The variable h is approximated in an element e by

$$h \approx h = \sum_{j=1}^4 h_j(t) N_j \quad (9)$$

where N_j and h_j are the basis function of element e and the amplitude of h , respectively, at nodal point j .

Using the Galerkin weighted residual procedure over the domain R, one obtains the following element matrix equation for element e:

$$[M_{ij}]\{\dot{h}_j\} + [S_{ij}]\{h_j\} + \{D_i\} + \{Q_i\} = 0 \quad (10)$$

where the temporal derivative of the head, h_i is given as:

$$\dot{h}_i = \frac{dh_i}{dt} \quad (11)$$

and where the matrix equation coefficients may be found in Yeh and Ward (1979), page 8.

Finite-difference methods are typically used in the approximation of the time derivative. Three time-marching methods are adopted in the present water flow model. In the first one, the central or Crank-Nicolson formulation is used, in which the required matrices are evaluated at $(t + \Delta t/2)$. In the second method the backward difference formulation is used in which the required matrices are evaluated at $t + \Delta t$. In the third optional method, the values of the unknown variables assumed to vary linearly with time during the time interval Δt . In this mid-difference method, the required matrices are all evaluated at $t + \Delta t/2$. This option has been shown superior to the central or backward-difference formulation, if the mass matrix is not lumped.

In summary, all element matrix equations presented in this section can be written as:

$$[C_{ij}]\{h_j\} = \{R_i\} - \{Q_i\} \quad (12)$$

where $[C_{ij}]$ is the element coefficient matrix, $\{h_j\}$ is the unknown vector to be found, and $\{R_i\}$ is the element load vector.

It is important to note that the model also applies the Galerkin technique to Darcy's law so as to produce a continuous flow field. This avoids discontinuities of the flow field at the nodes.

Probabilistic or Statistical Aspects--None.

Assumptions and Simplifications--The main assumptions are:

- Darcy's law is valid and hydraulic-head gradients are the only significant driving mechanisms for fluid flow.

- The nonlinear soil properties, F , and the hydraulic conductivity, K , are functions of the pressure head, h , only.

Structure and Level of Detail--FEMWATER models an aquifer either from an areal viewpoint or as a cross section. The domain is discretized using four-noded isoparametric finite elements of almost any quadrilateral shape. The time domain is discretized by finite-difference techniques.

Major Variables --Aside from the input parameters, the major variables are the hydraulic heads.

Applicability, Limitations, Validity and Completeness--This code is applicable to both saturated or unsaturated flow in a porous medium. This has evident advantages over codes that only model saturated flow. The code is limited to two-dimensional flow problems.

References--

- Yeh, G. T., and D. S. Ward. 1979. "FEMWATER: A finite-Element Model of Water Flow Through Saturated-Unsaturated Porous Media," Oak Ridge National Laboratory Report ORNL-5567.
- Yeh, G. T. (1982). "Training Course No.1: The Implementation of FEMWATER (ORNL-5567) Computer Program--Final Report." NUREG/CR-2705.
- Reeves, M., and J. O. Duguid. 1976. "Water Movement Through Saturated-Unsaturated Porous Media: A Finite-Element Galerkin Model," Oak Ridge National Laboratory Report ORNL-4927.

Acceptance and Adequacy--The physics of flow in the unsaturated zone is less fully understood than that for flow in the saturated zone. This code is based on state-of-the-art research and is generally accepted by the research community as being about as good as is possible given the present level of understanding.

Model Name: FEMWASTE

Code No. 25
Type: Transport

I. Summary of Code

Purpose and Scope--FEMWASTE (A Finite-Element Model of Waste Transport Through Saturated-Unsaturated Porous Media) was developed to simulate the transport of dissolved constituents by ground water through saturated-unsaturated subsurface systems.

Authors--FEMWASTE was developed at Oak Ridge National Laboratory by G. T. Yeh and D. S. Ward. It is an extension of work done by Duguid and Reeves (1976). Prime contact is:

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Code Functions--FEMWASTE is a finite element model for the transport of dissolved constituents by ground water through saturated-unsaturated porous media. Transport mechanisms include: advection, hydrodynamic dispersion, chemical sorption, and first-order decay. Implementation of quadrilateral isoparametric finite elements, bilinear spatial interpolation, asymmetric weighting functions, several time-marching techniques, and Gaussian elimination are employed in the numerical formulation. The waste transport model is compatible with the water flow model FEMWATER for predicting convective Darcy velocities in partially saturated porous media. FEMWATER is documented in Yeh and Ward (1979).

Potential Usage--FEMWASTE is capable of simulating the transport of dissolved constituents in a two-dimensional ground-water system. This system may have regions of saturated or unsaturated porous media. The velocity field for the ground water may be obtained by using the companion code FEMWATER.

Relation to NRC Issues--Not applicable as no list of issues currently exists for low-level radioactive waste treatment.

Restrictions--The code is in the public domain and is therefore available to the NRC.

Compatibility with Other NRC Codes--FEMWASTE is written in FORTRAN IV using no special equipment, hence it is compatible with other NRC codes.

II. Summary of Findings

General Critique--The code may be useful to the NRC for the analysis of contaminant concentration distributions in a saturated or unsaturated aquifer system. Boundary conditions consist of specified concentrations, specified flux or a mixture of the two (seasonal variation). The model analyzes an aquifer from a plane cross-sectional or arial viewpoint. However, radial coordinates have not been implemented; this would be a major disadvantage in the analysis of radial well flow problems.

FEMWASTE is an extension of the work performed by Duguid and Reeves (1976) in which the distribution of the pollutant constituent is obtained from mass balance equations.

Applicability to Medium--FEMWATER is designed to simulate the transport of dissolved constituents by ground water through saturated or unsaturated flow sytems subject to variable boundary or initial conditions. The code is applicable to most porous media as long as vertical or horizontal averaging is valid and a two-dimensional simulation is performed.

Sensitivity Analysis--A comparison is made with results obtained by the original code (Duguid and Reeves 1976; Reeves and Duguid 1976) using the original water movement model (Reeves and Duguid 1976) and the flow field produced by the companion code FEMWATER (Yeh and Ward 1979). The mass-balance error was reduced from 17% (old model) to 1% to 2% (new model), depending on the numerical scheme used.

Code Verification--A sample problem to which solutions had previously been obtained by other validated numerical models is studied in Yeh and Ward (1981). This problem is the seepage pond problem given in Duguid and Reeves (1976). In addition, results by all twelve alternative numerical schemes were compared with this example.

Field Validation--None.

III. General Description

Operating Characteristics--FEMWASTE is written in FORTRAN for use on an IBM 360 machine.

Inputs--Inputs for FEMWASTE include:

- Grid geometry
- Initial concentrations
- Prescribed concentration and flux boundary conditions
- Material properties
- Flow field velocity components

Outputs--Output for FEMWASTE consists of the pressure distribution and velocity field at each time step.

Available Documentation--FEMWASTE is documented in Yeh and Ward (1981) and in Yeh (1982).

IV. Review of Theory

Equations--The equation governing the distribution of a pollutant constituent in a two-dimensional subsurface porous system is obtained from the law of mass balance. It can be written in the form

$$\begin{aligned} L(c) = & \frac{\partial}{\partial t} (\theta c + \rho s) + (\theta c + \rho s) \alpha' \frac{\partial h}{\partial t} + \left(\frac{\partial V_x c}{\partial x} + \frac{\partial V_z c}{\partial z} \right) \\ & - \left[\frac{\partial}{\partial x} \left(\theta D_{xx} \frac{\partial c}{\partial x} + \theta D_{xz} \frac{\partial c}{\partial z} \right) + \frac{\partial}{\partial z} \left(\theta D_{zx} \frac{\partial c}{\partial x} + \theta D_{zz} \frac{\partial c}{\partial z} \right) \right] \\ & + \lambda (\theta c + \rho s) - M = 0 \end{aligned} \quad (1)$$

where θ is the moisture content; c is the concentration of dissolved constituent in the water; ρ is the bulk density of the solid; s is the concentration of the constituent that is adsorbed on the solid; α' is the modified coefficient of compressibility of the medium; h is pressure head of the water; D_{xx} , D_{xz} , D_{zx} , and D_{zz} are the dispersion coefficient tensor components; V_x and V_z are the Darcian velocity components in the x - and z -directions, respectively; λ is the decay constant; M is the artificial source; x and z are the horizontal and vertical coordinates, respectively; t is the time; and L is an operator.

Equation (1) expresses the mass balance in an initially small bulk volume. The first term represents the rate of change of total mass (including dissolved and adsorbed) in the element volume. The second term is the mass change due to the change of the bulk volume under pressure. The third and fourth terms represent the mass fluxes out and into the volume by advection and dispersion, respectively. The fifth term is the mass change due to the decay while the last term is the artificial input or withdrawal. Variables, θ , h , V_x , and V_z , in Equation (1) are obtained from the hydrodynamics of the subsurface flow system. The dispersion coefficient tensor is related to flow field and media properties as

$$\theta D_{xx} = a_T V + (a_L - a_T) V_x^2 / V + D_m \quad (2)$$

$$\theta D_{xz} = \theta D_{zx} = (a_L - a_T) V_x V_z / V \quad (3)$$

and

$$\theta D_{zz} = a_T V + (a_L - a_T) V_z^2 / V + D_m T, \quad (4)$$

where $V = \sqrt{V_x^2 + V_z^2}$; a_T and a_L are the transverse and longitudinal dispersivities, respectively; T is the tortuosity; and D_m is the molecular diffusion coefficient. The decay constant, λ , is a property of the constituent and ρ and α' are the properties of the porous media under consideration. The independent variables include: x , z , and t . Thus, there are two dependent unknowns, c and s , in Equation (1) to be determined. An additional equation is required to completely define the system. It is assumed that the adsorption of the constituent by the solid is to occur at a rapid rate (i.e., a fast exchange reaction) such that the dissolved material is in equilibrium with the material adsorbed by the solid. This is expressed by the linear equation:

$$s = K_d c, \quad (5)$$

where K_d is the distribution coefficient. Substituting (5) into (1), yields

$$\begin{aligned} L(c) = & \theta R_d \frac{\partial c}{\partial t} + \left(\frac{\partial V_x c}{\partial x} + \frac{\partial V_z c}{\partial z} \right) - \left[\frac{\partial}{\partial x} \left(\theta D_{xx} \frac{\partial c}{\partial x} + \theta D_{xz} \frac{\partial c}{\partial z} \right) \right. \\ & \left. + \frac{\partial}{\partial z} \left(\theta D_{zx} \frac{\partial c}{\partial x} + \theta D_{zz} \frac{\partial c}{\partial z} \right) \right] + \left(\frac{\partial \theta}{\partial t} + \alpha' \theta R_d \frac{\partial h}{\partial t} + \lambda \theta R_d \right) c - M = 0, \end{aligned} \quad (6)$$

where

$$R_d = 1 + \frac{\rho K_d}{\theta} \quad (7)$$

is the retardation factor, which is a measure of the delay of the breakthrough of the dissolved constituent.

Equation (6) is defined over a region R in the x - z plane. R is bounded by the curve $B(x,z)$ which is composed of four parts, one which is denoted as B_1 is the impervious part of the boundary. Three types of boundary conditions are considered in the program. These boundary conditions partition the remaining parts of B into B_1 , B_2 and B_3 .

The first type of boundary conditions occurs on the Dirichlet boundaries where the concentration is prescribed by

$$c = c_1(x, z, t) \quad \text{on } B_1, \quad (8)$$

where c_1 is a given function of time and (x, z) on B_1 . The second type occurs on the Neumann boundaries where the normal gradient of the concentration is prescribed by

$$\begin{aligned} & -\left(\theta D_{xx} \frac{\partial c}{\partial x} + \theta D_{xz} \frac{\partial c}{\partial z} - V_x c\right)n_x - \left(\theta D_{zx} \frac{\partial c}{\partial x} + \theta D_{zz} \frac{\partial c}{\partial z} - V_z c\right)n_z \\ & = q_2(x, z, t) + (V_x n_x + V_z n_z)c \quad \text{on } B_2, \end{aligned} \quad (9)$$

where n_x and n_z are the directional cosines of the outward unit vector normal to the B_2 portion of the curve B ; $q_2(x, z, t)$ is the given function of time, t , and (x, z) on B_2 . The right-hand side of (9) is zero when it is applied to impervious boundaries on which both $q_2(x, z, t)$ and the normal velocity, $(V_x n_x + V_z n_z)$, are equal to zero. If it is applied to the flow-through boundaries with outflows from the region, it becomes a concentration-dependent boundary condition and $q_2(x, z, t)$ is normally set to zero. When it is applied to the flow-through boundaries with inflows into the region, it degenerates into a third type (Cauchy) boundary condition

$$\begin{aligned} & -\left(D_{xx} \theta \frac{\partial c}{\partial x} + D_{xz} \theta \frac{\partial c}{\partial z} - V_x c\right)n_x - \left(D_{zx} \theta \frac{\partial c}{\partial x} + D_{zz} \theta \frac{\partial c}{\partial z} - V_z c\right)n_z \\ & = q_3(x, z, t) \quad \text{on } B_2, \end{aligned} \quad (10)$$

where q_3 is a given function of time and points (x, z) on B_3 portion of B .

