PROJECT ADMINISTRATION DATA SHEET

Project No. E-25-606
Project Director: G. G. Eichholz
Sponsor: E.I. DuPont de Nemours And Co., Inc., Aiken, SC 29808

Type Agreement: Purchase Order No. AX0654763
Award Period: From 7/1/84 To 6/30/85 (Performance) 6/30/85 (Reports)
Sponsor Amount: 
- Estimated: $49,957
- Funded: $49,957
Cost Sharing Amount: $n/a
Title: Transport Model for Radionuclide Migration in the SRP Lysimeters

ADMINISTRATIVE DATA
1) Sponsor Technical Contact: S. B. Oblath or J. A. Stone
   E. I. DuPont de Nemours and Co., Inc.
   Savannah River Plant
   Aiken, SC 29808
   (803)725-6211

2) Sponsor Admin/Contractual Matters: G. R. Parks, Jr.
   E. I. DuPont de Nemours and Co., Inc.
   Building 742-A, Room 154
   Savannah River Plant
   Aiken, SC 29808
   (803)725-6211

Defense Priority Rating: n/a
Military Security Classification: n/a

RESTRICTIONS
See Attached Supplemental Information Sheet for Additional Requirements.
Travel: Foreign travel must have prior approval — Contact OCA in each case. Domestic travel requires sponsor approval where total will exceed greater of $500 or 125% of approved proposal budget category.
Equipment: Title vests with none proposed.

COMMENTS:

CONTRACT AMENDMENTS:

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Sponsor I.D. #02.240.004, 84.004

FORM OCA 4.383
SPONSORED PROJECT TERMINATION/CLOSEOUT SHEET

Date August 1, 1985

Project No. E-25-606

Includes Subproject No.(s)

Project Director(s) C.G. Eichholz

School ME

GTRC / IXK

Sponsor E.I. DuPont de Nemours and Company, Inc. Aiken, SC 29808

Title Transport Model for Radionuclide Migration in the SRP Lysimeters

Effective Completion Date: 6/30/85 (Performance) 6/30/85 (Reports)

Grant/Contract Closeout Actions Remaining:

☐ None
☐ Final Invoice or Final Fiscal Report
☐ Closing Documents
☐ Final Report of Inventions
☐ Govt. Property Inventory & Related Certificate
☐ Classified Material Certificate
☐ Other

Continues Project No. Continued by Project No.

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Heyser

Jones

FORM OCA 69.285
Monthy Progress Report - Project E-25-606 (P.O. AX0654763)

Dear Dr. Oblath:

During the month a new contract was initiated under the above project number to continue previous work in support of the SRP lysimeter test. The major effort during the month was devoted to the completion of the Annual Report which was dispatched on July 24. In the meantime work has continued on residual moisture determinations and further development of the flow model.

To insert SRP data into the model we need to obtain some rainfall data for the period covered. We would appreciate if you would send us that information. We also acknowledge receipt of four drums of SRP soil for continuing test work.

Yours sincerely,

G.G. Eichholz
Regents' Professor

cc: O. H. Rodgers
Dear Dr. Oblath:

Work has progressed during the month mainly in determination of moisture profiles and drainage rates. Comparing sand and SRP soil samples we hope to find a generic correlation between porosity and clay content on the one hand and the gravity drainage coefficient and surface tension effects on the other. Conductivity probes have been calibrated for all four media and we are deriving rate constants for them at the moment.

No further measurements have been done on the flow divergence test; this will be resumed with new manpower at the start of the fall quarter.

The computer model is still undergoing some modifications to permit insertion of a steady or pulsed flow term and the use of the drainage rate coefficients to predict the drop to residual moisture content and recharge to saturated flow as appropriate.

At this point I would prefer leaving the setting of the date for a progress review till next month when I will have a clearer view of commitments.

Yours truly

Geoffrey G. Eichholz

cc: O.H. Rodgers (OCA)
Progress during the month has been unspectacular. Work has continued on adapting the computer code to handle rainfall data and SRP effluent results, but has been slowed by impending PhD Preliminary Exams.

Drainage coefficients are being obtained in column tests and we are continuing attempts to establish generic relationships. We are characterizing an intermediate sand/clay material available on the Georgia Tech Campus to bridge the gap between pure sand and SRP soils.

The flow divergence tests have been resumed. The barrel has been moved to a more convenient location and has been replaced. A new series of tests is under way in sand and, if we have enough SRP soil or something similar, we are planning to repeat the tests with that material. These results should help to provide input to the two-zone model.

We are also preparing some radioactive tracer tests to verify tracer movement in columns under unsaturated flow conditions.

We will discuss this work with you in more detail when you visit here on October 30.

Yours sincerely,

G.G. Eichholz
Regents' Professor

cc: O.H. Rodgers (OCA)
Dear Dr. Oblath:

During the past month work continued fairly steadily on the several phases of the project. The two-dimensional computer program is operating and is being tested at the moment and we welcome any input Dr. King can provide on his visit here tomorrow. We expect to run the program for the one-zone and two-zone case and to compare results with our laboratory test system. That system has been run with Georgia Tech sand and has demonstrated flow around the waste volume instead of through it. We are getting ready to repeat such tests with SRP soil and expect the results to be valuable, both to indicate flow pathways in the lysimeter and possible modifications in the source term assumed in the model.

We are also getting ready to run some tracer tests with cesium-137 in soil columns to demonstrate the magnitude of the retardation effect due to surface adsorption in the different soils.

It was useful to discuss progress and future directions for this project with Dr. Stone and yourself during your visit here last week. I expect to be at SRL on November 20, and will be available for further discussions if you have any questions.

Yours sincerely,

G.G. Eichholz
Regents Professor

GCE/swm
cc: O.H. Rodgers (OCA)
Dear Dr. Oblath:

During the past month work has progressed to combine the flow and transport codes and the program has been tested satisfactorily for saturated flow conditions. Column tests have been started on tracer tests to distinguish between water flow and retarded ion movement under unsaturated conditions.

Flow measurements on divergence tests clearly indicate water movement around, rather than through the waste volume for sand. The barrel has been repacked with GT sand and a new set of data are being obtained.

Both the model tests and the tracer work are continuing, though the Christmas break inevitably will bring some slowdown in activities.

With best wishes for the New Year.

Yours sincerely,

G.G. Eichholz
Regents' Professor

cc: O.H. Rodgers (OCA)

GGE/sm
Dear Dr. Oblath:

During the month work has continued to implement the matching of the two-dimensional flow and transport models. Some errors still exist that are ascribed to a sign error somewhere and attempts are being made to track it down. Several aspects on this work were discussed with Dr. Michael Grant on his visit here last week.

In experimental work, a series of glass funnel columns have been set up to determine hysteresis effects of wetting and drying on SRP soil samples. Changes in moisture content occur only slowly and the tests are relatively tedious.

The same applies to radioactive tracer tests on nuclide migration in laboratory columns, but data are being accumulated that should enable us to generate some retardation rates for incorporation in the model.

The drum test is being resumed for F P soil. The drum is being replaced and the deterioration of the previous simulated-waste sample may require assembly of a new "waste" sample.

I expect to meet with you and Dr. Stone on February 28, after the termination of the Reactor Safety Committee meeting.

Yours sincerely

G.G. Eichholz
Regents' Professor
Dear Dr. Oblath:

The status of this project was reviewed with you and Dr. Stone at SRP on February 28 and there is little to add beyond that point. We are still having some problems in the transport section of the 2D model, which I had thought that we had overcome, and I hope that this issue will be resolved shortly. Following your suggestion we will also check out again the water balance and material balance of the model.

Tracer tests on the soil columns have indicated that for unsaturated flow retardation remains proportional to water content, with constant K_d. Tests are continuing on measurements on hysteresis events to provide input data to the model on wetting and drying cycles.

The drum used in the flow divergence tests has been repacked with FP soil and measurements on moisture profiles are under way.

Contrary to my statement to you I find that de Sousa's thesis contains only documentation of the 1-D model; the 2-D model was not sufficiently finalized at this stage. We will send you a copy of the thesis for your records later this week and would appreciate your comments.

A copy of a paper on waste movement in unsaturated soil, prepared for presentation at the Tucson Waste Management Conference at the end of this month, has been sent to you for concurrence, which I hope to receive as soon as possible. Please call me if there are any questions in this regard.

Yours sincerely

Geoffrey G. Eichhold
Regents' Professor

GGE/swm

cc: P. Heitmuller
Dear Dr. Oblath:

During the past month further work has been done to solve the problem of matching the flow and transport models for the 2D model. This has been accomplished and has been tested for Van Genuchten's data and looks alright. However, Mr. Suh feels that it may be necessary to take into account the tensor characteristics of the diffusion coefficient and he is looking into that question.

We also expect to test the model with SRP data shortly, though there is a problem in terms of completeness and consistency of the available data.

It appears that the program is in a form compatible with the specifications you gave me for tape transmission to SRP. Work is under way to document fully the program as developed.

The flow divergence tests have been resumed with FP soil. Some problems arose when the injected water seemed to reach a steady distribution fairly rapidly with little drainage to the bottom of the drum. Some subsidence into the waste volume and cracking of the dry surface layer occurred, and we are evaluating whether this resulted in irreversible changes in the bed. Another run has been started and we await results.

A paper on waste movement in unsaturated soil was presented at the Waste Management 85 conference in Tucson, Ariz. on March 27, and was well received. The paper to be published in the Proceedings, was revised in accordance with your suggestions and received clearance.

A copy of the Sousa's thesis is in the mail. I apologize for the delay and would appreciate your comments.

Yours sincerely

G.G. Eichholz
Regents' Professor

GGE/swm

cc: P. Heitmuller (OCA)
Dear Dr. Oblath:

During the past month further work has been done to put the 2D model in final form. The cause of a residual oscillation has been located and corrected. Water balances have been obtained and look alright and attempts are being made to utilize existing experimental data in the model.

A major effort is being made to follow the moisture distribution in columns of SRP soil and to obtain drainage profiles using iodine-131 tracers. A source of I-131 has been found locally, that will make frequent re-supply convenient and inexpensive.

The flow divergence tests with the FP soil have been completed and the drum is being repacked to study flow patterns around a slanting soil-waste interface.

We look forward to discussing these various aspects of the project with you here May 22. I hope, also, we will be able to define several areas of continuing interest to you that you may wish us to study over the next few months.

Yours sincerely,

G.G. Eichholz
Regents' Professor

cc: Pat Heitmuller (OCA)
Dear Dr. Oblath:

Most of the present status of this project was discussed with you and Drs. Stone and Grant during your visit here on May 22 and there is not much to add. We are getting a tape and expect to send you the program on tape shortly. The code is being described and written up and will form part of our final report.

Experimental work has been resumed on the flow divergence test which we expect to conclude by the end of next week. The tracer tests on the laboratory columns have been held up by electronic problems, but we seem to have isolated the cause.

We plan to send you a preliminary proposal shortly for some further work in waste migration, which we hope will be of interest to SRP.

The next few weeks will be taken up with organizing our data and the preparation of the final report on this project.

Yours sincerely,

Geoffrey G. Eichholz
Regents' Professor

/ce:  P. Heitmuller (OCA)
TRANSPORT MODEL FOR RADIONUCLIDE MIGRATION
IN THE SRP LYSIMETERS

Final Report

Project E25-606 (SRP Purchase Order No. AX0654763)

Geoffrey G. Eichholz
Project Director

Submitted to

Waste Disposal Technology Division
Savannah River Laboratory
E. I. DuPont de Nemours & Company
Aiken, SC 29808

July 1984
Project Personnel (All part-time)

Geoffrey G. Eichholz, Ph.D
Fernando N. Carneiro de Sousa, MSHP
Jooho Whang, MSHP
M. Frank Petelka, MSHP
M. Christine Daily, B.S.
Harry K. Anderson, B.S.
Bruce W. Patton, B.S.