The initial condition for (6) is assumed to be known as:

$$c = c_0(x, z) \quad \text{at } t = 0 \text{ and } (x, z) \text{ in } R, \quad (11)$$

where c_0 is a given function of spatial coordinates, x and z ; R is a region bounded by the curve, $B(x, z) = 0$.

Numerical Approximations--Equations (6) through (10) are solved by the Galerkin finite-element method. The region of interest is subdivided into an assemblage of smaller subdomains called elements. Following the procedure of finite-element weighted-residual method, and employing quadrilateral bilinear elements for spatial discretization, approximate formulation of the concentration distribution, c , is obtained. The variable c is approximated in an element e by

$$c \approx \hat{c} = \sum_{j=1}^4 c_j(t) N_j , \quad (12)$$

where N_j and c_j are the basis functions (interpolating functions) of element e and the magnitude of c , respectively, at nodal point, j .

Using the Galerkin weighted-residual procedure over the domain R one obtains the following element matrix equation for element e

$$[M_{ij}] \{\dot{\hat{c}}_j\} + [S_{ij}] \{c_j\} + \{D_i\} + \{Q_i\} = 0 , \quad (13)$$

where

$$\dot{\hat{c}}_j = \frac{dc_j}{dt} . \quad (14)$$

The M_{ij} , S_{ij} , D_i and Q_i are defined in Yeh and Ward (1981), p. 13-14.

Finite-difference methods are typically used in the approximation of the time derivative. Three time-marching methods are adopted in the present water flow model. In the first one, the central or Crank-Nicolson formulation is used, in which the required matrices are evaluated at $(t + \Delta t/2)$. In the second method the backward difference formulation is used in which the required matrices are evaluated at $t + \Delta t$. In the third optional method, the values of the unknown variables assumed to vary linearly with time during the time interval Δt . In this mid-difference method, the required matrices are all evaluated at $t + \Delta t/2$. This option has been shown superior to the central or backward-difference formulation, if the mass matrix is not lumped.

In summary, all element matrix equations presented in this section can be written as:

$$[C_{ij}] \{c_j\} = \{R_i\} - \{Q_i\} \quad (15)$$

where $[C_{ij}]$ is the element coefficient matrix, $\{c_j\}$ is the unknown vector to be found, and $\{R_i\}$ is the element load vector.

Probabilistic or Statistical Aspects--None.

Assumptions and Simplifications--The main assumptions are:

Darcy's law holds

The system being studied is effectively two dimensional.

Structure and Level of Detail--FEMWASTE models an aquifer either from an areal viewpoint or as a cross section. The domain is discretized using four-noded isoparametric finite elements of almost any quadrilateral shape. The time domain is discretized by finite-difference techniques.

Major Variables--Aside from the input parameters, the major variables are the contaminant concentration.

Applicability, Limitations, Validity and Completeness--The code is limited to plane two-dimensional flow.

References--

Yeh, G. T., and D. S. Ward. 1981. "FEMWASTE: A Finite-Element Model of Waste Transport Through Saturated-Unsaturated Porous Media," Oak Ridge National Laboratory, Report ORNL-5601, April.

Yeh, G. T. 1982. "Training Course No. 2: The Implementation of FEMWATER (ORNL-5601) Computer Program--Final Report." NUREG/CR-2706.

Duguid, J. O., and M. Reeves. 1976. "Material Transport in Porous Media: A Finite-Element Galerkin Model," Oak Ridge National Laboratory, Report ORNL-4928.

Yeh, G. T., and D. S. Ward. 1979. "FEMWATER: A Finite-Element Model of Water Flow Through Saturated-Unsaturated Porous Media," Oak Ridge National Laboratory, Report ORNL-5567.

Reeves, M., and J. O. Duguid. 1976. "Water Movement Through Saturated-Unsaturated Porous Media: A Finite-Element Galerkin Model," Oak Ridge National Laboratory, Report ORNL-4927.

Acceptance and Adequacy--This code is based on state-of-the-art research and is generally accepted by the research community as being about as good as is possible given the present level of understanding.

I. Summary of Code

Purpose and Scope--UNSAT2 was developed to simulate nonsteady flow of water in saturated-unsaturated media.

Authors--UNSAT2 was developed by S. P. Neuman, R. A. Feddes and E. Bresler. The primary contact in the U.S. is

Dr. Shlomo P. Neuman
Department of Hydrology and Water Resources
University of Arizona
Tucson, AZ 85717
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FTS: (602)626-4434

Code Functions--UNSAT2 was designed to include the following list of features.

- Capability to treat nonuniform flow regions having irregular boundaries and arbitrary degrees of local anisotropy;
- Flow can occur in a vertical plane, a horizontal plane, or a three-dimensional system with radial symmetry;
- Atmospheric boundaries can be simulated;
- Water uptake by plant roots can be simulated;
- Flow to a fully- or partially-penetrating well of finite radius can be simulated.

Potential Usage--UNSAT2 can be used to investigate problems involving two spatial dimensions in the horizontal or vertical plane. Three-dimensional problems can be treated provided the flow pattern retains an axial symmetry about the vertical coordinate. The two-dimensional flow region may have any complex shape and it may consist of different soil materials arranged in arbitrary patterns. Each soil material may exhibit an arbitrary degree of local anisotropy, with the principal hydraulic conductivities oriented at any desired angle with respect to the coordinates.

A wide range of time-dependent boundary conditions can be treated; prescribed pressure head; prescribed flux normal to the boundary; seepage faces; and evaporation and infiltration boundaries where the maximum rate of flux is prescribed by atmospheric or other external conditions, whereas the actual rate is initially unknown. In addition, the program can handle water uptake by plants assuming that the maximum rate of transpiration is determined by

atmospheric conditions, whereas the actual rate of uptake depends on atmospheric as well as soil and plant conditions. Internal volumetric sinks or sources of prescribed strength can be included in the flow system at any stage of the computation. Finally, a special provision has been made for the analysis of axisymmetric flow to a well of finite radius partially penetrating an unconfined aquifer system and discharging at a prescribed time-dependent rate. The well may be partially cased and its capacity for storing water is taken into account. Several layers can be tapped by the well at the same time.

Restrictions on Use--This code is in the public domain and is listed in Neuman et al. (1974).

Compatibility with Other NRC Codes--UNSAT2 is written in FORTRAN IV using no special equipment, hence it is compatible with other FORTRAN codes.

II. Summary of Findings

General Critique--UNSAT2 has evolved over several years. Earlier versions have been successfully used in field studies abroad. The UNSAT2 code may be useful to the NRC for the analysis of pressure distributions in a saturated-unsaturated flow system. The capability of treating atmospheric boundaries as well as water loss by plant roots is essential for shallow waste repositories. It should be noted however that hysteresis is not included in the code and hence will restrict the code usage to a single cycle of the wetting-drying front problem.

Provisions are included to restart a previously interrupted run.

Sensitivity Analysis--No sensitivity analyses have been published.

Code Validation and Field Verification--Feddes et al. (1975) reports on comparison studies made using UNSAT2 simulations with field measurements for two problems. One of these problems is one-dimensional and has been simulated using finite-difference methods (Feddes et al. 1974). In this example the authors report,

"In general, there is excellent agreement between field transpiration data and the results obtained by both methods."

The second example is two-dimensional and reported by Feddes et al. (1973). Again quoting from Feddes et al. (1975)

"This example clearly demonstrates the flexibility of the finite element approach and its capability in treating complex situations which one often encounters in the field."

III. General Description

Operating Characteristics--UNSAT2 is written in FORTRAN IV and is operational on an IBM 370/165. It consists of some 13 subprograms.

Inputs--Input quantities for UNSAT2 include:

- Grid geometry and program options
- Initial heads and moisture conditions
- Well description
- Root zone description
- Root behavioral data
- Material properties.

Outputs--Virtually all output is to a line printer. It consists of a listing of all input information, a complete description of the finite element network, the boundary codes of all nodes, and the properties of each material. During each time step the program prints a listing of total head values, pressure head values, moisture content values, and discharge into or out of the system (*not flow through* the system) at all nodes. The rate of convergence of the iterative procedure is printed during each time step together with additional information pertaining to the particular problem at hand.

Available Documentation--The document by Neuman et al. (1974) is a User's Manual and includes a code listing.

IV. Review of Theory

Equations--The flow of water in an incompressible variably-saturated soil can be described by

$$L(\psi) = \sum_{i=1}^3 \sum_{j=1}^3 \frac{\partial}{\partial x_i} \left[K^r(\psi) K_{ij}^s \frac{\partial \psi}{\partial x_j} \right] + \sum_{i=1}^3 \frac{\partial}{\partial x_i} K^r(\psi) K_{i3}^s + S - C(\psi) \frac{\partial \psi}{\partial t} = 0 \quad (1)$$

where L is a quasilinear differential operator defined in the flow region; x_i ($i = 1, 2, 3$) are spatial coordinates (x_3 the vertical), K^r is relative hydraulic conductivity ($0 \leq K^r \leq 1$), K_{ij}^s is conductivity tensor at saturation (the separation of $K^r(\psi)$ and K_{ij}^s is a somewhat arbitrary assumption), ψ is pressure head, C is specific moisture capacity (defined as $d\theta/d\psi$), θ is volumetric moisture content, t is time, and S is a positive sink term (or, equivalently, a negative source term). In this case, S represents the volume of water taken up by the roots per unit bulk volume of the soil in unit time.

The sink term may be expressed as

$$S = K^r K_{11}^s (\psi - \psi_r) b' \quad (2)$$

where ψ_r is pressure head in the roots and K_{11}^s is principal conductivity parallel to the horizontal (x_1) axis (all diagonal components of K_{ij}^s are implicitly assumed to be zero in the root zone). The term b' is an empirical quantity, referred to herein as the root effectiveness function, b' represents the ratio between the specific surface area of the roots and the impedance (thickness divided by conductivity) of the soil-root interface.

Equation (1) must be supplemented by appropriate initial and boundary conditions. Hysteresis is not considered in the present case as ψ is a single-valued function of θ and therefore, the initial conditions are simply

$$\psi(x_i, 0) = \psi_0(x_i) \quad (3)$$

where ψ_0 is a prescribed function of x_i . In addition to this, one must specify either the pressure head or the normal flux at each point along the boundary. If Γ_1 is the segment of the boundary, Γ , along which pressure heads are prescribed, and Γ_2 is the complementary segment of Γ along which normal fluxes are prescribed, then the boundary conditions become:

$$\psi(x_i, t) = \Psi(x_i, t) \quad \text{on } \Gamma_1 \quad (4)$$

$$\sum_{i=1}^3 \sum_{j=1}^3 \left(K^r K_{ij}^s \frac{\partial \psi}{\partial x_j} \right) + \sum_{i=1}^3 K^r K_{i3}^s = -V(x_i, t) \quad \text{on } \Gamma_2 \quad (5)$$

Here Ψ and V are prescribed functions of x_i and t .

Along soil-air interfaces (in the absence of ponding) the soil can lose water to the atmosphere by evaporation or gain water by infiltration. While the potential (i.e., maximum possible) rate of evaporation from a given soil depends only on atmospheric conditions, the actual flux across the soil surface is limited by the ability of the porous medium to transmit water from below. Similarly, if the potential rate of infiltration (e.g., the rain intensity) exceeds the infiltration capacity of the soil, part of the water may be lost by surface runoff. Here, again, the potential rate of infiltration is controlled by atmospheric (or other) external conditions, whereas the actual flux depends on antecedent moisture conditions in the soil.

Thus, the exact boundary conditions to be assigned at the soil surface cannot be predicted *a priori*, and a solution must be sought by maximizing the absolute value of the flux (while maintaining the correct sign) subject to the requirements.

$$\left| \sum_{i=1}^3 \sum_{j=1}^3 \left(k^r k_{ij}^s \frac{\partial \psi}{\partial x_j} \right) + \sum_{i=1}^3 k^r k_{i3}^s \right| \leq |E_s^*| \quad (6)$$

$$\psi_L \leq \psi \leq 0 \quad (7)$$

where E_s^* is the prescribed potential surface flux and ψ_L is the minimum allowed pressure head at the soil surface. Both E_s^* and ψ_L may vary with time.

E_s^* and ψ_L are calculated by methods based on atmospheric data. The total potential evapotranspiration from both soil and crop, E^* , is calculated according to

$$E^* = \frac{\delta(R_n - G) + \rho_a C_p (e_z^* - e_z)/r_a}{(\delta + \gamma)L} \quad (8)$$

where δ is slope of saturation vapor pressure curve, R_n is net radiation flux, G is heat flux into soil, ρ_a is density of moist air, C_p is specific heat of air at constant pressure, e_z^* is saturated vapor pressure and e_z is unsaturated vapor pressure at elevation z and ambient temperature r_a is resistance to vapor diffusion through air layer around leaves, γ is psychrometric constant, and L is latent heat of water vaporization. The potential evaporation, E_s^* , is calculated from a simplified form of (8) by neglecting the aerodynamic term and taking into account only that fraction of R_n which reaches the soil surface.

$$E_s^* = [\delta/(\delta + \gamma)L]R_n \exp - 0.39(LAI) \quad (9)$$

where LAI is the leaf-area index.

The value of ψ_L in (7) is determined from equilibrium conditions between soil water and atmospheric vapor using the formula

$$\psi_L = (RT/Mg) \ln (f) \quad (10)$$

where R is universal gas constant, T is absolute temperature, M is molecular weight of water, g is acceleration due to gravity, and f is relative humidity of air.

The potential rate of transpiration by plants, E_{p1}^* , which we assume is equal to the maximum possible rate of water extraction by roots per unit horizontal area of the soil, is also dependent on atmospheric conditions. This quantity can be calculated directly from (8) and (9) according to

$$E_{p1}^* = E^* - E_s^* \quad (11)$$

This quantity will be required later in the text.

A seepage face is another kind of atmospheric boundary at which water seeps out from the saturated portion of a porous medium. The length of the seepage face varies with time in a manner that can never be predicted *a priori*. On the other hand, pressure head along the seepage face must be uniformly zero (if atmospheric pressure is also taken to be zero).

Numerical Approximations--Equation (1), together with appropriate initial and boundary conditions, is solved by the Galerkin finite-element method. Here the flow region is subdivided into a network of triangular elements. Let the corners of these elements be designated as nodal points and let x_i^0 ($i = 1, 2, 3$) represent the space coordinates of the n^{th} node. Also, let each element, e , be associated with a set of so-called local coordinate functions, $\xi_n^e(x_i)$, which may vary linearly inside the element, vanish outside the element, and satisfy the requirement $\xi_n^e(x_j^0) = \delta_{nm}$ where δ_{nm} is Kronecker delta. Then an approximate solution to the problem at any *given* time, t , is obtained as

$$\psi^N(x_i, t) = \sum_{n=1}^N \psi_n(t) \cup \xi_n^e(x_i) \quad (12)$$

where N is the total number of nodes, $\psi_n(t)$ is the value of ψ at node n , and the union sign is taken over all elements. The values of ψ_n must be determined so as to satisfy the initial and boundary conditions of the problem together with the orthogonality requirement

$$\sum_e \int_{\Omega^e} L(\psi^N) \xi_n^e d\Omega = 0; \quad n = 1, 2, \dots, N \quad (13)$$

where Ω^e is the interior of e .

Since the Galerkin method applies only at a given instant of time, the time derivative $\partial\psi/\partial t$ appearing in $L(\psi)$ [(see (1))] must be determined independently of the orthogonalization process. The nodal values of the time derivatives as defined as weighted averages over the entire flow region according to

$$\frac{\partial\psi_n}{\partial t} = \frac{\sum_e \int_{\Omega^e} C \frac{\partial\psi}{\partial t} \xi_n^e d\Omega}{\sum_e \int_{\Omega^e} C \xi_n^e d\Omega} \quad (14)$$

K_{ij}^s is assumed constant in each element while K^r and C vary linearly according to

$$K^r = \sum_{\ell} K_{\ell}^r \xi_{\ell}^e \quad (15)$$

$$C = \sum_{\ell} C_{\ell} \xi_{\ell}^e$$

where ℓ stands for the corners of the triangle. By combining (12), (13), (14), and (15) and using Green's first identity, one obtains a set of quasilinear first-order differential equations

$$A_{nm} \psi_m + F_{nm} \frac{d\psi_m}{dt} = Q_n - B_n - D_n \quad n, m = 1, 2, \dots, N \quad (16)$$

where the quantities A_{nm} , F_{nm} , Q_n , B_n and D_n are defined in Neuman et al. (1974).

The matrix with elements A_{nm} is sparse and symmetric. The matrix with elements F_{nm} is diagonal as a direct consequence of the averaging process implied by (14). The quantity Q_n is zero at all internal nodal points which do not act as sinks or sources. D_n represents the effects of water withdrawal by plant roots and B_n accounts for all other boundary values not accounted for in Q_n and B_n .

To integrate (16) the time domain is discretized into a sequence of finite intervals, Δt , and the time derivatives of ψ_n are replaced by finite differences. If the entire flow system remains unsaturated at all times, good results can be obtained by employing the time-centered scheme

$$\begin{aligned} \left(A_{nm}^{k+\frac{1}{2}} + \frac{2}{\Delta t^k} F_{nm}^{k+\frac{1}{2}} \right) \psi_m^{k+1} &= 2Q_n^{k+\frac{1}{2}} - 2B_n^{k+\frac{1}{2}} - 2D_n^{k+\frac{1}{2}} \\ - \left(A_{nm}^{k+\frac{1}{2}} - \frac{2}{\Delta t^k} F_{nm}^{k+\frac{1}{2}} \right) \psi_m^k & \quad n, m = 1, 2, \dots, N \end{aligned} \quad (17)$$

where k represents the time $t = t^k$ and $\Delta t^k = t^{k+1} - t^k$. In order to evaluate the coefficients in (17), one must know the values of $\psi_n^{k+\frac{1}{2}}$ at $t^{k+\frac{1}{2}} = t^k + \Delta t^k/2$. At the beginning of each time step, these are predicted by linear extrapolation from previously calculated values according to

$$\psi_n^{k+\frac{1}{2}} = \psi_n^k + \frac{\Delta t^k}{2\Delta t^{k-1}} (\psi_n^k - \psi_n^{k-1}). \quad (18)$$

The resulting set of simultaneous linear algebraic equations is then solved by a Gauss elimination algorithm (which takes account of the sparse and symmetric nature of A_{nm} and F_{nm}) for the values of ψ_n^{k+1} at all nodes.

Due to the nonlinear nature of (17), these results must be improved by an iterative process. At each iteration, the most recent values of ψ_n^{k+1} are used to obtain an improved estimate of $\psi_n^{k+\frac{1}{2}}$ from

$$\psi_n^{k+\frac{1}{2}} = 1/2 (\psi_n^k + \psi_n^{k+1}). \quad (19)$$

After having re-evaluated the coefficients, the equations are again solved by Gauss elimination for improved values of ψ_n^{k+1} . The iterative procedure continues as long as it is necessary to achieve a satisfactory degree of convergence.

If part of the system is saturated, the values of F_{nm} corresponding to nodal points in the saturated zone vanish because C is zero, and the governing equations there become elliptic. This means that sudden changes in boundary conditions around the saturated zone have an instantaneous effect on the values of ψ everywhere in this zone, and ψ is no longer a continuous function of time. For example, by imposing a certain boundary condition at time $t = t^k$, all values of ψ_n^k at the start of the time step, Δt^k , becomes unknown. Thus, the right-hand side of (17) is unknown, and the equations cannot be solved.

To overcome this problem, a fully implicit backward difference scheme in terms of ψ is used

$$\left(A_{nm}^{k+\frac{1}{2}} + \frac{1}{\Delta t_k} F_{nm}^{k+\frac{1}{2}} \right) \psi_m^{k+1} = Q_n^{k+\frac{1}{2}} - B_n^{k+\frac{1}{2}} - D_n^{k+\frac{1}{2}} + \frac{1}{\Delta t_k} F_{nm}^{k+\frac{1}{2}} \psi_m^k. \quad (20)$$

Here the coefficients are all evaluated at half the time step, $k + \frac{1}{2}$, this is done in order to dampen the tendency of ψ to oscillate around its limit.

With this scheme a solution can be obtained without knowing the values of ψ_n^k at the start of the time step in the saturated zone. The only exception to this rule occurs at nodes that pass from a state of saturation to a state of incomplete saturation during a time step. The values of $F_{nm}^{k+\frac{1}{2}}$ corresponding to such nodes may differ from zero and (20) can no longer be solved without knowing the values of ψ_n^k . However, $F_{nm}^{k+\frac{1}{2}}$ represents only storage due to changes in the moisture content, θ . Such changes occur only within the negative range of ψ values whereas when ψ is positive, $C = \partial\theta/\partial\psi$ is zero. Thus, whenever a value of ψ_n^k in the saturated zone becomes unknown due to a sudden change in the boundary conditions, one is justified in replacing this value by zero in (20).

As the numerical solution is developed the boundary conditions are imposed as needed. Neuman et al. (1974) describes the exact procedure used to treat multiple plant species root growth and atmospheric condition changes as a function of time.

Probabilistic or Statistical Aspects--None.

Assumptions and Simplifications--The main assumptions are:

- Darcy's law is valid and hydraulic-head gradients are the only significant driving mechanisms for fluid flow.
- The maximum rate of transpiration is determined by atmospheric conditions alone.
- The hydraulic conductivity at each point is expressed as a symmetric tensor $K_{ij} = K^r(\theta) K_{ij}^s$, where K_{ij}^s is the conductivity at saturation and $K^r(\theta)$ is the relative conductivity ($0 \leq K^r(\theta) \leq 1$) as a function of volumetric moisture content.

Structure and Level of Detail--UNSAT2 models a flow region either from an areal viewpoint, as a vertical cross section or as a radially symmetric (vertical) cylinder. The spatial domain is discretized using triangular isoparametric-finite elements. The time domain is discretized by finite difference methods.

Major Variables--Aside from the input parameters, the major variables are the hydraulic heads.

Applicability, Limitations, Validity and Completeness--This code is applicable to both saturated and unsaturated flow in porous media. The code is limited to two dimensions or three dimensions with axial symmetry.

References--

- Neuman, S. O., R. A. Feddes and E. Bresler. 1974. "Finite Element Simulation of Flow in Saturated-Unsaturated Soils Considering Water Uptake by Plants," Third Annual Report, Project ALO-SWC-77, Hydrodynamics and Hydraulic Engineering Laboratory Technion, Haifa, Israel.
- Feddes, R. A., S. O. Neuman and E. Bresler. 1975. "Finite Element Analysis of Two-Dimensional Flow in Soils Considering Water Uptake by Roots: II. Field Applications," Soil Science Society of America Proceedings 39(3):231-237, March-April.
- Feddes, R. A., E. Bresler and S. O. Neuman. 1974. "Field Test of a Modified Numerical Model for Water Uptake by Root Systems," Water Resources Research 10(6):1199-1206 (December).
- Feddes, R. A., and M. G. vanSteenbergen. 1973. "Subirrigation Field 'de Groeve'," Nota 735. Inst. for Land and Water Management Res. Wageningen, the Netherlands (in Dutch).

Acceptance and Adequacy--UNSAT2 is based on state-of-the-art research and is generally accepted by the research community both in the U.S. and abroad as being as good as is possible given the present level of understanding.

Model Name: VS2D

Code No. 45
Type: Flow

1. Summary of Code

Purpose and Scope--VS2D was developed to simulate multidimensional movement of liquid water in variably saturated porous media.

Author and Contacts--VS2D was developed at U.S. Geological Survey by E. G. Lappala. Prime contact for additional information is

Project Chief
U.S. Geological Survey
Box 25046, Mail Stop 420
Denver Federal Center
Lakewood, CO 80225

Lappala (1981) may be purchased by contacting

Open File Services Section
U.S. Geological Survey
Box 25425
Denver Federal Center
Denver, CO 80225
Phone: (303)235-5888
FTS: (303)234-5888

Code Functions--VS2D was designed to include the following list of features.

- Capability to handle problems in which part of the solution domain is saturated and part is unsaturated.
- Capability to handle "difficult" nonlinear problems, such as those caused by infiltration into dry soils, anisotropy, and discontinuities in permeabilities and porosities.
- Inclusion of general nonlinear source-sink terms to account for stresses such as evapotranspiration.
- Capability to analyze problems in one and two dimensions with planar, and cylindrical geometries.