Project Director
Graduate Research Assistant
Graduate Research Assistant
Graduate Research Assistant
Graduate Research Assistant
Graduate Research Assistant
Graduate Research Assistant

NOTE: Mr. De Sousa obtained his Ph. D degree in March, 1985, based in part on research conducted in connection with this project.
Summary

The Project described in this report was undertaken in support of current studies conducted by staff of the Savannah River Laboratory to model and simulate the migration of radionuclides from miscellaneous low-level wastes buried at the plant site in disposal trenches. These studies center on a number of lysimeters that have been installed to simulate various waste forms and burial conditions in local soil under actual climatic conditions. These tests have been running for several years and the work at Georgia Tech has been designed to provide supporting studies in the areas of model development and hydraulic and hydrological investigations to provide input data and to help verify the models.

This work was started in July 1983 and the first phase, to June 30, 1984, has been reported in a Final Report (Project E26-627), submitted a year ago. That report contained a description of the lysimeters and a bibliography of the related literature, which will not be repeated in this report.

The work described here addresses two related tasks:

1. Development of a finite-element two-dimensional model capable of describing waste migration under unsaturated conditions; and

2. Experimental tests on flow rates, drainage rates and flow patterns for various waste configurations and soil-moisture conditions.

Model development has been completed and a copy of the program has been delivered to SRL on tape. Various tests have demonstrated flow around the waste, rather than through it, under unsaturated conditions and several types of moisture profiles have been obtained.
INTRODUCTION

The potential migration of waste materials from the low-level burial trenches at the Savannah River Plant has been of continuing concern for several years. To allow prediction of any such effects, the type of waste and its burial conditions have been simulated by means of a series of lysimeters (Stone, 1984). These lysimeters have been operated for several years, but in the nature of such tests, little active material has, in fact, appeared at the sample points, as might be expected considering the relatively dry weather that has prevailed in the past few summers and the nature of the SRP soil.

In support of this work, the Health Physics group at Georgia Tech has worked with SRL staff to develop a two-dimensional computer model, capable of representing flow and transport conditions in unsaturated soil, and to conduct experimental work on the flow paths of infiltrated water around waste packages and on the effect of varying moisture concentrations.

This study was begun in July 1983 and the results of the first year were reported in a previous report (Eichholz, 1984) and will not be repeated here. Similarly, much of the background information will be found in that report.

At that time a one-dimensional model had been completed and tested against data in the literature. Since then a two-dimensional model has been developed as described in the next chapter. The program is listed in detail in the appendix and has been transcribed onto a tape, which has been delivered to SRL.

Experimental work has concentrated on flow path determinations, using conductivity probes, and on studies of the hysteresis effects in wetting/
drying cycles. No further work has been done on leach tests on the waste materials and, for the present, the source term in the model is assumed to be proportional to the rate of water movement through the waste zone.

Direct comparison of the model with output data from the lysimeter tests has been hampered by a scarcity of such data and uncertainty regarding the source term. It is hoped that future laboratory tests can serve to validate the model more directly.

We are indebted to Professor Mustafa Aral of the School of Civil Engineering at Georgia Tech for his continuing advice and assistance in the development of the hydrological models.
MODEL DEVELOPMENT

10 CFR Part 61 requires, as a condition of the licencing process, that the applicant for a waste disposal site will make detailed predictions of site performance over a 500 year period. To determine the suitability and performance of a proposed or existing site, modeling can be a valuable tool with which to calculate potential migration of radionuclides from the disposal site. Besides, modeling can be a useful tool with which to evaluate the effectiveness of design features such as cover systems and backfills, which are designed to minimize infiltration and contact of water with wastes buried in the site.

In general, the movement of radionuclides through soils is described by a couple of partial differential equations. Although the problem is to solve these equations simultaneously, normally the flow equation is shaped for computer modeling first and then the transport equation is coupled to it.

In this work, the finite element technique was used to develop a two-dimensional unsaturated flow and transport model. In the one-dimensional model that was developed by De Sousa (1985), simulations were done assuming that the soil parameters only vary in the vertical directions, and that the lateral movement of water can be neglected. However, in many cases, the use of a one-dimensional model may be useful only to gain insight of how the site works. A two-dimensional model presented here may describe the transportation of wastes in two directions, which is more suitable in simulating a real waste burial site. In this work, a two-dimensional model is presented with axisymmetric coordinates which would apply to the lysimeters under test in Savannah River Laboratory. The model includes a linear sorption isotherm as a geochemical process in the transport equation, and a first-order reaction for the radionuclide migration.
FLOW MODEL

The equation of unsaturated flow can be obtained by combining the continuity equation with Darcy's Law for unsaturated conditions. The generally used form of the unsaturated flow equation is given by

\[ L(\psi) = C^* \frac{\partial \psi}{\partial t} - \nabla \cdot (K \nabla \psi) + \frac{\partial K}{\partial x} = 0 \]  

(1)

where \( C^* \) is the specific soil-water capacity (L), given by

\[ C^* = \frac{\partial \theta}{\partial \psi} \]

\( \psi \) is the pressure head (L),

\( t \) is time (T),

\( K \) is the hydraulic Conductivity (LT\(^{-1}\))

\( X \) is the vertical coordinate (positive down) (L)

As is seen from equation (1), this equation only deals with water flow in soils. However, in the case of unsaturated flow, air (or vapor) and water move together and the existence of air in the pores affects the flow of water. In general, when dealing with flow in a large unsaturated zone in the field, the effect of air flow in neglected (Bear, 1979).

In equation (1), the specific soil-water capacity \( C^* \), and the hydraulic conductivity are function of either water content \( \theta \) or pressure head, and this makes equation (1) non-linear. In the model, these relationships can either be adopted from site-specific data or from empirical relations that are available.

Complete description of the unsaturated flow equation requires the initial and boundary conditions to be specified for the system under study. The initial condition is given by describing the distribution of pressure head at the beginning.

\[ \psi(x, r, z) \bigg|_{t=0} = \psi_0 (r, z) \]  

(2)
There are two types of boundary conditions: Dirichlet boundary, where the pressure head remains constant regardless of time,

$$\psi(\tau, r, z) = \tilde{\psi}(\tau, r, z)$$

on \( \Gamma_t \); or Neumann boundary, where the flux due to the gradient of the pressure head is constant,

$$\int_{A} q_0(x, r, z) \, dA = \int_{A} (k \nabla z + k \nabla \psi(x, r, z)) \, dA = \text{const.}$$

on \( \Gamma_s \) where \( \Gamma = \Gamma_t + \Gamma_s \) is the total boundary of the region.

The finite-element method is used to solve the differential equation which is dependent on position variables \( r \), and \( z \). Following Yeh (1982), the finite element technique is applied to the equation step by step:

1. Divide the region into elements and nodes.

An element in the axisymmetric coordinate is the volume confined in three circles which are made when rotating an area \( A \) \( B \) \( C \) around the axis. In each elemental volume the properties of soil or porous media are to be constants. The three circles made by rotating points \( A \), \( B \), and \( C \) represent nodes where the pressure head or the concentration of waste is calculated.

2. Define basis functions for each node.
The element used in the model was said to be a circle of volume. However, the area A B C in Figure 1 is used to determine the basis function as is the case in a Cartesian coordinate triangular element.

Pressure head, concentration, specific water capacity, and hydraulic conductivity are functions of position \((r,z)\). However, these values are calculated by linearly interpolating nodal values. In transient flow cases, the basis function is used to separate space variables \((r,z)\) from the time variable. The basis function defining a parameter in an element is given by

\[
N^e(r,z) = \frac{a^e + b^e r + c^e z}{2A^e}
\]  

(5)

where

\[
2A^e = (r_1 z_2 - r_2 z_1) + (r_3 z_1 - r_1 z_3) + (r_1 z_3 - r_2 z_3)
\]

(6)

Then, for example, the pressure head at points \(P (r,z)\) at the time \(t\) is given by

\[
\hat{\Psi} (t, r, z) = \sum_{\lambda=1}^{3} N^e_r (r, z) \Psi^\lambda(t)
\]

(7)
3 - Define the residual as the difference between hypothetical true solution and approximate solution. Galerkin's method requires that, when the trial solution is substituted into the differential equation, the residual, when weighted by each of the basis functions, be zero.

4 - Derive the matrix equation.

5 - Incorporate boundary conditions to the matrix equation.

6 - Use initial conditions to advance the solution through time.

**FINITE ELEMENT FORMULATION**

The Galerkin technique is used to determine approximate solutions to equation (1) under the appropriate initial and boundary conditions. For each element, the interpolated equation is multiplied by the basis function \( N_i (r, Z) \), and integrated over the element. Since the type of an element is a triangle with three basis functions, three equations are formed in an element. Trial solutions are chosen of the form:

\[
\hat{u} = \sum_{\lambda=1}^{3} \psi_{\lambda} N_{\lambda} \tag{8}
\]

\[
\hat{K} = \sum_{L=1}^{3} K_{L} N_{L} \tag{9}
\]

\[
\hat{C} = \sum_{L=1}^{3} \hat{C}_{L}^{k} N_{L} \tag{10}
\]
In the Galerkin procedure, the trial solution \( \hat{\psi} \) is substituted into the differential equation \( L(\psi) = 0 \) (eq. 1), and this expression is set orthogonal to all the functions \( N_i \) of the system. (J. F. Pickens, R. W. Gillham and D. R. Cameron, 1979). Thus, the residual can be minimized in the following form:

\[
\int_V C^* (\psi) \frac{\partial \psi}{\partial x} N_j \, dV = \int_V \nabla \cdot \left\{ k(\psi) \left( \nabla \psi - \kappa \mathbf{Z} \right) \right\} N_j \, dV
\]  

Equation (11) can be separated, in a general form, as follows:

\[
\int_V C^* (\psi) \frac{\partial \psi}{\partial x} N_j \, dV = \int_V \nabla \cdot \left\{ k(\psi) \left( \nabla \psi - \kappa \mathbf{Z} \right) N_j \right\} dV - \int_V \left\{ k(\psi) \left( \nabla \psi - \kappa \mathbf{Z} \right) \cdot \nabla N_j \right\} dV
\]  

Equation (12) can be shaped in matrix and vector form

\[
[M] \left\{ \frac{\partial \psi}{\partial x} \right\} = [Q] - [S] \left\{ \psi \right\} + [P]
\]
where \([ M ]\), \([ Q ]\), \([ S ]\), \([ F ]\) matrixes represent the left-hand side term, the first term on the right hand-side, the second term, and the third term of equation (12), respectively.

To obtain numerical stability of the time derivatives, the nodal values of the time derivatives are defined as weighted averages over the entire flow region (Neuman, 1973). The time derivative appearing in equation (12) is the time derivative of the pressure head, \( \frac{\partial \psi}{\partial t} \).

For each term, a matrix element can be made, making use of functionals as follows:

\[
m_j = \sum_{L=1}^{3} \int_{V} C^* N_L N_j \, dV = \sum_{L=1}^{3} C^* \int_{V} N_L N_j \, dV
\]  

(14)

\[
S_{ij} = \sum_{L=1}^{3} \int_{V} K_L N_L \nabla N_i \cdot \nabla N_j \, dV = \nabla N_i \cdot \nabla N_j \sum_{L=1}^{3} K_L \int_{V} N_L \, dV
\]  

(15)

\[
P_{ij} = \sum_{L=1}^{3} \int_{V} K_L N_L \frac{\partial N_j}{\partial z} \, dV = \frac{\partial N_j}{\partial z} \sum_{L=1}^{3} K_L \int_{V} N_L \, dV
\]  

(16)

\[
q_{ij} = - \int_{\Gamma_z} \vec{n}_{\Gamma_z} \cdot q_{ij} \, d\Gamma_z
\]  

(17)

The time-dependent nature of equation (13) can be accommodated by employing a finite-difference scheme to approximate the time derivatives. In this work, the Crank-Nicolson method is used.
\[
[M] \frac{\psi^{k+1} - \psi^k}{\Delta t} = [Q] - \left[ S \right] \frac{\psi^{k+1} + \psi^k}{2} + [P] \tag{18}
\]

Equation (18) can be written as,

\[
\{ [M] + \left[ S \right] \} \frac{\psi^{k+1}}{\Delta t} = \left[ [M] - \left[ S \right] \right] \frac{\psi^k}{\Delta t} + [Q] + [P] \tag{19}
\]

Other steps to solve the matrix differential equation described above are the assembly of a global matrix with boundary conditions, and solving the matrixes, which are discussed in other sections of this work.
HYDRAULIC PROPERTIES

The following hydraulic properties are accommodated in the model. The user may select and decide which hydraulic property is to be used. However, if there exist experimental data on these hydraulic properties, the data can be fitted to each model and coefficients should be obtained.