Potential Usage--Recharge to aquifer systems generally occurs through overlying materials that are variably saturated. Land-use activities may alter both quantity and quality of recharge. Prediction of the fate of pollutants applied to the land surface or buried above the zone of permanent saturation often can be most readily accomplished with numerical models of variably saturated flow. VS2D provides a user-oriented tool for examining these types of

problems. Although an attempt has been made to make VS2D general enough to handle most field situations, its use should be accompanied by a thorough understanding of the theoretical and practical limitations described herein. Field applications exist for which this model is not adequate; an example would be evapotranspiration in which significant anisothermal movement of water vapor as well as liquid water occurs. However, these types of problems can be analyzed using modified versions of the basic isothermal model. This version of the model does not include solution of the equations for movement of solutes.

Restrictions on Use--This code is in the public domain and is available from USGS.

Compatibility with Other NRC Codes--Since VS2D is written in FORTRAN the output files are directly usable by other FORTRAN codes.

II. Summary of Findings

General Critique--The VS2D code may be useful to the NRC for the analysis of the pressure distributions in a saturated-unsaturated flow system. Boundary conditions consist of specified head, specified flux or a mixture of the two (seasonal variation). The model analyzes flow systems from a plane cross-sectional or areal viewpoint. Cylindrical coordinates have been included in the code.

Understanding the occurrence and movement of water in variably saturated systems is important in developing predictive tools for managing both quantity and quality of ground-water systems. Recharge to aquifer systems generally occurs through overlying materials that are variably saturated. Land-use activities may alter both quantity and quality of recharge. Prediction of the fate of pollutants applied to the land surface or buried above the zone of permanent saturation often can be most readily accomplished with numerical models of variably saturated flow. The VS2D model provides a user-oriented tool for examining these types of problems. An attempt has been made to make the model general enough to handle most field situations. Field applications exist for which this model is not adequate; an example would be evapotranspiration in which significant anisothermal movement of water vapor as well as liquid water occurs. However, these types of problems can be analyzed using modified versions of the basic isothermal model. The current version of the code does not include solution of the equations for movement of solutes.

VS2D was designed to handle the "difficult" nonlinear problems caused by infiltration into dry soils, anisotropy, and discontinuities in permeabilities and porosities. This capability is met by using finite differences to discretize spatial and temporal domains. Adequate solutions of nonlinear equations using finite elements discretization in space require such numerical tricks as lumping the capacity (storage) term over each element. The upstream weighting of relative hydraulic conductivities that may be required to prevent numerical oscillations is more difficult with finite elements than with finite differences. Finally, algebraic equations resulting from a finite-element

spatial discretization scheme generally require more computer core storage and time to solve than those resulting from a finite difference scheme. General nonlinear source-sink terms are included to account for stresses, such as evapotranspiration.

Sensitivity Analysis--No sensitivity analyses were reported.

Code Validation--The computer code VS2D was verified on several test problems. Owing to the nonlinearity of the descriptive flow equation closed-form analytic solutions are not available for all possible problems to which the code might be applied. However, a few analytic solutions are available for one-dimensional geometries and specific nonlinearities. Tests of the numerical solutions against a few of these solutions are described by Lappala (1981). Also described are two tests of linear forms of the flow equation to verify the code for rectangular and radial coordinates.

Field Verification--None.

III. General Description

Operating Characteristics--VS2D is written in FORTRAN and consists of 24 subprograms.

Inputs--Inputs for VS2D include:

- Grid geometry and program options
- Initial heads or moisture content conditions
- Source/Sink strengths
- Material properties

Outputs--Output may be obtained on six files. The files used and their contents depend on input specifications. In general these files and their contents are:

File 2--Total head and saturation at selected observation points for every time step.

File 6--Printer file--echo of all input data, initial conditions, boundary conditions; mass balance summary heads and saturations and maximum ΔH /iteration for every KTH time step.

File 7--Cumulative and evapotranspiration--elapsed time for each time step.

File 8--Total head and saturation at all nodes at selected times.

File 9--Mass balance summary as a function of elapsed time.

File 10--Number of iterations/time step as a function of time.

Available Documentation--VS2D is documented in Lappala (1981).

IV. Review of Theory

Equations--The equation that describes the transient movement of liquid water under isothermal and isohaline conditions is developed by combining the equation for continuity of mass for water with auxiliary equations for fluid flux and storage. These relationships are developed for elementary volume elements or cells obtained by the spatial discretization procedure applied to the solution domain. The resulting equation for each volume element, or cell, of the solution domain is

$$v \left[\rho (\phi c_m + s\beta + s\phi\alpha) \right] \frac{\partial H}{\partial t} - \sum_{k=1}^m \frac{A_k \rho^2}{\mu} g \bar{K}_r \frac{\partial H}{\partial n_k} + \rho W = 0. \quad (1)$$

where

v = volume of the cell, L^3

ρ = liquid density, ML^{-3} ;

ϕ = porosity, L^0 ;

s = liquid saturation, L^0 ;

$c_m = \left(\frac{\partial s}{\partial h} \right)_{\rho\phi}$ = specific moisture capacity, which is the slope of the moisture retention or pressure-saturation curve, L^{-1} ;

$\beta = \left(\frac{\partial \phi}{\partial h} \right)_{\rho s}$ = matrix compressibility, L^{-1} ;

$\alpha = \frac{1}{\rho} \left(\frac{\partial \rho}{\partial h} \right)_{\phi s}$ = fluid compressibility, L^{-1} ;

h = pressure potential, L ;

H = total potential of the fluid, expressed as the height of a column of the liquid, L ;

t = time, T ;

m = number of faces on the cell;

A_k = area of k^{th} face on the cell, L^2 ;

μ = dynamic viscosity of the liquid, $ML^{-1}T^{-1}$;

g = gravitational acceleration, LT^{-2} ;

$\bar{K}$ = intrinsic permeability of the medium, L^2 ;

$K_r(s)$ = relative hydraulic conductivity to liquid as a function of liquid saturation (s)L°;

n_k = direction orthogonal to face A_k of the cell;

W = volumetric source/sink term for the cell, L^3T^{-1} .

Retention of the volume and area factors in (1) facilitates the use of either rectangular or cylindrical coordinate systems.

The program solves for the total potential, H , as the principal dependant variable.

The solution to (1) requires that initial values of H be specified everywhere in the solution domain. These initial conditions usually represent some type of steady state or equilibrium. However, this need not be the case. If initial conditions are used that do not represent steady state, any simulation results will include transient effects from the difference between specified initial conditions and equilibrium conditions. Since (13) is nonlinear, it is not permissible to use the principle of superposition to subtract out the effects of transient initial conditions, as is often done in simulating fully saturated ground-water systems.

Solutions to (13) require boundary conditions that specify either the flux or liquid across the boundary, or the total potential along the boundaries. Boundary conditions of the first type are defined as:

$$\rho \vec{u}_k = f_1(x_k, t, \nabla H_k) \quad (2)$$

where $\vec{u}_k$ is the liquid flux normal to boundary face k , L^3T^{-1} ; $f_1(x_k, t, \nabla H_k)$ is a general function that depends upon location, time, and the gradient in total hydraulic potential across the face.

Boundary conditions of the second type are defined as:

$$H_k = f_2(x, t)_k \quad (3)$$

where f_2 is a general time-dependent function.

Three phenomena exist in flow through variably saturated media that may make *a priori* specification of the boundary condition type impossible: infiltration, evaporation, and discharge through seepage faces.

Numerical Approximations--The spatial derivatives in (13) are approximated by finite differences. The values of the differenced variables are

assumed to be located at the volumetric center of the cell. For a two-dimensional rectangular grid the number of faces [m in (1)] of the cell is 6. However, two of the faces are not explicitly included because generally no liquid flow occurs across them.

The spatial derivatives of total potential, $\partial H / \partial n_k$, in (1) are approximated at the cell boundaries using the sign convention that flow into the cell as positive and flow out of the cell as negative. Replacement of the $\partial H / \partial n_k$ terms in (1) by difference approximations results in a differential-difference equation for each cell. The coefficients in the difference parts of these equations, called conductances, are linear functions of the product $\rho^2 \bar{K} K_r$ which are evaluated at the cell boundaries. Each parameter in this product is averaged by a separate method. The liquid density ρ at a cell boundary is taken as the arithmetic average of ρ for the two cells sharing the boundary. The intrinsic permeabilities, $\bar{K}$, are computed by a distance weighted, harmonic-mean formula. The hydraulic conductivity K_r is computed by either a weighted arithmetic mean (the weights are specified in the input data) and a geometric mean, depending on the option chosen in the input data.

The time derivatives in (1) are replaced with a weighted difference scheme permitting the choice, by specifying an input parameter, of the Crank-Nicolson method, the fully implicit method or a "weighted average" of the two methods. The resulting system of difference equations can be written in matrix form as

$$[A^{i-\frac{1}{2}}] \{H^i\} = \{R\} \quad (4)$$

where i is the time step index; $[A]$ is a square matrix that includes all implicit or unknown parts of the conductance, storage and source/sink terms; and $\{R\}$ is a vector of all explicit or known parts of the conductance, storage and source/sink terms. The elements of the matrix A are functions of the implicit parts of conductance terms, the storage term and the source/sink terms and are evaluated at some approximation to the midpoint in time between t^i and t^{i-1} . It is the dependence of the parameters in these terms on H that makes (4) nonlinear.

VS2D allows the user to select the method of dealing with the nonlinearity of (4). An iterative method is used which is analogous to that used in treating the temporal discretization of (1). At one extreme the explicit method no iteration is used. That is A is computed based on conditions at time t^{i-1} . At the other extreme, the fully-implicit method, the elements of A are computed based on the conditions at time t^i . To deal with the iterative determination of A at t^i VS2D uses a procedure called implicit linearization. Further options include using the Newton-Raphson method to speed convergence.

At each iteration a system of linear equations is solved. Two methods are available in VS2D, a direct method based on Gaussian elimination, and an iterative method known as line successive over relaxation or LSOR. The method used is specified in the input data.

Probabilistic or Statistical Aspects--None.

Assumptions and Simplifications--The main assumptions are:

- Darcy's law is valid and hydraulic-head gradients are the only significant driving mechanisms for fluid flow.
- The pressure head is a function of volumetric moisture content only.
- The volumetric moisture content, relative hydraulic conductivity, porosity, and fluid density are functions of pressure head only.
- Root activity is a function of depth, time and volumetric moisture content.
- The coordinate axes used for a given problem are colinear with the axes of the intrinsic permeability tensor.

Structure and Level of Detail--VS2D models a variably saturated groundwater system as either a cross section or as a cylinder using standard finite difference methods. A maximum of 100 cells made from at most 100 dimensions in the horizontal or radial direction and at most 200 divisions in the vertical direction is permitted.

Major Variables--Aside from the input parameters the major variables are the total potential of the fluid expressed as the height of a column of liquid.

Applicability, Limitations, Validity and Completeness--The code is applicable to both saturated and unsaturated flow in porous media. The code is limited to plane two-dimensional flow. Steeply dipping beds cannot be adequately simulated.

Reference--

Lappala, E. G. 1981. "Documentation of Computer Program to Solve the Equations of Fluid Flow in Variably Saturated Porous Media," August Preliminary Report, Eventually to be issued as USGS Open-File Report 81-XXX.

Acceptance and Adequacy--This code is based on state-of-the-art research and is generally accepted by the research community as being about as good as is possible given the present level of understanding.

Model Name: MLTRAN

Code No. 54
Type: Transport

I. Summary of Code

Purpose and Scope--MLTRAN was designed as a nondispersive kinetic transport model of two-dimensional transport of dissolved contaminants through mine tailings, pit linings and layered geologic sediments of varying hydraulic characteristics.

Authors--MLTRAN was developed by A. E. Reisenauer, S. K. Gupta, R. W. Nelson, C. R. Cole, and C. A. Newbill at Battelle, Pacific Northwest Laboratories, Richland, Washington. The primary contact is:

A. E. Reisenauer
Battelle, Pacific Northwest Laboratory
P.O. Box 999
Richland, Washington 99352
Telephone: (509) 376-8338

Code Functions--MLTRAN is designed to work in conjunction with the flow code TRUST which solves the transient unsaturated flow problem. MLTRAN utilizes the fluxes defined by TRUST along with media properties and grid configurations to calculate pathlines, fronts and contaminant movement. The method used is based on pathline kinematics. The code utilizes PNL graphics software and relies heavily on graphical hardware for use in an interactive mode.

Potential Usage--MLTRAN was specifically designed to study "worst-case" situations of low level waste storage sites, where the media is unsaturated. The model is capable of simulating in one- or two-dimensional geometries.

Relation to NRC Issues--Not applicable as no list of issues currently exists for low level radioactive waste treatment.

Restrictions--The code is in the public domain and is therefore available to NRC.

Compatibility with Other NRC Codes--MLTRAN is written in FORTRAN. It utilizes PNL graphics software and relies heavily on graphical hardware for use in the interactive mode. This special software is compatible with FORTRAN and thus should not create problems with respect to input/output files and their compatibility with other NRC codes.

II. Summary of Findings

General Critique--The transport model MLTRAN, consists of six separate subcodes MLSTRT, MLFLUX, MTRVL, MLFRNT, MLPLOR and MLGRID. The model uses finite element principles for the pathline and transport calculations. Using

the integrated finite difference grid points and distances linking each pair of nodes and the finite element grid description of the TRUST element nodes. MLSTRT generates the direct access files for use by the other MLTRAN subprograms. MLFLUX uses the TRUST flow rates between each pair of nodes for each time plane to estimate the net flow vectors at each finite element node. MLTRVL estimates pathlines and travel times from any given point in the space and time domains.

MLTRVL is executed three times during an analysis of the waste transport analysis problem. First to determine the water flow travel pathlines, second to estimate the acid front, and third to estimate the radionuclide transport as a function of the position of the acid front. For the acid and radionuclide travel time, the laboratory measured retardation coefficients of the contaminant for the different soils are incorporated into the model. MLFRNT is also executed three times to delineate the travel time of the water, acid and radionuclide front at specified times of interest. MLPLOR plots the moisture content and pressure head for selected times. MLGRID plots the grid details and material number of each node to verify input geometry.

MLTRAN is designed for interactive graphic oriented computation. The user may exploit these graphics capabilities to insure proper input data prior to executing the computation parts including TRUST, of the model.

Applicability to Medium--MLTRAN is designed to simulate solute transport through variably saturated media subject to variable initial and boundary conditions. The code is applicable to most porous media transport problems which can be adequately modeled in two-dimensions and for which a nondispersive simulation is adequate.

Sensitivity Analysis--No sensitivity analyses have been published.

Code Verification--Checks have been made with other codes and analytical solutions but no results have been published.

Field Verification--None published.

III. General Description

Operating Characteristics--MLTRAN is written in FORTRAN IV and is operational on Digital Equipment Corporation's PDP 11/45 and PDP 11/20 computers with 32k core memory of 16-bit words. It relies heavily on graphic capabilities.

Inputs--MLTRAN requires access to the input files used by the program TRUST (Reisenauer, et al. 1982) as well as the file of flux values produced by TRUST. TRUST does not require element node location so these must be input to MLTRAN. Also required are parameters for the plotting device, and plots, cycle specification (water, acid or contaminant), starting point for pathlines to be traced, starting and ending times.

Outputs--MLTRAN produces both plotted and printed hardcopy. The plots include not only the initial grid definitions for the TRUST integrated finite difference cells but also the pathlines specified for water acid, and/or contaminants. Also, contour plots are made for moisture content, and pressure heads at selected points in time.

Available Documentation--MLTRAN is documented in Reisenauer, et al. (1981) which serves as a user's manual.

IV. Review of the Theory

Equations--Consider a fluid particle at a given time t_0 , at location x_0, y_0 in a velocity field $\vec{V}(x, y, t)$ interior to a porous flow system. Let a function $\psi(x, y, t)$ follow the particular fluid particle. The convective derivative of ψ must vanish along the path traveled by the fluid particle

$$\frac{D\psi}{Dt} = \frac{\partial\psi}{\partial t} + v_x \frac{\partial\psi}{\partial x} + v_y \frac{\partial\psi}{\partial y} = 0 \quad (1)$$

where, using Darcy's Law and the volumetric moisture content θ , for partially saturated soil, the pore velocity components are given by

$$v_x = - \frac{K}{\theta} \frac{\partial\phi}{\partial x} \quad (2)$$

$$v_y = - \frac{K}{\theta} \frac{\partial\phi}{\partial y} \quad (3)$$

where K is the partially saturated hydraulic conductivity, and ϕ is the energy potential. Substituting (2) and (3) into (1) produces a first order partial differential equation in ψ which is solved by the method of characteristics. The characteristic equations are

$$\frac{dx}{dt} = - \frac{K}{\theta} \frac{\partial\phi}{\partial x} \quad (4)$$

$$\frac{dy}{dt} = - \frac{K}{\theta} \frac{\partial\phi}{\partial y} \quad (5)$$

which are nothing more than the velocity components expressed as differential displacements on the pathline differential equations that pass through the starting point x_0, y_0 at t_0 .

Now consider a contaminant tracer particle which interacts with the porous matrix in such a way that it is effectively retarded. The above derivation can be carried out but using the retarded time T rather than water travel time. That is in (2) and (3) let

$$v_x = \left(1 + \frac{B_b K_d}{\theta}\right) V_x = - \frac{K}{\theta} \frac{\partial \phi}{\partial x} \quad (6)$$

$$v_y = \left(1 + \frac{B_b K_d}{\theta}\right) V_y = - \frac{K}{\theta} \frac{\partial \phi}{\partial y} \quad (7)$$

Equations (6) and (7) can be solved for the contaminant particle velocities, V_x and V_y . The path followed by the contaminant particle yields

$$\frac{D\psi_c}{DT} = \frac{\partial \psi_c}{\partial t} + V_x \frac{\partial \psi_c}{\partial x} + V_y \frac{\partial \psi_c}{\partial y} = 0 \quad (8)$$

where ψ_c is a function following the contaminant particle. Substituting (6) and (7) into (8) yields a first order partial differential equation which is solved by the method of characteristics. The characteristic equations are

$$\frac{dx}{dT} = \frac{1}{R} \frac{q_x}{\theta} \quad (9)$$

$$\frac{dy}{dT} = \frac{1}{R} \frac{q_y}{\theta} \quad (10)$$

where

$$q_x = - K \frac{\partial \phi}{\partial x} \quad (11)$$

$$q_y = - K \frac{\partial \phi}{\partial y} \quad (12)$$

which are the Darcian flux components;

$$R = \frac{1}{1+\beta K_d} \quad (13)$$

is the retardation factor; and

$$\beta = \frac{B_d}{\theta} \quad (14)$$

is the bulk density of the matrix divided by the volumetric moisture content.

The MLTRAN code solves (9) and (10) numerically to yield pathlines, fronts and contaminant movement throughout the porous matrix.

Numerical Approximations--For TRUST there is no description of elemental nodal coordinates. It primarily needs the node pairs, distance between the node pairs and the orthogonal distance, representing the intercepted distance of the flow between the given pairs of nodes. For discretization of a given problem the user normally locates the nodes and constructs the integrated finite difference element.

For the purpose of generating pathlines from the velocity vectors stored at each time plane, it is convenient to shift from an integrated finite difference grid to a finite element grid system. The grid point locations are maintained and a new file is required which describes the linking in the finite element quadrature notation, i.e., four points linked in a counter clockwise pattern.

MLTRAN uses linear quadrilateral elements of four nodes while the integrated finite difference grid may have elements formed with more than four sides. In some cases the element might be a triangle. If the integrated finite difference element is not of four sides, the user may be required to redefine the element node of integrated finite difference element by four-sided finite element.

The TRUST code estimation of the flux between nodes is based on the assumption that the potential associated with each nodal point is a function of time only, and the spatial variation of the average properties are independent of time. The flux rate between elements is represented by a simple linear relationship.

Under unsaturated conditions the hydraulic conductivity (K) and the moisture retention (C) are functions of the potential and elevation. Hence, the governing partial differential equation is nonlinear. For numerical simulation, an iterative technique is used until convergence of the potentials used

for estimating K and C, and the predicted potentials are within prescribed limits. The TRUST code adjusts the time steps automatically, starting from small initial values. The initial time frames are very small and generally have insignificant impact on the estimation of the contaminant transport. TRUST values for mass flux between element nodes pairs, and the estimated potentials at pre-selected time planes are saved on magnetic tape or disk files.

Let X_0, Y_0 and X_1, Y_1 be the coordinates of two nodes 0 and 1 and let D be the orthogonal intercepted distance between the elements. TRUST saves the total mass flux m_0^1 between 0 and 1 passing through intercept D during a given time increment Δt . The following steps are used to calculate the net velocity vector V_x^{01} and V_y^{01} at element node 0.

1. The mass flow M_0^1 is converted to a volume flow rate
2. The estimated Q is resolved into its components parallel to the x and y coordinate system by the following transformation

$$Q_{x_0}^{01} = A_0^1 \cos(\alpha) \quad (15)$$

$$Q_{y_0}^{01} = Q_0^1 \sin(\alpha) \quad (16)$$

where

$$\alpha = \tan^{-1} \left(\frac{y_1 - y_0}{x_1 - x_0} \right) \quad (17)$$

3. The above procedure is repeated to estimate Q_x^{0i} and Q_y^{0i} where $i = 1, 2, \dots, n$ (n = number of nodes connected to element node 0).
4. To estimate the Darcian flux components q_x and q_y the sum

$$Q_x^0 = Q_x^{01} + Q_x^{02} + \dots + Q_x^{0n} \quad (18)$$

is divided by the sum of the associated y projections of all the intercepts

$$y_p = \sum_{i=1}^h \left| 0_i \sin \alpha_i \right| \quad (19)$$

$$q_y^0 = q_x^0 / y_p \quad (20)$$

Similarly,

$$q_y^0 = q_y^{01} + q_y^{02} \dots + q_y^{0n} \quad (21)$$

$$x_p = \sum_{i=1}^n \left| 0_i \cos \alpha_i \right| \quad (22)$$

and

$$q_y = q_y^0 / x_p \quad (23)$$

5. Using the estimated potential of element node 0 and moisture retention properties of the material associated with element 0, the moisture content θ , is estimated.
6. The net pore water velocity vector at element node 0, is then defined by

$$v_x^0 = q_x^0 / \theta \quad (24)$$

$$v_y^0 = q_y^0 / \theta \quad (25)$$

where the vectors are along the x and y axis, respectively.

7. The above process is repeated for all the nodes in the flow system and the results stored in a direct access file for efficient retrieval during pathline estimation.

The subprogram MLCNP plots the contours of TRUST estimated potentials and moisture contents of interactively specified time planes. Along with contours the nodal values of potential or moisture content at specified nodes are also plotted. Contours and the nodal values provide a means of checking the TRUST results before tracing pathlines and fronts. The finite elements are defined by four corner points, an interpolation function is defined by the basic functions. This interpolation function is used to construct the contours plotted by MLCNP.

Probabilistic or Statistical Aspects--None.

Assumptions and Simplifications--The main assumptions are:

- Darcy's Law is valid and the hydraulic-head gradients are the only significant driving mechanisms for fluid flow.
- The flux between discretization elements is linear.

Structure and Level of Detail--The integrated finite difference grid of TRUST and the corresponding finite element grid of MLTRAN permit the user to place smaller elements where more detail is wanted and larger elements where detail is less important. The code is confined to two-dimensions.

Major Variables--The primary variables are the pathline coordinates, contaminant particle travel times, and contaminant concentration values.

Applicability, Limitations, Validity and Completeness--The primary limitations are the restriction to nondispersive transport in two dimensions, and the dependence on plotting capabilities. This latter limitation is one which could be removed by software modification. The TRUST code is applicable to both saturated and unsaturated flow problems. Thus, MLTRAN which relies on TRUST for the flux components is applicable to both saturated and unsaturated problems.

References--

- Reisenauer, A. E., S. K. Gupta, R. W. Nelson, and C. A. Newbill. 1981. "Advective Radionuclide Transport with Soil Interaction Under Variably Saturated Flow Conditions." PNL-3994, Pacific Northwest Laboratory, Richland, Washington.
- Reisenauer, A. E., K. T. Key, T. N. Narasimhan, and R. W. Nelson. 1982. "TRUST: A Computer Program for Variably Saturated Flow in Multidimensional, Deformable Media." NUREG/CR-2360, PNL-3975. Prepared for U.S. Nuclear Regulatory Commission by Pacific Northwest Laboratory, Richland, Washington.

Acceptance and Adequacy--MLTRAN is based on state-of-the-art research and is generally accepted by the research community as being as good as is possible at the current level of understanding.