WARRICK MODEL

The Warrick Model can be used by assigning \(iTM = 0\).

\[
\begin{align*}
\Theta &= \begin{cases} 
0.6829 - 0.09524 \ln 141 & \psi \leq -29.484 \\
0.4531 - 0.02732 \ln 141 & -29.484 < \psi \leq -14.495 \\
19.34 \times 10^5 \, 141^{3.4095} & -14.495 < \psi \\
516.8 \, 141^{-0.097814} & -29.484 < \psi \\
0.09524 / 141 & -29.484 < \psi \leq -14.495 \\
0.02732 / 141 & \psi < -29.484
\end{cases}
\end{align*}
\]

VAN GENUCHTEN MODEL

It can be used by assigning \(iTM=1\).

\[
\Theta = \Theta_r + (\theta - \Theta_r) \left( \frac{1}{1 + (\psi \lambda)^m} \right)
\]

\[
C^* = m (\theta - \Theta_r) \lambda (\psi \lambda)^{m+1} \left( \frac{1}{1 + (\psi \lambda)^m} \right)^{m+1}
\]

\[
K = K_s \sqrt{\Theta} \left[ 1 - (1 - \Theta^m)^m \right]^2
\]
where $\theta_r$ is the residual water content, 
n is the porosity, 
$k_s$ is the saturation hydraulic conductivity, 
$M = 1 - \frac{1}{n}$, and 
$\beta = (\theta - \theta_r) / (n - \theta_r)$.

**BROOKS AND COREY MODEL**

It can be used by assigning iTM = 2.

$$\theta = \theta_r + (n - \theta_r) \left( \frac{\psi_s}{\psi} \right)^\lambda$$

$$k = k_s \left( \frac{\theta - \theta_r}{n - \theta_r} \right)^\lambda$$

$$c^* = (n - \theta_r) \lambda \frac{1}{\psi_s} \left( \frac{\theta - \theta_r}{n - \theta_r} \right)^{1+\frac{1}{\lambda}}$$

where $\psi_s$ is the air-entry value.
HAVERKAMP MODEL

It can be used by assigning iTM = 3.

\[
\theta = \theta_r + \alpha \left( \frac{n - \theta_r}{\alpha + \psi^A} \right)
\]

\[
C^* = \lambda \alpha \frac{(n - \theta_r)}{(\alpha + \psi^A)^2} \psi^{\lambda-1}
\]

\[
K = K_s \left( \frac{\beta}{\beta + \psi^A} \right)
\]

SATURATION CASE

It can be used by assigning iTM = -1.

\[
\theta = n
\]

\[
C^* = 0
\]

\[
K = K_s
\]

\[
\psi = \psi_s
\]
By assigning the variable iTM with different numbers, other variables in the program are made to change as follows:

<table>
<thead>
<tr>
<th>iTM</th>
<th>SER</th>
<th>SES</th>
<th>HES</th>
<th>CKS</th>
<th>RMM</th>
<th>APH</th>
</tr>
</thead>
<tbody>
<tr>
<td>-1</td>
<td>n</td>
<td>$\psi_s$</td>
<td>$\kappa_s$</td>
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<td>$\kappa_s$</td>
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<td>n</td>
<td>$\beta$</td>
<td>$\kappa_s$</td>
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-16-
TRANSPORT MODEL

The governing partial differential equation used to describe the movement of solutes through porous materials is based on the principle of conservation of mass (Yeh, 1982; Van Genuchten, 1978). The advection-dispersion equation for the transport of a solute in a saturated-unsaturated soil can be formulated in a general form as

$$\frac{\partial (\Theta C)}{\partial t} + q K_d \frac{\partial C}{\partial x} = \nabla \cdot (\Theta D \nabla C - q C) + \lambda \Theta C + \beta \Theta K_d C + \gamma \Theta$$  \hspace{1cm} (20)

where $\Theta$ is the volumetric water content,
$C$ is the concentration of solute in solution,
$\Theta$ is the soil bulk density,
$K_d$ is the distribution coefficient,
$D$ is the hydrodynamic dispersion coefficient,
$q$ is the volumetric flux
$\lambda$ is the first-order rate constant (liquid phase),
$\beta$ is the first-order rate constant (solid phase), and
$\gamma$ is the zero-order rate constant (liquid phase).
Equation (20) assumed the linear isotherm for adsorption of solute on soil, which has the relation of

$$S = K_d C$$  \hspace{1cm} (21)

where $S$ is the adsorbed concentration.

A retardation factor may be incorporated into equation (20), which results in

$$\frac{\partial (\Theta C)}{\partial t} = \nabla \cdot (\Theta D \nabla C - \psi C) + \alpha \Theta C + \beta \psi K_d C + \gamma \theta$$  \hspace{1cm} (22)

where $R$ is the retardation factor representing

$$R = 1 + \frac{\psi K_d}{\Theta}$$  \hspace{1cm} (23)

If the reactions of the solute with soil are only adsorption and radioactive decay, coefficients $\alpha$ and $\beta$ become both equivalent to a decay constant of the radionuclide in question, and $\gamma$ becomes zero. However, for the purpose of verification of the model with published results, those coefficients are left in the model.
Ignoring the last term $\gamma \theta$ in equation (22) and differentiating the left-hand side term, equation (22) can be rewritten as

$$\theta R \frac{\partial c}{\partial t} = \nabla \cdot (\theta \tilde{D} \cdot \nabla c - \tilde{q} c) + \tilde{a}' c$$

(24)

where

$$\tilde{a}' = (\alpha \theta + \beta \gamma k - \frac{\partial \theta}{\partial t})$$

(25)

Multiplying equation (24) by $N_j$ of an element, and integrating over the element would give

$$\int \theta R N_j \frac{\partial c}{\partial t} dV = \int (\theta \tilde{D} \cdot \nabla c - \tilde{q} c) \cdot \vec{n} d\Gamma + \int \theta \tilde{D} \cdot \nabla N_j dV + \int \tilde{q} c \cdot \nabla N_j dV + \int \tilde{a}' c N_j dV$$

(26)

which results in the following form:

$$[M] \left\{ \frac{\partial c}{\partial t} \right\} = [Q] - [A] \{ c \} + [B] \{ c \} + [F] \{ c \}$$

(27)

Making use of the lumping method as was used in the flow equation, we have

$$m_{\tilde{a}} = \sum_{L=1}^{2} (\theta R) L \int N_L N_{\tilde{a}} dV$$

(28)
\[ q_i = \int ( \Theta \mathbf{D} \cdot \nabla C - \mathbf{q} C ) \cdot \hat{n}_i \, d\mathbf{r} = - \mathbf{q}_0 \cdot C_0 \int d\mathbf{r} \]  

(29)

where \( \mathbf{q}_0 \) is the surface flux of water and \( C_0 \) is the concentration of solute.

\[ b_{j; i} = \int \mathbf{K} \left( \frac{\partial N_j}{\partial x}, \frac{\partial N_j}{\partial y}, \frac{\partial N_j}{\partial z} \right) N_i \, d\mathbf{r} \]  

(30)

\[ b_{j; i} = \int \mathbf{K}(0, 1) \left( \frac{\partial N_j}{\partial x}, \frac{\partial N_j}{\partial y}, \frac{\partial N_j}{\partial z} \right) N_i \, d\mathbf{r} - \int \mathbf{K}(1, 0) \left( \frac{\partial N_j}{\partial x}, \frac{\partial N_j}{\partial y}, \frac{\partial N_j}{\partial z} \right) N_i \, d\mathbf{r} \]  

(31)

\[ = \sum_{l=1}^{\infty} K_l \int N_{i; l} N_{j; l} \, d\mathbf{r} \left\{ - \sum_{k} \frac{\partial N_k}{\partial z} \nabla N_k \cdot \nabla N_j \right\} \]  

(32)

\[ f_{j; i} = \sum_{l=1}^{\infty} \left( \partial \Theta + \beta \Theta K_d - \frac{\partial \Theta}{\partial z} \right) \int N_{i; l} N_{j; l} \, d\mathbf{r} \]  

(33)

The second term of the right-hand side of equation (26) can be expressed as follows:
\[ \nabla \cdot (\theta \frac{\partial}{\partial r} \nabla C) = \left( \frac{\partial}{\partial r}, \frac{\partial}{\partial z} \right) \begin{pmatrix} \Theta D_{rr} & \Theta D_{rz} \\ \Theta D_{rz} & \Theta D_{zz} \end{pmatrix} \left( \frac{\partial C}{\partial r}, \frac{\partial C}{\partial z} \right) \]  

(34)

where the hydrodynamic coefficients are

\[ D_{rr} = D_d^* + \left( \frac{d_d^*}{v} \right) / v \]  

(35)

\[ D_{rz} = D_d = \left( \frac{d_d}{v} - \frac{d_d^*}{v} \right) \frac{v_r v_z}{v} \]  

(36)

\[ D_{zz} = D_d^* + \left( \frac{d_d^*}{v} \right) / v \]  

(37)

In equation (35), (36), and (37),

\[ \vec{v} = \vec{q} / \Theta \]  

(38)

is the velocity of water

\[ |v| = \sqrt{v_r^2 + v_z^2} \]  

(39)
and flux is given by

$$\vec{q} = K \vec{\nabla} (Z - \Phi)$$  \hspace{1cm} (40)$$

where, for each direction

$$\vec{q}_x = K (1 - \partial \Phi / \partial z)$$  \hspace{1cm} (41)$$

$$\vec{q}_r = -K \partial \Phi / \partial r$$  \hspace{1cm} (42)$$

Thus, the water velocity for each direction is

$$\vec{v}_r = K (r, z) (-\partial \Phi / \partial r) / \Theta (r, z)$$  \hspace{1cm} (43)$$

$$\vec{v}_z = K (r, z) (1 - \partial \Phi / \partial z) / \Theta (r, z)$$  \hspace{1cm} (44)$$

Substituting equation (43), (44), and (39) into equation (35), (36), and (37) and multiplying them by $\Theta$, we have
\[ \theta D_{rr} = D_d^x \theta(r,z) + k(r,z) \frac{c_l \left[ (- \frac{\partial \psi}{\partial r})^2 + c_r (1 - \frac{\partial \psi}{\partial z})^2 \right]}{\sqrt{(- \frac{\partial \psi}{\partial r})^2 + (1 - \frac{\partial \psi}{\partial z})^2}} \] (45)

\[ \theta D_{rz} = \theta D_{zr} = k(r,z) \frac{c_l \left[ (- \frac{\partial \psi}{\partial r}) (1 - \frac{\partial \psi}{\partial z}) \right]}{\sqrt{(- \frac{\partial \psi}{\partial r})^2 + (1 - \frac{\partial \psi}{\partial z})^2}} \] (46)

\[ \theta D_{zz} = D_d^z \theta(r,z) + k(r,z) \frac{c_l (1 - \frac{\partial \psi}{\partial z})^2 + c_r (- \frac{\partial \psi}{\partial z})^2}{\sqrt{(- \frac{\partial \psi}{\partial r})^2 + (1 - \frac{\partial \psi}{\partial z})^2}} \] (47)

Van Genuchten (1978) showed that very accurate solutions of the one-dimensional convective-dispersive equation can be obtained through the introduction of appropriate dispersion corrections. The corrections are

\[ D^- = D - \frac{\Delta t}{6} \theta R \] (48)

\[ D^+ = D + \frac{\Delta t}{6} \theta R \] (49)
Thus, equations (35), (36), and (37) are given by

\[ D_{rr}^\pm = D_{rr} \pm \phi_{rr}^2 \Delta t / 6 \theta^2 R \]  

\[ D_{rz}^\pm = D_{rz} \pm \phi_{rz}^2 \Delta t / 6 \theta^2 R \]  

\[ D_{zz}^\pm = D_{zz} \pm \phi_{zz}^2 \Delta t / 6 \theta^2 R \]

These correction factors are applied to the dispersion coefficients such that the correction factors are different for the old and new time steps.