APPENDIX E

PARTIALLY SATURATED AND MULTIPHASE CODES INVENTORIED--SHORT SUMMARIES

CODE: 6

TYPE: Transport

CODE NAME: BACHMAT

METHOD USED:

PRINCIPAL CONTACT: Y. Bachmat
Hydrological Service
P.O. Box 6381
Jerusalem, Israel

DOCUMENTATION: listings and cards available on request

- OTHER: ● designed for predicting the concentration of nitrogen compounds in one dimensional surface water or groundwater streams
- coded in FORTRAN IV
 - operational on CDC 6400

CODE: 7

TYPE: Flow

CODE NAME: UNFLOW

METHOD USED: 2-dimensional Galerkin finite element

PRINCIPAL CONTACT: John F. Pickens
Dept. of Earth Sciences
Univ. of Waterloo
Waterloo, Ontario
Canada N2L 3G1

DOCUMENTATION: listings and operating instructions available
from Principal Contact

- OTHER: ● designed to simulate 2-dimensional (cross-sectional)
transient movement of water in full or partially
saturated soils
- coded in FORTRAN IV
 - operational on IBM 370/158

CODE: 8

TYPE: Flow

CODE NAME: VERGE

METHOD USED: 3-dimensional Galerkin finite element

PRINCIPAL CONTACT: M.J. Verge
Dept. of Earth Science
University of Waterloo
Waterloo, Ontario
Canada N2L 3G1

DOCUMENTATION: User's Guide, listings in M.J. Verge
"A Three-Dimensional Saturated-Unsaturated
Groundwater Flow Model for Practical
Application" Ph.D. Thesis, Univ. of Waterloo,
Waterloo, Ontario, Canada (1976).

- OTHER: ● designed to determine hydraulic head in
3-dim. saturated-unsaturated groundwater
flow system
- coded in FORTRAN IV

CODE: 9

TYPE: Coupled Flow and Transport

CODE NAME: SEGOL

METHOD USED: 3-dimensional Galerkin finite element

PRINCIPAL CONTACT: Genevieve Segol
Bechtel Civil and Minerals, Inc.
P.O. Box 3965
San Francisco, CA 94119
Phone: (415) 768-7159

DOCUMENTATION: User's Guide in: Genevieve Segol "A Three-Dimensional Galerkin Finite Transport in Variably Saturated Porous Media, User's Manual", Dept. of Earth Sciences, Univ. of Waterloo, Waterloo, Ontario, Canada N2L 3G1 (June 1976).

- OTHER:
- designed to determine transient concentration of conservative on non-conservative solute in groundwater flow systems
 - coded in FORTRAN IV
 - operational on IBM 360/75

CODE: 10

TYPE: Flow

CODE NAME: UNSAT

METHOD USED: 1-dimensional finite differences

PRINCIPAL CONTACT: Frederick W. Bond
Battelle Northwest
P. O. Box 999
Richland, WA 99352

DOCUMENTATION: ● early version described in:
S.K. Gupta, K.K. Tanji, D.R. Nielsen
J.W. Biggar, C.S. Simmons, J.L. McIntyre
"Field Simulation of Soil-Water Movement
with Crop Water Estimation", Univ. of Calif.
at Davis, Water Science and Engineering Paper
No. 4013, (Jan. 1978).

● A user's manual is currently being prepared and
will be distributed by EPRI.

OTHER: ● designed to simulate infiltration, vertical seepage
and uptake by plant roots as related to the hydraulic
properties of a soil, soil layering, the root growth
characteristics of a given crop in a given soil profile
evapotranspiration rates, and frequency rate and amount
of irrigation.

● coded in FORTRAN IV

● operational on DEC PDP 11/70

CODE: 11

TYPE: Flow and Transport

CODE NAME: SUNATRA-1

METHOD USED: 1-dimensional, Hermitian (cubic) finite elements

PRINCIPAL CONTACT: Dr. M. Th. van Genuchten

USDA

U.S. Salinity Lab.

4500 Glenwood Drive

Riverside, CA 92501

Phone: (714) 683-0172

DOCUMENTATION: code listing in: M.Th. van Genuchten, "Mass Transport in Saturated - Unsaturated Media: One-dimensional Solutions", document no.78-WR-11 Princeton University, Princeton, NJ

- OTHER:
- designed to simulate the simultaneous flow of water and solutes in a one-dimensional (vertical) soil profile under transient saturated - unsaturated conditions
 - coded in FORTRAN IV
 - the method for solving the flow equations is essentially the same as that used in Code No. 28 (UNSAT1).

CODE: 12

TYPE: Flow and Transport

CODE NAME: TRANSONE

METHOD USED: One-dimensional Hermitian finite elements
used with Galerkin's approximation

PRINCIPAL CONTACT: Dr. M. Th. van Genuchten
USDA
U.S. Salinity Lab.
4500 Glenwood Dr.
Riverside, CA 92501
phone: 714-683-0172

DOCUMENTATION:

OTHER: ● designed to solve the equations governing
one-dimensional mass transport through
unsaturated and saturated porous media

CODE: 13

TYPE: Flow and Transport

CODE NAME: TRANSTWO

METHOD USED: 2-dimensional finite differences

PRINCIPAL CONTACT: Allen Shapiro

DOCUMENTATION: In preparation (1976)

OTHER: ● designed to solve the equations governing two-dimensional mass transport in unsaturated and saturated groundwater flow.

CODE: 14

TYPE: Flow and Transport

CODE NAME: MOBIDIC

METHOD USED: Finite difference used to obtain a system of differential differences equations which are then integrated using a variable step Runge Kutta method.

PRINCIPAL CONTACT: Ph. Couchat
Service de Radioagronomic
C.E.N. Cadamache
13115 - Saint-Paul-lez-Durance

DOCUMENTATION: model description given in "notices": DIFSOL, DFMOD, MULTISOL (in French), Internal report by Cisi Cadarache and G. Le Cardinal.

OTHER: ● designed to predict water transfer from soil to plants in a one-dimensional multi-layered soil or 2-dimensional homogeneous soil

CODE: 15

TYPE: Flow and Transport

CODE NAME: NMODEL

METHOD USED: Finite differences

PRINCIPAL CONTACT: H.M. Selim
Soil Science Department
University of Florida
Gainesville, FL 32611

DOCUMENTATION:

- OTHER: ● designed to predict water and nitrogen transport and transformation under transient and steady unsaturated water flow in homogeneous or multi-layered soils
- coded in FORTRAN

CODE: 16

TYPE: Flow and Transport

CODE NAME: WATSOL

METHOD USED: 1-dimensional finite difference

PRINCIPAL CONTACT: J.P. Gaudet or R. Haverkamp
Institute de Mecanique de Grenoble
B.P. 53 - Centre de Tri
38041 Grenoble Cedex - France

- DOCUMENTATION:
- theory and application for water flow:
R. Haverkamp, M. Vauchin, J. Touma, P.J. Wierenga,
G. Vachaud, "A Comparison of Numerical Simulation
Models for One-dimensional Infiltration", to appear
in SOIL SCIENCE SOC PROC AM April 1977.
 - for solute transport: J.P. Gaudet, "Transfer d'eau
et de solute dans la zone non-saturee des sols:
Mesures et Modelisation", Thesis, Universiti de
Grenoble 1977.
 - listings available on request
 - operating instruction not written (as of Feb. 10, 1977)
- OTHER:
- designed to simulate and predict water flow with or
without solute through the unsaturated zone
 - coded in FORTRAN IV - Level H
 - operational on IBM 1130
IBM 360/67
CII-IRIS 80 (SIRIS8)

CODE: 17

TYPE: Transport

CODE NAME: FECTRA

METHOD USED: 2-dimensional Galerkin- finite element with Adams-Moulton
predictor - corrector algorithm

PRINCIPAL CONTACT: Robert G. Baca or Alan Lu
Research Department
Rockwell Hanford Operations
P.O. Box 250
Richland, WA 99352

DOCUMENTATION: User's Manual: document no. RHO-MA-250
Rockwell Hanford Operations
P.O. Box 250
Richland, WA 99352

- OTHER: ● designed to simulate constituent transport
in saturated or unsaturated porous media
with complicated or arbitrary geometry
- coded in FORTRAN IV
 - operational on CDC 6600, CYBER 74, UNIVAC 1108

CODE: 18

TYPE: Flow and Transport

CODE NAME: TARGET

METHOD USED: 2-and 3-dimensional integrated finite differences

PRINCIPAL CONTACT: D. Sharma
Dames and Moore
250 East Broadway, Suite 200
Salt Lake City, Utah 84111
Phone (801) 521-9255

DOCUMENTATION: D. Sharma, "A Comprehensive Mathematical Model
Capable of Predicting Flow, Heat Transfer as well
as Chemical-Species Transport in Porous Media",
Dames and Moore, Advanced Tech. Group Rep. TN-DN-42

- OTHER:
- designed to simultaneously solve the transient hydrodynamic and chemical transport equations in unsaturated or saturated media
 - coded in FORTRAN IV
 - operation on CDC-6600
 - Proprietary code

CODE: 19

TYPE: Transport

CODE NAME: DUGUID-REEVES

METHOD USED: Galerkin finite element in 2-dimensions

PRINCIPAL CONTACT:

DOCUMENTATION: Comprehensive description and listing in:
J.O. Duguid and M. Reeves, "Material Transport
through Porous Media: A finite-element Model",
Oak Ridge National Laboratory, Oak Ridge, TN
ORNL-4928 (March 1976)

- OTHER: ● designed to solve the governing transport
equations when both absorption and decay of
the dissolved constituent are present.
- coded in FORTRAN IV

CODE: 20

TYPE: Coupled Flow and Transport

CODE NAME: McCANN

METHOD USED: 2-dimensional finite differences

PRINCIPAL CONTACT: R.A. McCann or L.E. Wiles
Battelle Northwest
P.O. Box 999
Richland, WA 99352
Phone (509) 375-2488

DOCUMENTATION: analytical developments: L.E. Wiles and
R.A. McCann, "Water Coning in Porous Media
Reservoirs for Compressed Air Energy Storage",
Battelle Northwest, Richland, WA PNL-3470
(June 1981)

OTHER: ● coded in FORTRAN IV
● operational on UNIVAC 1110

CODE: 21

TYPE: Flow

CODE NAME: ALPURS

METHOD USED: 3-dimensional finite difference
(fully implicit)

PRINCIPAL CONTACT: P.P. Bansal or A.S. Odeh
Mobil Research and Development Corp.
Dallas, TX
Phone: (214) 333-6231 (Odeh's phone)

DOCUMENTATION: technical discussion in: P.P. Bansal, J.L. Harper,
A.E. McDonald, E.E. Moreland, A.S. Odeh and
R.H. Trimble, "A strongly coupled, fully implicit,
three-dimensional, three phase reservoir simulator"
SPE 8329 (1979)

application: Aziz S. Odeh, "Comparison of solutions
to a three-dimensional black oil reservoir simulation
problem", J. OF PET. TECH (Jan 1981) pp. 13-25

- OTHER:
- designed to solve the equation for three-dimensional
three phase, multiwell black oil reservoir
 - operational on CDC cyber 172 and 175
 - proprietary code

CODE: 22

TYPE: Flow

CODE NAME: REEVES-DUGUID

METHOD USED: 2-dimensional Galerkin finite element

PRINCIPAL CONTACT:

DOCUMENTATION: User's manual and listing in: M. Reeves
and J.O. Dugeid, "Water movement through
saturated-unsaturated porous media: A finite
element Galerkin model", Oak Ridge National
Laboratory, Oak Ridge, TN ORNL-s4927 (Feb. 1975)

OTHER: ● coded in FORTRAN IV

CODE: 23

TYPE: Flow and Transport

CODE NAME: TRANS

METHOD USED: 2-dimensional Galerkin finite element

PRINCIPAL CONTACT: Wynn R. Walker
Colorado State University

DOCUMENTATION: analytical discussion and code listing in:
Wynn R. Walker, James D. Sabey and Duane R. Hampton
"Studies of Heat Transfer and Water Migration in
Soils", final report May 1, 1979 to September 30, 1980
to U.S. DOE Solar Energy Applications Laboratory,
Colorado State University (April 1981)

OTHER: ● designed for the solution of transient coupled heat
and moisture flow problems in soils or aquifers for
axisymmetric problems

● coded in FORTRAN

CODE: 24

TYPE: Flow

CODE NAME: FEMWATER

METHOD USED: finite-element Galerkin

PRINCIPAL CONTACT: George T. Yeh
Room 203
Bldg. 1505
Oak Ridge National Laboratory
P. O. Box X
Oak Ridge, TN 37830
FTS phone: 624-7285

DOCUMENTATION: analytical discussion and code listing in:
G.T. Yeh and D.S. Ward "FEMWATER: a finite
element model of water flow through saturated
unsaturated porous media. Oak Ridge National
Laboratory, Oak Ridge, TN ORNL-5567 (1979)

User's manual in: Yeh, G. T. (1982). "TRAINING
COURSE NO. 1: The implementation of FEMWATER
(ORNL-5567) Computer Program - Final Report"
NUREG/CR-2705

REFERENCES: Pickens, J.F. and G.E. Grisak, "Finite element
analysis of liquid flow, heat transport and
solute transport in a groundwater flow system:
governing equations and model formulation.
AECL-TEC-REC-81, National Hydrology Research
Institute Inland Waters Directorate, Environment
Canada, for Atomic Energy of Canada Limited,
Whiteshell Nuclear Research Establishment.
(September 1979)

OTHER: • written in FORTRAN IV

CODE NO: 25

TYPE: Transport

CODE NAME: FEMWASTE

METHOD USED: 2-dimensional Galerkin finite element

PRINCIPAL CONTACT: George T. Yeh
Room 203
Bldg 1505
Oak Ridge National Laboratory
P. O. Box X
Oak Ridge, TN 37830
FTS phone 624-7285

DOCUMENTATION: analytical discussion and code listing in:
G.T. Yeh and D.S. Ward, "FEMWASTE: a finite
element model of waste transport through
porous media, Oak Ridge National Laboratory,
Oak Ridge, TN ORNL-5601 (April 1981)

User's manual in: Yey, G. T. (1982). "TRAINING
COURSE NO. 2: The implementation of FEMWASTE
(ORNL-5601) Computer Program - Final Report"
NUREG/CR-2706

- OTHER: ● transport mechanisms include: convection,
hydrodynamic dispersion, chemical sorption
and first-order decay.
- coded in FORTRAN IV

CODE NO: 26

TYPE: Flow

CODE NAME: UNSAT2

METHOD USED: 2-dimensional finite-element

PRINCIPAL CONTACT: Shlomo P. Neuman
Dept. of Hydrology & Water Resources
University of Arizona
Tucson, AZ 85717
Phone: (602) 884-4434
FTS: (602) 626-4434

DOCUMENTATION: User's guide and listing in:
S.P. Neuman, R.A. Feddes, and
E. Bresler, "Finite element simulation
of flow in saturated-unsaturated soils
considering water uptake by plants",
3rd ann. report, Project AL0-SWC-77,
Hydrodynamics and Hydraulic Engineering Lab,
Technion, Haifa, Israel (1974)

- OTHER:
- designed to compute hydraulic heads, pressure heads, water content, boundary flumes and internal sinks and sources in a saturated-unsaturated non-uniform anisotropic porous medium under nonsteady state conditions. Soil evaporation and evapotranspiration due to plants uptake may also be computed
 - written in FORTRAN IV
 - operational on IBM 360-370's

CODE NO: 27

TYPE: Flow

CODE NAME: STGWT/MOGWT

METHOD USED: 1-dimensional finite differences

PRINCIPAL CONTACT: F. De Smedt
Dept. of Hydrology
Faculty of Applied Sciences
Vrije Universiteit
Brussel, Pleinlaan 2
B-1040
Brussels - Belgium

DOCUMENTATION: code listing in: F. De Smedt and A. van Beker,
"The groundwater flow in the unsaturated zone"
Dept. of Hydrology, Faculty of Applied Sciences,
Vrije Universiteit, Brussel, Pleinlaan 2, B-1040
Brussels - Belgium (Sept. 1974)

OTHER: ● designed to solve problems of one-dimensional
vertical, unsaturated flow in homogeneous soil
● coded in FORTRAN extended version 4

CODE NO: 28

TYPE: Flow

CODE NAME: UNSAT1

METHOD USED: 1-dimensional Hermitian (cubic) finite element

PRINCIPAL CONTACT: Dr. M.Th. van Genuchten
USDA
U.S. Salinity Laboratory
4500 Glenwood Drive
Riverside, CA 92501
Phone: (714) 683-0172

DOCUMENTATION: analytical discussion and code listing in:
M.th. van Genuchten, "Numerical solutions of
the one-dimensional saturated-unsaturated flow
equation", 78-WR-09, Princeton University

OTHER: ● coded in FORTRAN IV
● This code is very similar to the flow part of
Code No. 11 (SUMATRA-1).

CODE NO: 29

TYPE: Flow

CODE NAME: COOK

METHOD USED: 2-dimensional finite difference

PRINCIPAL CONTACT:

DOCUMENTATION: analytical discussion in: R.E. Cook,
R.H. Jacoby and A.B. Ramesh, "A Beta-Type
Reservoir Simulation for Approximating
Compositional Effects During Gas Injection",
SOC. PET. ENGR. J. (Oct. 1974)

- OTHER: ● designed to solve 2-dimensional, 2-phase
(oil and gas) problems where the fluid
compositional effects are significant
- proprietary code

CODE NO: 30

TYPE: Flow

CODE NAME: GANDALF

METHOD USED:

PRINCIPAL CONTACT: Frank A. Morrison
Lawrence Livermore Laboratory
Livermore, CA

DOCUMENTATION: analytical discussion and code listing in:
Frank A. Morrison, Jr., "Stability of flow from
a nuclear cavity" UCRL-13799 July 1977

- OTHER: ● designed to calculate velocities, saturations,
marginal stability conditions, and growth rates
of instability for multiphase multicomponent
flow in porous media. Design problem was cavity
generated by underground nuclear explosion.
- coded in FORTRAN IV
 - operational on IBM 360

CODE NO: 31

TYPE: FLOW

CODE NAME: GPSIM (General Purpose Reservoir Simulator)

METHOD USED: finite, semi implicit, three dimensional

PRINCIPAL CONTACT: Exxon Production Research

DOCUMENTATION: analytical discussion contained in:
A.G. Spillette, J.G. Hillestad and H.L. Stone
"A High-Stability Sequential Solution Approach
to Reservoir Simulation" SPE 4542. Presented
at 48th Annual Fall Meeting of SPE's of AIME,
Las Vegas, Nev., September 30-October 3, 1973.

Application: Aziz S. Odeh, "Comparison of
Solutions to a Three-Dimensional Black-Oil
Reservoir Simulation Problem", J&PET TECH
(Jan. 1981) pp. 13-25.

- OTHER: ● designed to solve the equations governing
three-dimensional, three phase black oil
reservoirs. It can also treat fewer phases
and/or dimensions.
- operational on Amdahl 470/V5, IBM 370/168
 - proprietary code

CODE NO: 32

TYPE: FLOW

CODE NAME: TS&E

METHOD USED:

PRINCIPAL CONTACT: Technical Software & Engineering Inc.
P.O. Box 19533
Dallas, TX 75219
phone (214) 691-4869

DOCUMENTATION: analytical discussion contained in SPE
paper no. SPE-4979 which was presented at
the 49th annual fall meeting of SPE's of
AIME at Houston, October 1974.

OTHER: ● Universal Black Oil Reservoir
Simulator, designed to solve the governing
equations for three-phase, three-
dimensional black oil reservoir.
It can be used on fewer phases and/or
dimensions.

● proprietary code

CODE NO: 33

TYPE: Flow

CODE NAME: BRUTSAERT1

METHOD USED: finite differences

PRINCIPAL CONTACT: Willem F. Brutsaert
351 Hubert Hall
University of Maine
Dept. of Civil Engineering
Orono, ME 04473
Phone (207) 581-7693

DOCUMENTATION: analytical discussion and code listing in
NSF funded project:
The Transition Problem in Pumped Wells
Project No. ENG 75-10179.

- OTHER:
- designed to forecast potentiometric head
in an initially confined aquifer as it
transgresses to water table conditions
 - coded in FORTRAN IV
 - operational on IBM 370

CODE NO: 34

TYPE: Flow and Transport

CODE NAME: WHC (Water, Heat, Chemical Transport)

METHOD USED: Integrated Compartment Method

PRINCIPAL CONTACT: George T. Yeh
Room 203
Bldg. 1505
Oak Ridge National Laboratory
P. O. Box X
Oak Ridge, TN 37830
FTS phone: 624-7285

DOCUMENTATION: analytical discussion and code listing in:
E.A. Crooks and G.T. Yeh, "WHC: a multi-
dimensional model of water movement, heat
flow, and chemical transport in complex
aquifer systems", ORNL/TM 7564, Oak Ridge, TN

- OTHER: ● designed to solve the governing equations for
pressure head, temperature and chemical
distribution in saturated-unsaturated porous
media.
- coded in FORTRAN IV

CODE NO: 35

TYPE: Transport

CODE NAME: SCAT1D (one-dimensional)

METHOD USED: finite differences, uncertain velocity input
is used to generate dispersion

PRINCIPAL CONTACT: C.A. Oster
P.O. Box 999
Battelle Northwest
Richland, WA 99352
Phone: (509) 375-2979

DOCUMENTATION: analytical discussion contained in:

C.A. Oster, A.G. Gibbs and D.H. Tang,
"Analysis of a numerical solution to the
one-dimension stochastic convection equation"
ADV WATER RESOURCES vol. 4, 1981 (Mar. 81)

- OTHER: ● requires user to furnish velocity covariance
functions. For examples see J.L. Devary and
P.G. Doctor. "Geostatistical modeling of Pore
Velocity", PNL-3789, Pacific Northwest Labs,
Richland, Wa (1981).
- coded in FORTRAN IV
 - operational on DEC 11/70

CODE NO: 36

TYPE: Transport

CODE NAME: SCAT2D (two-dimensional)

METHOD USED: finite differences, uncertain velocity input
is used to generate dispersion

PRINCIPAL CONTACT: C.A. Oster
Battelle Northwest
P. O. Box 999
Richland, WA 99352
Phone: (509) 375-2979

DOCUMENTATION: analytical discussion contained in:
C.A. Oster and A.G. Gibbs "A numerical
procedure for obtaining the mean solution
and variance of the two-dimensional stochastic
convection equation". Submitted for publication
in ADV. WATER RESOURCES

- OTHER: ● requires user to furnish velocity covariance
functions. For examples see J.L. Devary and
P.G. Doctor. "Geostatistical modeling of Pore
Velocity", PNL-3789, Pacific Northwest Labs,
Richland, Wa (1981).
- coded in FORTRAN IV
 - operational on DECPDP 11/70

CODE NO: 37

TYPE: Flow

CODE NAME: AMOCO

METHOD USED: 3-dimensional IMPES (implicit with semi-implicit adjustment in well rates. Finite difference

PRINCIPAL CONTACT: Amoco Production

DOCUMENTATION: application: Aziz S. Odeh, "Comparison of solutions to a three-dimensional black-oil reservoir simulation problem", J. OF PET. TECH. (Jan 1981) pp. 13-25

OTHER: ● operational on IBM 3033, IBM 370/168, Amdahl V/6
● proprietary code

CODE NO: 38

TYPE: Flow

CODE NAME: CMG

METHOD USED: 3-dimensional finite differences

PRINCIPAL CONTACT: Computer Modelling Group
Calgary, Alberta, Canada

DOCUMENTATION: application: Aziz S. Odeh, "Comparison of
solutions to a three-dimensional black-oil
reservoir simulation problem", J. OF PET
TECH (Jan 1981) pp. 13-25

OTHER: ● operational on Honeywell 6000 DPS
● proprietary code

CODE NO: 39

TYPE: Flow

CODE NAME: BRUTSAERT2

METHOD USED: 2-dimensional, fully implicit finite differences

PRINCIPAL CONTACT: Willem F. Brutsaert
351 Aubert Hall
University of Maine
Dept. of Civil Engineering
Orono, ME 04473
phone (207) 581-7693

DOCUMENTATION: analytical discussion in:

W. Brutsaert, "A functional iteration technique for solving Richard's Equation Applied to two-dimensional infiltration problems", WATER RESERVOIR RESEARCH vol 6, No. 7, (Dec 1971)

- OTHER: ● designed to compute the temporal and spatial variation of moisture content and water table response, as caused by precipitation, artificial recharge, and irrigation, in a heterogeneous (layered) anisotropic soil profile
- coded in FORTRAN IV
 - operational on IBM 360

CODE NO: 40

TYPE: Flow

CODE NAME: BETA-II

METHOD USED: 3-dimensional finite difference

PRINCIPAL CONTACT: INTERCOMP Resources Development Corporation
1201 Dairy Ashford
Suite 200
Houston, TX 77079

DOCUMENTATION: application: Aziz S. Odeh, "Comparison of solutions to a three-dimensional black-oil reservoir simulation problem", J OF PET TECH (Jan 1981) pp. 13-25

- OTHER:
- designed to simulate two-and three-phase compressible flow in heterogeneous hydrocarbon reservoirs
 - operation on Cray-1, Harris/7
 - proprietary code

CODE NO: 41

TYPE: Flow

CODE NAME: SSC

METHOD USED: 3-dimensional finite differences
(adaptive implicit method)

PRINCIPAL CONTACT: Scientific Software Corporation
Denver, CO

DOCUMENTATION: application: Aziz S. Odeh, "Comparison
of Solutions to a Three-Dimensional
Black-Oil Reservoir Simulation Problem",
J. OF PET. TECH. (Jan. 1981) pp. 13-25

OTHER: ● operational on CDC CYBER 75
● proprietary code

CODE NO: 42

TYPE: Flow

CODE NAME: SHELL

METHOD USED: 3-dimensional finite differences (IMPES and Implicit)

PRINCIPAL CONTACT: Shell Development Co.