Substituting equation (50), (51), and (52) into the second term of the right-hand side of equation (26), the array for \( [A] \) in equation (27) becomes as follows:
Finally $[A]$ in equation (26) has an array of

$$
\alpha_{ji} = \sum_{L=1}^{N} \left[ \begin{pmatrix} \Theta_{D_{rr}} \Theta_{D_{rL}} \\ \Theta_{D_{rL}} \Theta_{D_{zz}} \end{pmatrix} \begin{pmatrix} \varphi \varphi \varphi \varphi \varphi \end{pmatrix} \right]^T \begin{pmatrix} \varphi \varphi \varphi \varphi \varphi \end{pmatrix}
$$

($54$)

Substituting equation (53) into equation (27) and separating the term $[A]$ into two, i.e.,

$$
[A^+] = [A] \pm [AD]
$$

($55$)
where \([ A D ]\) is the correction term in equation (48) and (49), the \([ A ]\) term becomes, with use of the Crank-Nicolson method,

\[
[A^+][C] = [A^+][\frac{C^1}{2}] + [A^-][\frac{C^{1+\Delta t}}{2}]
\]  \hspace{1cm} (56)

Equation (27), with the Crank-Nicolson time step, becomes

\[
[\frac{\Delta t}{2}][A][B][F][-AD][C^{1+\Delta t}] = [\frac{\Delta t}{2}[M] - [A][AN][B][F]][C^1] + [Q]
\]  \hspace{1cm} (57)

Other steps toward solving equation (57) are the same as were done for equation (19).

A flowchart of the main program follows.
FLOW-CHART OF MAIN PROGRAM.

start

read input

prepare coefficients of basis functions

integrate basis functions & their combinations for future use

write initial conditions

101

\[ \psi^s = \psi^t \]

103

\[ \psi^{s+1} = \psi^s + (\psi^s - \psi^t) \Delta t^t / \Delta t^{t+\alpha \Delta t^t} \]

\[ \psi^t = \psi^s \]

102
$\psi^t = (\psi^t + \psi^{t+\Delta t})/2$

first iteration?

- yes
  - determine $\theta, K, C^*$
  - make global matrix
  - solve matrix for new $\psi^{t+\Delta t}$
  - converge?
    - yes
      - too many inner iterations?
        - yes
          - reduce $\Delta t$
        - no
          - too few iterations?
            - yes
              - enlarge $\Delta t$
            - no
              - solve transportation
  - no
    - transportation?
      - yes
        - small $\Delta t$?
          - yes
            - stop
          - no
            - too few iterations?
              - yes
                - enlarge $\Delta t$
              - no
                - solve transportation
\[ t = t + \Delta t \]

- Time for output:
  - Yes: Write
  - No: Time to change condition

- Time to change condition:
  - Yes: Adjust \( t \), \( \Delta t \), and change condition
  - No: Stop

- Time to stop?
  - Yes: Stop
  - No: 101
Soil-Water Characteristic Curve and Hysteresis Effect

Introduction.

The soil-water characteristic curve is a graphical representation of a function that relates the suction with the amount of water remaining in the soil at equilibrium (Childs, 1969). Figure 1 shows that the amount of remaining water is also a function of the particle-size distribution and of texture. If a slight suction is applied to water in saturated soil, no outflow may occur until, as suction increased, a certain critical value is exceeded. Above the critical value, the largest pores begin to lose the water that filled them. This critical suction is called the air-entry suction, which is point A for each curve in Figure 1-a, and Figure 2. The soils which are more uniform in size (poorly-graded soil) may exhibit critical capillary head more distinctly and sharply than do less uniform soils (well-graded soil). It can be seen from Figure 1-b that the soil-moisture characteristic curve is strongly affected by the soil texture. The greater the clay content, the greater the water retention at any particular suction and the more gradual the slope of the curve becomes (Bear, 1979).

The practical use of the characteristic curve is limited to the soil in question and the measured range of soil suction values: For a curve to be used in groundwater modeling, a curve for the specific soil in
Figure I Typical retention curves in soil during drainage. (a) Schematic curves. (b) Curves obtained during desaturation (after Richards and Weaver, 1944).
Figure 2 - Soil-Water Characteristics
question has to be obtained experimentally, i.e., there exists no generic curve. However, if the data of a curve are available, they can either be used directly or fitted to empirical equations in the groundwater model. Empirical equations used in the model were described in the previous section.

So far, only the soil-water characteristic that is applicable for drainage has been discussed. By wetting an initially dry soil sample while reducing the suction, another relation between suction and soil moisture content can be obtained, which yields a continuous curve but is not identical to the one obtained while draining. This dependence of the equilibrium moisture content and the suction upon the direction of the process is called hysteresis (Hillel, 1980a). It is also possible to start the wetting process on the drainage curve or to start the drainage process on the wetting curve, which will give the lines connecting the boundary drainage curve to the boundary wetting curve. These lines are called scanning curves (Bear, 1979).

Hillel (1980a) reported several aspects that cause the effect of hysteresis:

a. The ink bottle effect, resulting from the geometric non-uniformity of the individual pores.

b. The contact-angle effect by which the contact angle is greater and hence the radius of curvature is greater in an advancing meniscus than in the case of a receding one.

c. Entrapped air in the wetting process.

d. Swelling, shrinkage or aging phenomena that depend on the wetting and drying history of the sample.

Comparing those aspects, Wilson (1980) reported that the hysteresis effect is mainly caused by entrapped air in the pore space during wetting.

The hydraulic conductivity of unsaturated soils is a function of the
water content $\theta$, or similarly, of the hydraulic head. The relation between the hydraulic conductivity and the water content is assumed to be nonhysteretic. This nonhysteretic behavior has been substantiated by Topp and Miller (1966), Topp (1969), and others. However, hysteretic hydraulic conductivity as a function of the water content was reported by Poulavassilis and Tzimas (1975). The relation between the hydraulic conductivity and the suction head is considered to be affected by hysteresis, since the relation between the suction head and water content are very much hysteretic. Mualem (1976) found substantial hysteresis in the relation between the hydraulic conductivity and the suction head, whereas hysteresis in the relation between hydraulic conductivity and the water content was of much less importance. However, for practical purposes, the majority of published data indicate that the relation between hydraulic conductivity and the water content can be considered nonhysteretic.

The importance of the hysteresis effect in groundwater problems is that the hydraulic conductivity is a function of either the water content or the suction head. The empirical equations of the hydraulic conductivity indicate that a small change of the water content may lead to a great change in the hydraulic conductivity, which will result in a great error in calculated amount of infiltrated water through a porous material. Pickens and Gillham (1980) reported from a simulation of a vertical column, that the pressure head profile for the hysteretic case lay between the profiles for nonhysteretic drying and nonhysteretic wetting, but the water content profile exhibited quite a different shape. Hoa et al. (1977) compared the numerical simulation with experimental results and reported that a numerical simulation in which the hysteresis effect is ignored may introduce important errors in the water content profile.
The water content and its related hydraulic conductivity are important parameters in determining the source term of the low level waste burial site. Besides, when one tries to simulate and predict a long-term effect of precipitation to the release of waste materials from the site, cyclic wetting and drying of the site together with the hysteresis effect had better be taken into consideration to be close to reality.

Experimental

For a laboratory method to obtain soil-water characteristic curves down to negative pressures of -800 cm of water, the modified Haines method is usually recommended.

The modified Haines method employs equipment shown on Figure 3.

In this work, the Haines method was modified such that, instead of soil cores, soil is placed on a fritted glass bead plate and several Buchner funnels are employed to produce different negative pressures.

(Because of the strength of the fritted glass bead plate employed, the negative pressure one can apply was limited up to 15 psi.)

The cores are weighed after the soil water has equilibrated with each successive negative head. At the end of the test, the soil cores are overdried and intermediate masses are converted to volumetric water content values. (EPA-600).

The procedure for obtaining a desorption curve (Wet to Dry) is as follows:

1. Fill the column and Buchner funnel with distilled water.
2. Lower the end of the column to the lowest height possible and let the system stay there for 24 hr. This step removes air from the system.
Figure 3 - Hanging Column (Wilson, 1980)
3. Place the soil in question in the funnel making sure that sizes of particles are well distributed. The amount of soil used was 15±1 ml which is air dried, sieved through #14 size mesh and compacted by tapping. The resulting height of soil from the fritted glass bead is about 1 cm. In placing soil in the funnel, the end of the column (top of the pipet connected to rubber tubing) is maintained 100 cm lower than the funnel.

4. Saturate the soil by lifting the water level 40 cm above the surface of the soil in the funnel. Continual supply of water through the end of column is necessary.

5. Wait until the water seeped through the soil forms a 1 cm layer above the surface of the soil. Then tap the funnel to remove entrapped air in the soil.

6. Lower the end of column to a desired suction value.

7. Wait until no water drips out of the pipet and then watch to see if the water level changes.

8. When the level of water starts going down, sample the soil in the funnel and use the oven-dry method to obtain water content.

The procedure for obtaining a sorption curve is the same as the one for desorption through Step 1. However, in this procedure the level of water is lowered down to a value at which the water content is the residual water content. After Step 7, the level of water is lifted up to a desired value. The most important thing to do in this step is to maintain the desired water level constant until sampling of the soil is finished.

To decide when to sample, at least three funnels with the same value are required. Each funnel is sampled after a long enough time has elapsed. For each funnel, the time interval is chosen to be different. If the water
contents of soil from three funnels are the same, the shortest time for a
given funnel will indicate the appropriate sampling time. If different
results are obtained, one must try again, taking longer times for
equilibrium.

Results

The resultant soil-water characteristic curves are shown in Figures 2
and 4. De Sousa (1985) obtained the soil-water characteristic curves in
Figure 2 for three types of soils: SRP1, SRP2, and GT sand, for which the
soil parameters are reported in Eichholz (1984). The three curves in
Figure 2 show several aspects of soil characteristics; first, all three
curves present the same general shape; second, the air-entry value of each
soil is different from each other; third, each type of soil has its own
residual water content.

The general shape of the soil-water characteristic curve is such that
there is a region of constant water content, then the water content drops
rapidly as the magnitude of the pressure head increases, and finally the
water content reaches the residual value of constant water content (De
Sousa, 1985). However, the curve for GT sand presents a very sharp
decrease in the pressure region right after the air-entry value, which was
expected due to the fact that the GT sand was a poorly graded soil. Two
other curves for SRP soils show a more gradual decrease since they are
well-graded soils.

Looking at the differences of the air-entry values for the three
curves, we can tell, without identifying the samples, which soil has more
clay and bigger pores, since the smaller the particle size or pore size,
the bigger the force attracting the water to the soil particles becomes,
and, consequently, the greater the force to remove water from a soil is
required.
FIGURE 4 - HYSTERETIC SOIL-WATER CHARACTERISTICS OF SRP #1.
The residual water content of each curve represents the amount of water left after a mobile fraction of the water has been removed by applying the negative pressure. For the rest, the surface tension of the water films covering the soil particles is so large that no more water can be removed even at high pressure. However, the residual water contents obtained by the Modified Haines Method (the hanging column method) are higher than the ones obtained by Whang (1984). Whang (1984) measured electrical conductivities of soils using electrodes embedded in soil. The residual water content defined in that work was the one at which electric current could no longer be sustained. At that water content, the films of water covering the soil particles would no longer be connected, so that no current flows. To reach the residual water content in a draining soil column took a long period of time (3 weeks for short columns, Whang (1984), 3 months for long columns by De Sousa (1985).

Figure 4 includes two curves representing the hysteretic nature of the soil-water characteristic curve of SRP1 soil. The two curves, for drying and wetting conditions, are boundary curves which form a closed loop. It is also possible to start the wetting process from any point on the drying curve, or to start the drying process from any point on the wetting curve, leading to many curves, called scanning curves. This is what makes it hard to incorporate a general $\psi = \psi_s$ equation into a computer model. However, as long as the soil remains stable (i.e., no consolidation), the hysteresis loop can be traced repeatedly.
The shape of the drying curve in Figure 4 looks different from that of
the SRP1 curve in Figure 2. That is because the bulk density of soil in the
Buchner filter was different for each case. In obtaining the curves in
Figure 2, the soil sample was compressed to give a consistent bulk density.

The three curves in Figure 2, were fitted to two empirical relations,
the Brooks and Corey relation, and the Van Genuchten relation. The least
square method was applied to the experimental data of each soil to fit the
Brooks and Corey relation. It was found, that for the Brooks and Corey
relation the pressure head region from 0 to $\psi_5$ cannot be fitted to the
relation, so that it was assumed that the water content was equal to the
porosity of the soil. For the Van Genuchten relation, the method used to
fit the experimental data was the one described by Van Genuchten (1978).
Table 1 shows the results obtained.
TABLE 1 - CURVE FITTING PARAMETERS (DeSousa, 1985)

<table>
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<th>BROOKS AND COREY</th>
<th>VAN GENUCHTEN</th>
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<tr>
<td></td>
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</table>
FLOW DIVERGENCE TESTS

In the previous report (Eichholz, 1984) various test configurations were described, which, on a small scale, were intended to examine the flow paths through and around simulated waste packages. For this purpose a 55 gallon drum was employed, which was filled to a height of about 5 inches with a gravel bed for drainage, and above that, a soil bed in which simulated laboratory waste was emplaced inside some perforated plastic bags. Details were shown in the previous report.

Water movement has been monitored by means of a series of conductivity probes, that were calibrated for that type of soil and were located at various horizons throughout the bed, both within the central column and in the annular outside region.

The results reported here were obtained with FP soil, a synthetic mixture of SRP soil and sand, which was expected to be a little more permeable than SRP soil and whose characteristics has been described before (Eichholz, 1984). The purpose of Test No. 3 was to determine if lateral inflow would occur into the region containing the waste. Test No. 4 was set up with the waste forming a sloping interface to study the resulting flow paths. Each test consisted of two runs to check for consistency. Because of the poor condition of the waste package after the first three tests, a new simulated waste package, similar to the previous one was used for Test No. 4.
DETAILS OF TEST WORK

Test No. 3 was set up with F P Soil with the electrodes inserted in the locations shown in Figure 5. Two separate runs were conducted, 28 days apart, so that some of the original water was still contained in the bed for the second run. The results are plotted in Figures 6 and 7 which show the rapid rise in moisture content for the top layer, followed by very slow drainage as indicated also by the slow rise in moisture content at the "middle" horizon. It is evident that there was no real pulse front moving through the bed and even after 600 hr the bottom layer showed only a very slight rise in moisture content. The onset of the second run indicates that there was a slight but uniform retention of moisture in the upper half of the test bed, with no particular puddle formation around the waste material and no special indication of any lateral movement.

In Test No. 4 the waste material was emplaced in a slanting position and the electrodes installed as shown in Figure 8. In the first run (Figure 9) the top layer peaked after 10 minutes at 88% saturation. Electrodes 4, 5, and 6 indicated the gradual progression of moisture down the top of the waste, with some more rapid loss at No. 6 indicated by the slower rise. Note the logarithmic time scale on the graphs; No. 4 peaked at 5.5 hr., No. 5 at 14.5 hr. and No. 6 at 95 hr. No. 12 did not show any increase until after more than 50 hr and the other electrodes even then showed no increase in moisture content. This clearly indicated that most of the water flow was diverted along the top of the waste through the wetter contact layer.

The second run, starting with slighter moister soil looks strikingly different (Figure 10), possibly because of some drying and cracking of the top layer which was observed between runs, though it was smoothed over superficially.
Figure 5. Configuration for Test No. 3
Figure 6. Test No. 3, Run 1
Figure 7. Test No. 3 Run 2
Top layer (electrodes 1, 2, & 3), located 2" below the surface.

The waste is at a 30° angle, with electrodes 4, 5, and 6 placed on the surface. All electrodes except 13 and 14 are located in the same plane.

Figure 8. Configuration for Test No. 4
Figure 9. Test No. 4 Run 1

Time (hours)

% Saturation

top
Figure 10. Test No. 4 Run 2
The surface of the waste itself was wetted to saturation very rapidly and water drained off in a matter of hours, leaving the top of the bed at low moisture levels throughout the test. It is evident that even under these conditions water movement occurred around the waste, not through. Very little moisture was ever detected at electrode No. 10 below the waste. Since this is a significant departure and it is desirable to obtain more data to compare this effect with model predictions, this test is being repeated.
CONCLUSION

The principal objective of this project has been the development of a two-dimensional model capable of simulating the behavior of the Savannah River Plant lysimeters and the validation of this model. Such a model has been developed and has been tested against the published data for Van-Genuchten's model as applied to the experimental results of Warrick. Because of the limited nature of the test results of the SRP lysimeter runs to date, a direct comparison has not been accomplished so far, but that is obviously something that will have to be attempted in the near future.

Since most of the experimental work in the literature was obtained for saturated flow conditions, much effort has been devoted to learn about the behavior of SRP soil and water flow through it under unsaturated conditions. Some results have been reported here on wetting and drying conditions and on flow patterns around simulated waste, but further test work appears to be necessary to obtain adequate numerical data for the various operational parameters that will help to make the model credible.

Qualitatively it is evident that the SRP lysimeters will operate under unsaturated conditions much of the time. It is highly probable that water flow will occur around the embedded waste rather than through it, except during saturated episodes. The soil is relatively slow to drain, but though the clay content of SRP soil is higher than our FP soil, the different size distribution has resulted in comparable drainability. It appears highly desirable to obtain laboratory data on some of these parameters to permit realistic validation of the computer model soon enough so that it can be used in the design of future low-level waste disposal trenches.
This work has benefitted greatly from the advice and guidance of Dr. Maustafa Aral of the Georgia Tech School of Civil Engineering in the formulation of the computer model. The research described here profited considerably from frequent, active interaction with Drs. S. B. Oblath and J. A. Stone of the Savannah River Laboratory. Some early phases of the work were supported indirectly by parallel work done for the DOE Low-level Waste Management Program sponsored through EG&G Idaho-Inc.
REFERENCES


18. Y. Mualem - A New Model for Predicting the Hydraulic Conductivity of Unsaturated Porous Media. Water Resources Res. 12, 513-522 (1976)


APPENDIX

INPUT Description

The 1st Line
TITLE : 60 characters for titling. (FORMAT 12A5)

The 2nd Line, AL, IL, ER, DTMAX, DTMIN, DT

AL : Time difference equation option

0 forward difference equation
1 Backward difference equation
.5 Crank-Nicholson's Method

IL : Maximum number of inner iterations. If the number of iterations are larger than IL, time interval is changed, number of iterations is set to 0.

ER : Error Bound of inner iteration

ER > MAX \left( \frac{U_i^k - U_i^{k-1}}{U_i^{k-1}} \right) \quad \text{where} \quad i=1, 2 \cdots \text{ND}

DTMAX : Maximum time interval in hour. Time interval is kept less than this value.

DTMIN : Minimum time interval in hour. If time interval is less than this value, it means that model is very unstable and it terminates the program.

DT : The initial time interval in hour

The 3rd Line

ITRSP : 0 not to solve transportation equation
1 to solve transportation equation

If ITRSP=1, next line is inserted as coefficients in transport equation.

The (3+ITRSP)th Line

RH, DOT, AFL, AFT, DK, ALF, BET, GAM, CBT

RH \quad \varphi, \quad \text{The bulk density of fluid (g/cm)}

DOT \quad D_{\alphaT}, \quad \text{where} \quad D_{\alpha} \quad \text{is the molecular diffusion coefficient (cm/day)}
\quad \text{and} \quad \tau \quad \text{is the tortuosity factor}.

AFL \quad \alpha_L, \quad \text{Longitudinal dispersivity of the porous medium}

AFT \quad \alpha_T, \quad \text{Transversal dispersivity of the porous medium}

DK \quad K_d, \quad \text{The empirical coefficient for absorbed concentration (cm/g)}
\quad \text{absorbed concentration} \quad S = \frac{K_d C}{R + \frac{1}{\theta}}
\quad \text{total concentration} \quad = \theta C + \frac{1}{\theta}
\quad \text{where} \quad R = 1 + \frac{\varphi K_d}{\theta}
ALF \( a \) a First order rate constant (liquid phase) (day)

BET \( b \) a First order rate constant (solid phase) (day)

GAM \( \gamma \) a zeroth order rate constant (liquid phase) (g/cm · day)

CST Concentration at the bottom for boundary condition of constant concentration.

The (4+ITRSP)th Line NS, HDBT

NS The number of steps of different boundary conditions
HDBT The hydraulic head at the bottom for boundary condition of constant head at the bottom.

The (5+ITRSP~4+ITRSP+NS)th Lines
TB(NS), IBC(NS), Q(NS), (IBCC(NS), CI(NS)) () only when ITRSP=1

TB Up to the moment, following BC is applied (hr)
IBC Top Boundary condition option of flow model
0 constant head, Q(i) is the hydraulic head (cm)
1 constant flux, Q(i) is the flux (cm/day)
IBCC Top boundary condition option of transport model
0 constant concentration, CI(i) is the concentration (g/cm · water).
1 constant flux, CI(i) is the concentration in inlet fluid (g/cm · water).

The (5+ITRSP+NS)th Line ISF(IHO)
ISF(i), i=1, IHO-1 The element numbers, one of whose surfaces are on the top where IHO is the number of nodes on the top.

The (6+ITRSP+NS)th Line IPRIN
IPRIN The number of printings the result

The (7+ITRSP+NS)th Line, PTIME(IPRIN)
PTIME(i), i=1~IPRIN The time to print the result.

The (8+ITRSP+NS~7+ITRSP+NS+NE)th Lines NOD(NE, 3)
NOD(i, j), j=1, 3 The number of nodes of the i-th element

The (8+ITRSP+NS+NE~7+ITRSP+NS+NE+ND)th Lines R(ND), Z(ND), HD(ND), (CON(ND)) () only when ITRSP=1

R The radial coordinate of the node (cm)
Z The axial coordinate of the mode (cm)
HD The initial hydraulic head at the nodes (cm), HD < 0
CON The initial concentration at the node (g/cm · water)

The (8+ITRSP+NS+NE+ND)th Line, IDFF
IDFF=0 Homogeneous case
IDFF=1 Heterogeneous case
If IDFF=1 next two lines are needed.
The (8+ITRSP+NS+NE+ND+1 or 2)th Lines
NBE, NEE
RHD, DOTD, AFLD, AFTD, DKD, ALFD, BETD

NBE–NEE The element number of different region should be in a row.
NBE and NEE are the first and last element number of the set.

RHD, DOTD, AFLD, AFTD, DKD, ALFD, and BETD are $\rho$, $\rho_\tau$, $\phi_L$, $\phi_T$, $k_d$, $\alpha$ and $\beta$ in the different region.

The (8+ITRSP+NS+NE+ND+IDFF*2)th Line , ITM
The option for the relationships of $\Theta$, $K$ and $C$ to $\psi$ in normal region.

The (9+ITRSP+NS+NE+ND+IDFF*2)th Line , Coefficients with respect to the value of ITM. See below.

Next lines are needed only when IDFF=1.