DOCUMENTATION: application: Aziz S. Odeh, "Comparison of solutions to a three-dimensional black-oil reservoir simulation problem", J. OF PET. TECH. (Jan. 1981) pp.13-25

OTHER: ● operational on UNIVAC 1110/2C Level 36

● proprietary code

CODE NO: 43

TYPE: Flow and Transport

CODE NAME: SHAMTU

METHOD USED: 1-dimension finite difference, implicit

PRINCIPAL CONTACT: M. Vauclin
Institut de Mecanique de Grenoble
B.P. 53 - Centre de Tri
38041 - Grenoble - Cedex - France

DOCUMENTATION: description, theory and application in:
M. Vauclin, G. Hamon, R. Haverkamp, G. Vachaud
"Simulation des transferts couples mass-chaieur
in milie poreus partiellement - application a la
prediction de levaporation sur sol nu in-situ"
Communication to Sixth International Heat Transfer
Conference (7-11 Aug 1978) Toronto, Canada

- OTHER:
- designed to predict simultaneous heat and mass transport in the unsaturated zone
 - coded in FORTRAN IV Level H
 - operational on IBM 1130, 360/67, CII-IRIS 80

CODE NO: 44

TYPE: Transport

CODE NAME: MMT-DPRW

METHOD USED: 2-dimensional, discrete-parcel-random-walk
(DPRW)

PRINCIPAL CONTACT: H.P Foote
Battelle, Pacific Northwest Laboratories
P.O. Box 999
Richland, WA 99352
Phone: (509) 376-8418
FTS: (509) 444-8418

DOCUMENTATION:

- OTHER: ● designed to predict the movement of
radionuclides and other contaminants
in groundwater and in the vadose zone
- coded in FORTRAN IV
- operational on PDP 11/70, 11/45

CODE NO: 45

TYPE: Flow

CODE NAME: VS2D

METHOD USED: 2-dimensional finite differences,
either fully implicit or Crank-
Nicholson time discretization

PRINCIPAL CONTACT: E. G. Lappala
Senior Hydrogeologist
Ertec Western, Inc.
3777 Long Beach, CA 90807
Phone: (213) 595-6611/976-1721

DOCUMENTATION: Analytical discussion, user instruction
and program listing are contained in:
E. G. Lappala, "Documentation of Computer
Program to Solve the Equations of Fluid
Flow in Variably Saturated Porous Media",
August 1981, Preliminary report, eventually
to be issued as USGS open-file report 81-xxx.

OTHER: ● coded in FORTRAN

- Capable of treating problems in which part
of the solution domain is saturated and
part is unsaturated.
- Includes general nonlinear source-sink
terms to account for stresses, such as
evapotranspiration.
- Either rectangular or cylindrical
coordinates may be used.

CODE NO: 46

TYPE: Flow

CODE NAME: SUM-2

METHOD USED: 2-dimensional finite element

PRINCIPAL CONTACT: National Institute for Water Supply
P.O. Box 150
Leinschendam, The Netherlands

DOCUMENTATION: P.J.M. DeLaat, C. van den Akker and
Van Dener, "Consequences of Groundwater
extraction on evapotranspiration and
saturated-unsaturated flow", Symposium on
Application of Mathematical Models in Hydrology,
Bratislava, IAHS Publication No. 1.5, pp. 67-76
(1965)

- OTHER: ● designed to simulate a field size composite
groundwater-soil mixture system
- coded in FORTRAN IV
 - operational on IBM 370/158

CODE NO: 47

TYPE: Flow

CODE NAME: SUPERMOCK

METHOD USED: 2-dimensional finite difference,
alternating-direction-implicit

PRINCIPAL CONTACT: J.E. Reed
Hydrologist, U.S. Geological Survey
2301 Federal Office Bldg.
Little Rock, AR

DOCUMENTATION: Model description and program listing appear in:
J.E. Read, M.S. Bedinger and J.E. Terry
"Simulation Procedure for Modeling Transient
Water-Table and Artesian Stress and Response"
Open File Report 76-792 (1976)

OTHER: ● designed to simulate water tables and
artesian stress and response
● coded in FORTRAN IV - H level

CODE NO: 48

TYPE: Flow

CODE NAME: DELAAT

METHOD USED: 2-dimensional, finite element (variational)

PRINCIPAL CONTACT: P.J.M. de Laat
International Institute for Hydraulic
and Environmental Engineering
Oude Delft 95
Delft, The Netherlands

DOCUMENTATION: P.J.M. de Laat, "Groundwater extraction and
crop production", thesis

- OTHER: ● designed to predict consequences of
groundwater extraction on polymetric
heads, water balance and crop production
- coded in FORTRAN IV - Level G

CODE NO: 49

TYPE: Flow

CODE NAME: PORES

METHOD USED: 3-dimensional finite difference (fully implicit)

PRINCIPAL CONTACT: U.K. Atomic Energy Authority
Harwell Research Laboratory
Berkshire, England

DOCUMENTATION:

OTHER: ● designed to solve the governing equations
for three-dimensional, three phase,
multiwell black oil reservoir

CODE NO: 50

TYPE: Fluid Flow

CODE NAME: WAFE

METHOD USED: 2-dimensional finite difference

PRINCIPAL CONTACT: Bryan J. Travis
Los Alamos National Laboratory
MS F665
P.O. Box 1663
Los Alamos, NM 87545
phone FTS: 843-1254

DOCUMENTATION: In preparation.

- OTHER: ● Special features: coupled heat and two-phase mass transport (air vapor and liquid), accurate treatment of water, separate velocity field for each phase.
- Past applications: confined underground radioactive waste disposal, in-situ fossil energy recovery studies, two-phase flow and tracer studies.

CODE NO: 51

TYPE: Fluid Flow

CODE NAME: TRIPM

METHOD USED: 2-dimensional finite element

PRINCIPAL CONTACT: Dr. A. B. Gureghian
Project Management Division
Performance Analysis Department
Battelle Columbus
505 King Avenue
Columbus, OH 43201

DOCUMENTATION: A.B. Gureghian, "A two-dimensional finite-element model for the simultaneous transport of water and reacting solutes through saturated-unsaturated porous media TRIPM", Argonne National Laboratory, Argonne, IL (1981) ANL/ES-114 (in press Oct. 1981)

REFERENCES: A.B. Gureghian, "Migration of Radionuclide Chains in a Non-Homogeneous Aquifer under Transient Saturated-Unsaturated Flow Conditions", Presented at the 4th Annual Symposium on Uranium Mill Tailings Management, Colorado State University, Fort Collins, Colorado, Oct. 26-27, (1981)

OTHER: includes three-membered radionuclide decay chains

written in FORTRAN IV

Run on IBM 371 95

CODE NO: 52

TYPE: Flow

CODE NAME: MOMOLS

METHOD USED: 1-dimensional finite difference solution
of Richard's equation

PRINCIPAL CONTACT: Stuart Alan Rojstocyer

DOCUMENTATION: Stuart Alan Rojstocyer "Moisture movement
through layered soils of highly contracting
texture", M.S. Thesis U. of Ill., Urbana, Ill
(1981)

OTHER: ● coded in FORTRAN 77
listing appears in above thesis

● operational on CDC Cyber 174 or 175

CODE NO: 53

TYPE: Flow Transport

CODE NAME: MARINO

METHOD USED: 2-dimensional Galerkin finite element

PRINCIPAL CONTACT: Professor Miguel A. Marino
Dept. of Land, Air and Water Resources
and Dept. of Civil Engineering
University of California
Davis, CA 95616

DOCUMENTATION: Miguel A. Marino, "Saturated-Unsaturated Modeling of Groundwater Quality in Unconfined Aquifer Systems", QUALITY OF GROUNDWATER, Proceedings of an International Symposium, Noordwijkerhout, The Netherlands, 23-27 March 1981, W. van Duijvenbooden, P. Glasbergen and H. van Lelyveld (Eds.), STUDIES IN ENVIRONMENTAL SCIENCE vol. 17 Elsevier Scientific Publishing Co., pp. 979-984

OTHER: model includes a term for solutes which undergo first order reactions such as radioactive decay

CODE NO: 54

TYPE: Transport

CODE NAME: MLTRAN

METHOD USED: 2-dimensional finite elements

PRINCIPAL CONTACT: A.E. Reisenauer, R.W. Nelson, C.A. Newbill
Battelle Northwest
P.O. Box 999
Richland, Wa 99352
Phone (509) 376-8338
FTS 444-8338

DOCUMENTATION: A.E. Reisenauer, S.K. Gupta, R.W. Nelson
C.A. Newbill "Advective Radionuclide Transport
with soil Interaction Under Variably Saturated
Flow Conditions" PNL-3994, Pacific Northwest
Laboratory, Richland, Wa. 99352 (Sept. 1981)

OTHER: ● Uses data files generated by the program TRUST,
Code No 4, for the flow field calculation.

● Operational on DEC PDP11/45 computer.

CODE NO: 55

TYPE: Flow

CODE NAME: TRACR3D

METHOD USED: 3-dimensional integrated
finite differences

PRINCIPAL CONTACT: Bryan J. Travis
Los Alamos National Laboratory
MS F665
P. O. Box 1663
Los Alamos, NM 87545
Phone FTS: 843-1254

DOCUMENTATION: In preparation.

- OTHER: ● Special features: one or two phase
flow with tracer in either phase
(air or water) Freundlich, Langmuir
sorption, radioactive decay,
capillary effects.
- Past applications: tracer flow in
unsaturated conditions, radionuclide
transport, tracer flow in fractured
system.

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NRC FORM 335 <small>(11-81)</small>		U.S. NUCLEAR REGULATORY COMMISSION BIBLIOGRAPHIC DATA SHEET		1. REPORT NUMBER (Assigned by DDC) NUREG/CR-2917 PNL-4427	
4. TITLE AND SUBTITLE (Add Volume No., if appropriate) Review of Ground-Water Flow and Transport Models in the Unsaturated Zone				2. (Leave blank)	
				3. RECIPIENT'S ACCESSION NO.	
7. AUTHOR(S) C. A. Oster				5. DATE REPORT COMPLETED MONTH: October YEAR: 1982	
9. PERFORMING ORGANIZATION NAME AND MAILING ADDRESS (Include Zip Code) Battelle Pacific Northwest Laboratory P. O. Box 999 Richland, Washington 99352				DATE REPORT ISSUED MONTH: November YEAR: 1982	
				6. (Leave blank)	
12. SPONSORING ORGANIZATION NAME AND MAILING ADDRESS (Include Zip Code) Division of Waste Management Office of Nuclear Material Safety and Safeguards U.S. Nuclear Regulatory Commission				8. (Leave blank)	
				10. PROJECT/TASK/WORK UNIT NO.	
11. FIN NO. B2220				11. FIN NO. B2220	
				11. FIN NO. B2220	
13. TYPE OF REPORT Technical Report			PERIOD COVERED (Inclusive dates)		
15. SUPPLEMENTARY NOTES				14. (Leave blank)	
16. ABSTRACT (200 words or less) Models of partially saturated flow and transport in porous media have application in the analysis of existing as well as future low-level radioactive waste facilities located above the water table. An extensive literature search along with telephone and mail correspondence with recognized leading experts in the field, was conducted to identify computer models suitable for studies of low-level radioactive waste facilities located in the unsaturated zone. Fifty-five existing models were identified as potentially useful. Ten of these models were selected for further examination.					
17. KEY WORDS AND DOCUMENT ANALYSIS unsaturated zone ground water ground-water models			17a. DESCRIPTORS		
17b. IDENTIFIERS/OPEN-ENDED TERMS					
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