The (10+ITRSP+NS+NE+ND+IDFF*2)th Line , ITMD
The option for the relationships of $\Theta$, $K$ and $C$ to $\psi$ in different region.

The (11+ITRSP+NS+NE+ND+IDFF*2)th Line , Coefficients with respect to the value of ITMD. See below.

MODEL

<table>
<thead>
<tr>
<th>MODEL</th>
<th>ITM</th>
<th>SER</th>
<th>SES</th>
<th>APH</th>
<th>RMM</th>
<th>CKS</th>
<th>HES</th>
</tr>
</thead>
<tbody>
<tr>
<td>Saturation</td>
<td>-1</td>
<td>n</td>
<td>n</td>
<td>$K_4$</td>
<td>$\psi_4$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Warrick Sand</td>
<td>0</td>
<td>n</td>
<td>n</td>
<td>$K_4$</td>
<td>$\psi_4$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Van Genuchten</td>
<td>1</td>
<td>$\Theta$</td>
<td>$n$</td>
<td>$\alpha$</td>
<td>$\times$</td>
<td>$K_4$</td>
<td>$\psi_4$</td>
</tr>
<tr>
<td>Brooks and Corey</td>
<td>2</td>
<td>$\Theta$</td>
<td>$n$</td>
<td>$\alpha$</td>
<td>$\times$</td>
<td>$K_4$</td>
<td>$\psi_4$</td>
</tr>
<tr>
<td>Haverkamp</td>
<td>3</td>
<td>$\Theta$</td>
<td>$n$</td>
<td>$\alpha$</td>
<td>$\times$</td>
<td>$K_4$</td>
<td>$\beta$</td>
</tr>
</tbody>
</table>

HES = $|\psi_4|$ $>$ 0

-58-
Symbolic Constants

These constants should be assigned before using the program. The use of these constants are easily explained with the following example.

NE : number of elements
ND : number of nodes
iHO: number of nodes on the top of the region
NOD: number of nodes in different region when the program deals with multi-region problem.

(Example)

The shaded area represents the region with different hydraulic properties from surrounding region.

\[
\begin{array}{ccc}
1 & 2 & 3 \\
4 & 5 & 6 \\
7 & 8 & 9 \\
\end{array}
\]

\[
\begin{array}{c}
\circ \ 0 \\
\circ \ 1 \\
\circ \ 2 \\
\circ \ 3 \\
\circ \ 4 \\
\circ \ 5 \\
\circ \ 6 \\
\circ \ 7 \\
\circ \ 8 \\
\end{array}
\]

\[
\begin{array}{c}
\text{NE} = 8 \\
\text{ND} = 9 \\
\text{iHO} = 3 (1, 2, 3) \\
\text{NOD} = 4 (4, 5, 7, 8) \\
\end{array}
\]
Variables in Main Program

Variables with postfix D represent the variables in the region with different hydraulic properties.

A (NE,3) : $a_i^e$, one of the coefficient of basis function, i.e.,
the i-th basis function of e-th element is

$$N_i^e = a_i^e + b_i^e r + C_i^e Z$$

AFL, AFLD: $\alpha_L$, the longitudinal dispersivity [L]
AFT, AFTD: $\alpha_T$, the transverse dispersivity [L]

AL: The optional parameter to select the method to solve time-difference equation

$$AL = \begin{cases} 
1. & \text{back-ward difference scheme} \\
0.5 & \text{Crank-Nicolson method} \\
0 & \text{forward difference scheme}
\end{cases}$$

ALF, ALFD: $\lambda$, the first-order rate constant in transport equation
(liquid phase) [T⁻¹]
APH, APHD: see page for Hydraulic Properties.

AR: \( A^e \), the area of an element, See A(NE,3)

B: \( b^e_i \), see A(NE,3)

BDC (IHO): dummy matrix for boundary condition on the top of region

BET, BETD: the first-order rate constant (solid phase) \([T^{-1}]\)

C: \( c^e_i \), see A(NE,3)

CBT: Concentration of solute at the bottom. This is used for the boundary condition at the bottom of the region.

CC (ND), CCD (NDD): \( C^* \), the specific water capacity \([L^{-1}]\)

\( C_i \) (NS): the array for changeable boundary condition.
NS: the number of boundary condition changes

TB(NS): new boundary condition is applied up to this moment [T]

iBC(NS): option for the boundary condition at the top of flow region

iBCC(NS): option for the boundary condition at the top of transport region

\[ Q_i(NS) \text{ iBC}(i) = 0, \quad Q_i(i) \text{ is constant hydraulic head on the top } [L], \]
i.e., B.C. of constant head.

\[ Q_i(NS) \text{ iBC}(i) = 1, \quad Q_i(i) \text{ is constant water flux on the top } [LT^{-1}], \text{ i.e., B.C. of constant water flux.} \]

\[ C_i(NS) \text{ iBCC}(i) = 0, \quad C_i(i) \text{ is constant concentration at the top } [M/L^3], \]
i.e., B.C. of constant concentration

\[ C_i(NS) \text{ iBCC}(i) = 1, \quad C_i(i) \text{ is the solution concentration in incoming water} \]

CKTIME, QM, IQ, CQ, and iQC are TB, QI, IBC, CI and IBCC for current boundary condition on the top, respectively.

CK, CKD: k, the hydraulic conductivity [LT^{-1}]

CKS, CKSD: see APH.
CKTiME: the time limit for current boundary condition.

\[ T \]

CNE (NE,9): see subroutine ITGL.

CON (ND): the solution concentration \([M/L^3]\).

CQ: see Ci

CSE: see CNE

DK, DKD: \(k_d\), the distribution coefficient with which the retardation factor is defined as

\[ R = 1 + \phi k_d / \theta \]

where \(\phi\) is the bulk density \([M/L^3]\) of porous medium, and \(\theta\) is the volumetric water content \([L^3/L^3]\).

DT: \(\Delta t\), the current time interval

DTL: \(\Delta t\), the previous time interval

DTLL: \(\Delta t\), the buffer for time interval when time is adjusted to CKTiME at the end of current boundary condition.

DTMAX: see input
**DTMIN:** see INPUT

**DOT, DOTD:** see INPUT

**ER:** the error limit in inner iteration.

**ERROR:**

\[
\text{ERROR} = \left| \frac{\psi_j^{i+1} - \psi_j^i}{\psi_j^{i+1}} \right|
\]

where \( \psi_j^i \) is the pressure head at the j-th node at the i-th iteration.

**ERR:** The maximum value of \( \text{ERROR} \) among j nodes.

It is used as follows:

\( \text{ERR} > \text{ER} \): Do more iteration

\( \text{ERR} < \text{ER} \): Go to next time step

**GAM:** see INPUT

**HD (ND):** \( \psi^t + \Delta t \), the pressure head at \( t + \Delta t \)

**ADH (ND):** \( \psi^t + \Delta t / 2 \), the pressure head at \( t + \Delta t / 2 \)

\[
\psi^t + \Delta t / 2 = \psi^t_+ (\psi^t_+ - \psi^t_- \Delta t') \Delta t / 2 \Delta t' \text{ at the beginning of inner iteration (extrapolation)}
\]

\[
\psi^t + \Delta t / 2 = (\psi^t_+ \Delta t - \psi^t) / 2 \text{ during inner iteration (interpolation)}
\]

**HDL (ND):** \( \psi^t \), the pressure head at \( t \)
HDLL (ND): $\Psi^{t+} \Delta t$, the pressure head at $t + \Delta t$ at the previous iteration.

HDS (ND): buffer for $\Psi^t$ at the beginning of inner iteration.

HES, HESD: see SER

HOUR: Time in hour for print out.

iBC, IBCC: see CI.

IDFF: the option for homogeneity. See INPUT.

IFLAG: the condition of solved matrix

$$\begin{align*}
\text{IFLAG} &= 0 .... \text{good matrix to have as many roots as its order.} \\
\text{IFLAG} &= i .... \text{bad matrix, to have } i \text{ indefinite roots} \\
\text{IFLAG} &= 100 .... \text{singular matrix}
\end{align*}$$

IHD: see symbolic constants.

IL: the limit to number of iteration. See INPUT

IPNT: the order of printing time

IPRIN: the number of steps to print

IPPP: the flag to check whether the current time and the time interval are defined by CKTIME for boundary-condition changes.

$$\begin{align*}
\text{IPPP} &= 0 .... \text{normal case} \\
\text{IPPP} &= 1 .... \text{they are defined by CKTIME.}
\end{align*}$$
IQ, IQC, IQIN: see CI.

ISF (IHO): element numbers one of whose surfaces is on the top.

IT: the number of inner iterations compared by IL.

ITM, ITMD: see page for O, X, C* of $\Psi$.

ITRSP: 
\[
\begin{cases}
= 0, & \text{transport is not considered.} \\
= 1, & \text{transport is considered}
\end{cases}
\]

LHS (ND, ND): the left-hand side matrix used for both flow equation and transport equation. e.g.

\[
[A](x) = \{B\}
\]

\[
[A] = \text{LHS (nxn)}
\]

\[
\{X\} = \text{unknown (nx1) which can either be } \Psi \text{ or } C
\]

\[
\{B\} = \text{RHS (nx1)}
\]

After the subroutine (GAUSSE, LHS and RHS becomes an unit matrix (nxn), and X(nx1) respectively.

NBE, NEE: see INPUT

ND, NDD, NE: see symbolic constants.
NOD (NE, 3): see INPUT.

NODD (NDD): the number of nodes occupied by different region.

NS: see CI

PTIME: see INPUT

Q (20): see INPUT or CI

QM: see CI

R (ND): the radical coordinate. see INPUT

RH, RHD: the bulk density of soil or porous material

RHS: see LHS.

RMM, RMMD: see hydraulic properties

SER, SERD: see hydraulic properties

SES, SESD: see hydraulic properties

SUM 1: summation of water contents at all nodes.

SUM 2: summation of concentration multiplied by water contents at all nodes.
TB (20): see CI

TH, THD: $\theta^{t+\Delta t}$, the water content at $t + \Delta t$

TIME: $t + \Delta t$, the current time

TIMEL: $t$, the previous time

TPRNT: see IPNT

V(NE): The volumes of elements $[L^3]$

\[ V(i) = \int_0^1 \int_0^2 \pi r^d r dr dz \]

Z (ND): the axial coordinate, see INPUT.

**SUBROUTINES**

**SUBROUTINE ABC:** it prepares the coefficients of basis functions.

**INPUT:** NOD (NE, 3), K (ND), Z (ND)

**OUTPUT:** A (NE, 3), B (NE, 3), C(NE,3), AR (NE)

**SUBROUTINE ITGL:** it integrates the basis functions and their combinations over each element volume, which is to be used in iteration loop.

**INPUT:** NOD (NE,3), R(ND), Z (ND), A(NE,3), B(NE,3), C(NE,3), AR (NE,3).

**OUTPUT:** It consist of the first, second, and third order of integrations of combination of basis functions.
\[
\text{CNE}(E,i) = \int_{v_e} N_k^e N_{l}^e \, dv, \quad \text{............(a)}
\]

\[
\text{CNE}(E,i) = \int_{v_e} N_k^e \, dv, \quad \text{............(b), or}
\]

\[
\text{CNE}(E,i) = \int_{v_e} N_k^e N_{l}^e N_{M}^e \, dv, \quad \text{............(c)}
\]

k, l, and m are 1, 2, or 3, respectively, and
\[
i = 1 \sim 6 \quad \text{for (a),} \quad i = 7 \sim 9 \quad \text{for (b), and}
\]
\[
i = 1 \sim 10 \quad \text{for (c)}
\]

\[
\text{CSE}(E,j,k) = \int_{v_e} \nabla N_j^e \cdot \nabla N_k^e \, dv
\]

**SUBROUTINE TMDP:** It calculates water content, hydraulic conductivity, and specific water capacity at all nodes as functions of pressure head.

**INPUT:**

- NOD (NE,3), HD (NE,3)
- COMMON/TMD/SER,SES,HES,CKS,RMM,APH,iTM.

**OUTPUT:**

- TH(ND), CK(ND), CC (ND).

**SUBROUTINE TMDPD:** It calculates water content, hydraulic conductivity, and specific water capacity in different region. **INPUT** and **OUTPUT** variables are the same as those in subroutine TMDP except that NODD (NDD) replaces NOD (NE,3). NDD is the number of nodes in different region. NODD is the node numbers of the nodes involved in different region. This array is generated in MAIN.
SUBROUTINE SYS: The global matrix is generated to calculate hydraulic head at next time step.

OUTPUT: LHS(ND,ND), RHS(ND), BDC (IHO)

Important variables are:

\[ CM(I) = \sum_{j=1}^{3} \sum_{i=1}^{3} C_{ij}^{e} \int_{V} N_{j}^{e} N_{i}^{e} \, dV \]

\[ CS(I,J) = \sum_{k=1}^{3} \nabla N_{k}^{e} \cdot \nabla N_{j}^{e} \sum_{i=1}^{3} K_{k}^{e} \int_{V} N_{i}^{e} \, dV \]

\[ CP(I) = \sum_{k=1}^{3} \frac{3}{\alpha Z} \sum_{k=1}^{3} K_{k}^{e} \int_{V} N_{k}^{e} \, dV \]

\[ LHS(I,J) = AL * CS(I,J) + CM(I) / DT \]

\[ RHS(I) = CP(I) + CM(I) / DT \times HDL(I) - \sum_{J=1}^{ND} CS(I,J) \times (1-AL) \times HDL(J) \]

SUBROUTINE TRANSP: It generates the global matrix to calculate concentration at next time step.

OUTPUT: LHS (ND,ND), HMS (ND, ND)

Important variables are:

\[ DM(I) = \sum_{j=1}^{3} \sum_{i=1}^{3} \Theta_{ij}^{e} R_{j}^{e} \int_{V} N_{j}^{e} N_{i}^{e} \, dV \]

\[ DA(I,J) = \sum_{k=1}^{3} \sum_{i=1}^{3} \Theta_{k}^{e} \left( D_{k}^{e} \cdot \nabla N_{k}^{e} \cdot \nabla N_{j}^{e} \right) \int_{V} N_{i}^{e} \, dV \]

\[ DAD(I,J) = \sum_{k=1}^{3} \sum_{i=1}^{3} \Theta_{k}^{e} \left( D_{k}^{e} \cdot \nabla N_{k}^{e} \cdot \nabla N_{j}^{e} \right) \int_{V} N_{i}^{e} \, dV \]

\[ DOB(I,J) = \sum_{k=1}^{3} \sum_{i=1}^{3} \Theta_{k}^{e} \left( \nabla N_{k}^{e} \cdot \nabla N_{j}^{e} \right) K_{k}^{e} \int_{V} N_{i}^{e} \, dV \]

\[ DF(I,J) = \sum_{k=1}^{3} \sum_{i=1}^{3} \left( -\frac{3 \Theta_{k}^{e}}{\alpha Z} + \phi \Theta_{k}^{e} + \beta K_{d} \right) \int_{V} N_{i}^{e} N_{j}^{e} N_{k}^{e} \, dV \]
where $D$ is the dispersion coefficient tensor and $\tilde{D}$ is the corrected dispersion coefficient tensor.

$$\text{LHS}(I,J) = \frac{\text{DM}(I)}{\text{DTL}} - (\text{DDB}(I,J) - \text{DA}(I,J) + \text{DF}(I,J) - \text{DAD}(I,J)) / 2$$

$$\text{RHS}(I) = \frac{\text{DM}(I)}{\text{DTL}} * (\text{ON}(I) + (\text{DDB}(I,J) - \text{DA}(I,J) + \text{DF}(I,J) + \text{DAD}(I,J)) / 2$$

**SUBROUTINE Q Q:** It generates dispersion coefficient tensors.

**OUTPUT:**

$\text{DRR}(\text{ND})$, $\text{DRZ}(\text{ND})$, and $\text{DZZ}(\text{ND})$ are the dispersion coefficient tensors in normal region, which represent $D_{rr}$, $D_{rz} = D_{zr}$ and $D_{zz}$ respectively.

$\text{DRRD}(\text{NDD})$, $\text{DRZD}(\text{NDD})$, and $\text{DZZD}(\text{NDD})$ are the corrected tensors in normal region, which represent $D'_{rr}$, $D'_{rz} = D'_{zr}$, and $D'_{zz}$, respectively.

$\text{DRD}(\text{NDD})$, $\text{DZD}(\text{NDD})$, $\text{DXD}(\text{NDD})$ are the dispersion coefficient tensors in different region, which represent $D_{rr}$, $D_{zz}$, and $D_{rz} = D_{zr}$ respectively.

$\text{DRDD}(\text{NDD})$, $\text{DZDD}(\text{NDD})$, and $\text{DKDD}(\text{NDD})$ are the corrected tensors in different region, which represent $D'_{rr}$, $D'_{zz}$, and $D'_{rz} = D'_{zr}$ respectively.

Important variables are:

- $\text{QR}(\text{ND})$ which is $\bar{q}_r$, radial flux, at a node,
- $\text{QZ}(\text{ND})$ which is $\bar{q}_z$, axial flux, at a node,

$$\text{QR}(I) = \sum_{k=1}^{3} \sum_{\lambda}^{1} 2 \kappa_k^e \psi_\lambda^e \frac{\partial N_\lambda}{\partial r} \int_{V_k} N_k dV / V^e$$

$$\text{QZ}(I) = \sum_{k=1}^{3} \sum_{\lambda}^{1} (1 + \psi_\lambda^e \frac{\partial N_\lambda}{\partial z}) \kappa_k^e \int_{V_k} N_k dV / V^e$$

$$\text{QA}(I) = \sqrt{\text{QR}^2(I) + \text{QZ}^2(I)}$$
SUBROUTINE GAUSSE: It solves ND-th order matrix equation of which the form is \[ A \{ x \} = \{ b \} \].

INPUT:  
LHS (ND,ND) ..... \{ A \}  
RHS (ND) ..... \{ b \}  

OUTPUT  
LHS (ND,ND)...
unit matrix  
RHS (ND) .... X, unknown matrix.

FUNCTION CZ (IP, I, J, K): It assigns a value to

\[ \int_\Omega N_i^e N_j^e N_k^e \, dv \]

OUTPUT:  CNEE (IP,10) where IP is element number.
**RAIN**

**ASYMMETRIC TWO DIMENSIONAL**

**FINITE ELEMENT METHOD**

**UNSATURATED FLOW MODEL**

**AND TRANSPORT MODEL**

**BOUNDARY CONDITION**

**TOP**

- CONSTANT WATER CONTENT AND/OR CONCENTRATION
- CONSTANT FLUX

**BOTTOM**

- CONSTANT WATER CONTENT AND/OR CONCENTRATION
- FREE DRAINING

**PROGRAM MAIN**(IN, OUT, TAPE5=IN, TAPE6=OUT)

PARAMETER(NE=20, ND=22, IHO=2, NDD=1)

REAL LHS
COMMON/LR/LHS (ND, ND), RHS (ND)
COMMON/CK/C (ND), CC (ND)
COMMON/CCKD/C (NDD), CCD (NDD), NODD (NDD), NBE, NEE
COMMON/TMD/SER, SES, HES, CKS, RMM, APH, ITM
COMMON/TMDD/SERD, SESD, HESD, CKSD, RMDD, APHD, ITMD
COMMON/CNEE/CNEE (NE, 10)
COMMON/ECE/CNEE (NE, 9), CSE (NE, 3, 3)
COMMON/RZA/R (ND), Z (ND), A (NE, 3), B (NE, 3), C (NE, 3), AR (NE), ISF (IHO)
DIMENSION NOD (NE, 3), HD (ND), HDL (ND), HDH (ND), HDL (ND), HDLL (ND)
1, Q (20), TB (20), IBC (20), IBCC (20), CI (20)
1, TH (ND), CON (ND), BDC (IHO), PTIME (20), V (NE)
1, THD (NDD), THLD (NDD)
CHARACTER*5 TITLE (12)
COMMON/TRA/RH, DK, DOT, AFL, AFT, GAM, ALF, BET
COMMON/TRAD/RHD, DKD, DOTD, AFLD, AFTD, ALFD, BETD
READ (5, 302) TITLE
! 302 ! FORMAT (12A5)
WRITE (6, 304) TITLE
! 304 ! FORMAT (1//5X, 12A5, ///)

**TRANSPORTATION(1), OR NOT(0) ?**

IF 1, READ COEFFICIENTS FOR TRANSPORT MODEL

**RH** : BULK DENSITY OF FLUID

**DZZ** = AFT*VR**2/V + AFL*VZ**2/V + DOT

**CBI** : CONCENTRATION AT THE BOTTOM

---
READ(5,*)ITRSP
 IF(ITRSP.EQ.1)READ(5,*)RH,DOT,AFL,AFT,DK,ALF,BET,GAM,CBT
***************************************************************************
* NS 	 : # OF BC CHANGING 
* TB 	 : IN HOUR, UP TO THIS MOMENT 
* IBC(I) 	 : 1 CONSTANT FLUX 	 Q(I)=Q0 < KS(SAT. COND.) 
* 0 CONSTANT HEAD 	 Q(I)=HD(0,T) 
* IBCC(I) 	 : 1 CONSTANT FLUX 	 CI(I)=C0*Q0 
* 0 CONSTANT CONCENT. 	 CI(I)=CON(0,T) 
* HDBT 	 : HEAD AT THE BOTTOM 
* CBT 	 : CONCENTRATION AT THE BOTTOM 
* ISF 	 : ELEMENT NUMBERS( ONE OF THEIR SURFACE IS TOP SURFACE) 
***************************************************************************
READ (5, *) NS, HDBT 
IF(ITRSP.EQ.0)READ(5, *)(TB(I), IBC(I), Q(I), I=1,NS) 
IF(ITRSP.EQ.1)READ(5, *)(TB(I), IBC(I), Q(I), IBCC(I) , CI(I), I=1,NS) 
READ(5, *) (ISF(I), I=1, IH0-1) 
IQIN=1 
CKTIME=TB(IQIN)/24. 
QM=Q(IQIN) 
IQ=IBC(IQIN) 
IF(ITRSP.EQ.1)THEN 
CQ=CI(IQIN) 
IQC=IBCC(IQIN) 
ENDIF
***************************************************************************
* PRINTING OPTION 
* IPRIN : NO. OF STEPS TO PRINT 
* PTIME TIMES (IN HOUR) 
***************************************************************************
READ(5,*)IPRIN 
READ(5, *)(PTIME(I),I=1,IPRIN) 
IPNT=1 
TPRNT=0. 
IPPP=0 
***************************************************************************
***** NOD : NODE NUMBERS OF EACH ELEMENT  **********************
***** R, Z 	 : COORDINATES OF NODE IN CM  ****************************
***** HD, CON : INITIAL VALUE OF HEAD, CONCENTRATION 
***************************************************************************
DO 10 I=1,NE 
READ(5, *)(NOD(I,J), J=1,3) 
10 CONTINUE 
DO 20 J=1,ND 
IF(ITRSP.NE.1)READ(5,*)R(J), Z(J), HD(J) 
IF(ITRSP.EQ.1)READ(5,*)R(J), Z(J), HD(J), CON(J) 
20 HDL(J)=HD(J) 
***************************************************************************
* IDFF =0 HOMOGENEOUS CASE 
* =1 THERE IS A DIFFERENT REGION. 
* NBE THE FIRST ELEMENT # OF DIFF. REGION 
* NEE THE LAST ELEMENT # OF DIFF. REGION 
* ( THE ELEMENTS # OF DIFF. REGION SHOULD BE IN A ROW.) 
***************************************************************************
READ(5,*)IDFF 
IF(IDFF.EQ.0)GO TO 99 
READ(5,*)NBE, NEE 
IF(ITRSP.EQ.1)READ(5,*)RHD, DOTD, AFLD, AFTD, DKD, ALFD, BETD
-74-
K=1
NODD(1)=NOD(NBE,1)
DO 98 I=NBE,NEE
DO 98 J=1,3
KK=NOD(I,J)
LL=K
DO 97 M=1,LL
97 IF(KK.EQ.NODD(M))GO TO 98
K=K+1
NODD(K)=KK
98 CONTINUE
99 CONTINUE
***************************************************************************
ITM = -1 SATURATION MODEL
= 0 WARRICK MODEL
= 1 VAN GENUCHTEN MODEL
= 2 BROOKS AND COLEY MODEL
= 3 HAVERKAMP MODEL
***************************************************************************
READ(5,*)ITM
IF(ITM.EQ. -1.0R.ITM.EQ.0)READ(5,*)SES,CKS,HES
IF(ITM.EQ.1)READ(5,*)SER,SES,ApH,RmM,Cks,HES
IF(ITM.EQ.2)READ(5,*)SER,SES,RMM,CKS,HES
IF(ITM.EQ.3)READ(5,*)SER,SES,AHP,RMM,CKS,HES
IF(IDFF.EQ.0)GO TO 96
READ(5,*)ITMD
IF(ITMD.EQ. -1.0R.ITMD.EQ.0)READ(5,*)SESD,CKSD,HESD
IF(ITMD.EQ.1)READ(5,*)SERD,SESD,ApHD,RMMD,CKSD,HESD
IF(ITMD.EQ.2)READ(5,*)SERD,SESD,RmmD,CKSD,HESD
IF(ITMD.EQ.3)READ(5,*)SERD,SESD,APHD,RMMD,CKSD,HESD
96 CONTINUE
***************************************************************************
END OF INPUT
***************************************************************************
CALCULATE INITIAL WATER CONTENT,K AND C
CALL TMDP(THL,HD,NOD)
IF(IDFF.EQ.1)CALL TMDPD(THLD,HD)
CALL ABC(NOD)
CALL ITGL(NOD,V)
DTL=DT
TIME=DT
TIMEL=0.
PRINT INITIAL STATE
HOUR=24.*TIME
WRITE(6,411)HOUR
WRITE(6,542)
DO 221 I=1,ND
221 WRITE(6,540)I,R(I),Z(I),THL(I),CON(I)
END
***************************************************************************
BEGINNING OF OUTER LOOP(NEXT TIME STEP)
***************************************************************************
CONTINUE
DO 31 I=1, ND
HDS(I)=HD(I)

BEGINNING OF INNER LOOP (NEW TIME INTERVAL)

DO 30 I=1, ND
HDH(I)=HDS(I)+(HDS(I)-HDL(I))/DTL*DT/2.
HDL(I)=RDS(I)

CONTINUE

BEGINNING OF INNER ITERATION (INCREMENT OF IT)

IT=0

CONTINUE
IF(IT.NE.0)THEN
DO 17 I=1, ND
HDH(I)=(HD(I)+HDL(I))*0.5
ENDIF

CALL TMDP(TH, HDH, NOD)
IF(IDFF.EQ.1)CALL TMDPD(THD, HDH)

CALL SYS(IQ, AL, DT, NOD, HDL, QM, BDC, HDBT, IDFF)
CALL GAUSSE(IFLAG)
IF(IFLAG.NE.0)WRITE(6, 515)
515 FORMAT(' *WARNING* MATRIX IS NOT GOOD. FLOW EQ. ')
ERR=0.
DO 40 I=1, ND
HDLL(I)=HD(I)
HD(I)=ABS(RHS(I))*(-1.)

CHECK CONVERGENCE -------
ERROR=ABS(((HDLL(I)-HD(I))/HD(I))
40 IF(ERROR.GE.ERR)ERR=ERROR
IT=IT+1
IF(IT.GT.IL)THEN
** TOO LARGE TIME INTERVAL, REDUCE IT. **
DT=DT/1.5
IF(DT.LT.DTMIN)THEN
WRITE(6, 400)
400 FORMAT(//' *FATAL* MODEL IS VERY UNSTABLE. '//)
STOP
ENDIF
TIME=TIMEL+DT

RESUME INNER LOOP WITH REDUCED TIME INTERVAL

ENDIF
RESUME INNER ITERATION FOR CONVERGENCE

ENDIF

FLOW EQUATION IS SOLVED, GO AHEAD.

IF(ITRSP.NE.1)GO TO 90

SOLVE TRANSPORT EQUATION.

CALL TRANSP(HD, HDL, TH, THL, NOD, DT, CQ, IQC, 1 BDC, HDH, V, CBT, IDFF, THD, THLD)
CALL GAUSSE(IFLAG)
IF(IFLAG.NE.0)WRITE(6, 514)
514 FORMAT(' *WARNING* MATRIX IS NOT GOOD. TRANSPORT EQ. ')

SUM UP WATER CONTENT AND (WATER CONTENT)X(CONCETRATION) --

SUM1=0.
SUM2=0.
DO 130 I=1, ND
SUM1 = SUM1 + TH(I)
IF (RHS(I).LE.0) RHS(I) = 0.
CON(I) = RHS(I)
SUM2 = SUM2 + CON(I) * TH(I)
HOUR = TIME * 24.
WRITE (6, 239) HOUR, SUM1, SUM2

FORMAT (' AT ', F7.2, ' HOUR', 2X,
1 ' W.C. SUM = ', F7.3, 2X, 'CON. SUM = ', F7.2, '/)

CONTINUE
*--------------- PREPARE NEXT TIME STEP -----------------------------*

TIMEL = TIME
DTL = DT
IF (IT.LT.2) DT = DT * 1.5
IF (DT.GE.DTMAX) DT = DTMAX
DO 911 I = 1, ND
THL(I) = TH(I)
911 HDL(I) = HD(I)
HOUR = TIMEL * 24.
IF (HOUR.LT.TPRNT) GO TO 555
*--------------- PRINT CURRENT RESULT ---------------------------------

IF (IPNT.GT.IPRIN) GO TO 555
TPRNT = PTIME(IPNT)
IPNT = IPNT + 1
WRITE (6, 411) HOUR

411 FORMAT (' AT THE TIME OF', F10.3, ' HOUR')
WRITE (6, 542)
DO 122 I = 1, ND
WRITE (6, 540) I, R(I), Z(I), TH(I), CON(I)
122 CONTINUE
542 FORMAT (///5X, 'NODE', T15, ' R AND Z', T30, 'WATER CONTENT',
4 T45, 'CONCENTRATION', ')
DO 541 I = 1, NDD
NN = NODD(I)
WRITE (6, 540) NN, R(NN), Z(NN), THD(I), CON(NN)
541 CONTINUE
540 FORMAT (5X, I5, 2F7.1, 2F15.3)
543 CONTINUE
502 FORMAT (F8.2, T16, ':', 2F10.3, 2F10.1)
WRITE (6, 401) IT
401 FORMAT (///5X, ' TIMES ITERATED')
555 CONTINUE

*------- CHECK IF IT IS THE TIME TO CHANGE BOUNDARY CONDITION. -----------*

IF (IPPP.EQ.1) THEN
DT = DTLL
IQIN = IQIN + 1
IF (IQIN.GT.NS) STOP
IQ = IBC(IQIN)
QM = Q(IQIN)
IF (ITRSP.EQ.1) THEN
CQ = CI(IQIN)
IQC = IBCC(IQIN)
ENDIF
CKTIME = TB(IQIN) / 24.
WRITE (6, 277) IQ, QM, TB(IQIN), IQC, CQ
ENDIF
IPPP = 0
TIME = TIME + DT
IF (TIME.GE.CKTIME) THEN
DTLL = DT

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TIME=CKTIME
DT=CKTIME-TIMEL
IPPP=1
ENDIF

277 FORMAT(//' IQ=' , I3 , ' QO=' , F7.2 , ' UP TO ' , F7.2 , ' HOUR' /
1     // ' IQC=' , I3 , ' CQ=' , F7.2 , '/)
***************************************************************************
* GO BACK FOR NEXT TIME STEP. -----------------------------------------*
***************************************************************************
GO TO 101
END
***************************************************************************
***************************************************************************
SUBROUTINE ABC(NOD)
PARAMETER(NE=20, ND=22, IHO=2, NDD=1)
COMMON/RZA/R(ND), Z(ND), A(NE, 3), B(NE, 3), C(NE, 3), AR(NE), ISF(IHO)
DIMENSION NOD(NE, 3)

DO 10 I=1, NE
DO 20 J=1, 3
K=NOD(I, J)
ZE(J)=Z(K)
R2(J)=R(K)
20 CONTINUE
A(I,1)=R2(2)*ZE(3)-R2(3)*ZE(2)
A(I,2)=R2(3)*ZE(1)-R2(1)*ZE(3)
A(I,3)=R2(1)*ZE(2)-R2(2)*ZE(1)
B(I,1)=ZE(2)-ZE(3)
B(I,2)=ZE(3)-ZE(1)
B(I,3)=ZE(1)-ZE(2)
C(I,1)=R2(3)-R2(2)
C(I,2)=R2(1)-R2(3)
C(I,3)=R2(2)-R2(1)
AR(I)=(A(I,1)+A(I, 2)+A(I, 3))/2.
10 CONTINUE
RETURN
END
***************************************************************************
***************************************************************************
SUBROUTINE ITGL(NOD, V)
PARAMETER(NE=20, ND=22, IHO=2, NDD=1)
COMMON/RZA/R(ND), Z(ND), A(NE, 3), B(NE, 3), C(NE, 3), AR(NE), ISF(IHO)
COMMON/CNEE/CNEE(NE, 10)

DO 11 I=1, NE
V(I)=0.
R1=10.E10
R3=0.
DO 10 J=1, 3
IF(R1.GE.R(NOD(I, J)))THEN
R1=R(NOD(I, J))
ILG=J
ENDIF
10 IF(R3.LE.R(NOD(I, J)))THEN

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R3=\text{R}(\text{NOD}(I,J))
\text{ISM}=J
\text{ENDIF}
10 \text{CONTINUE}
\text{Z1}=\text{Z}(\text{NOD}(I,\text{ILG}))
\text{Z3}=\text{Z}(\text{NOD}(I,\text{ISH}))
\text{IM}=6-\text{ISH}-\text{ILG}
\text{R2}=\text{R}(\text{NOD}(I,\text{IM}))
\text{Z2}=\text{Z}(\text{NOD}(I,\text{IM}))
\text{DR}=\frac{(\text{R3}-\text{R1})}{10.0000000001}
\text{DZ}=\text{DR}
\text{DO 12 } J=1,9
\text{CNEE}(I,J)=0.
\text{CNE}(I,J)=0.
\text{CNEE}(I,10)=0.
\text{DO 13 } RC=\text{R1},\text{R3},\text{DR}
\text{IF}(RC.<.\text{R2}) \text{THEN}
\text{Z11}=\frac{(\text{Z2}-\text{Z1})}{(\text{R2}-\text{R1})}*(\text{RC}-\text{R1})+\text{Z1}
\text{ELSE}
\text{Z11}=\frac{(\text{Z2}-\text{Z3})}{(\text{R2}-\text{R3})}*(\text{RC}-\text{R3})+\text{Z3}
\text{ENDIF}
\text{Z22}=\frac{(\text{Z3}-\text{Z1})}{(\text{R3}-\text{R1})}*(\text{RC}-\text{R1})+\text{Z1}
\text{IF}(\text{Z11}.\geq.\text{Z22}) \text{THEN}
\text{BUFF}=\text{Z11}
\text{Z11}=\text{Z22}
\text{Z22}=\text{BUFF}
\text{ENDIF}
\text{DO 13 } ZC=\text{Z11},\text{Z22},\text{DZ}
\text{DV}=2*P*RC*DR*DZ
\text{V}(I)=\text{V}(I)+\text{DV}
\text{CN1}=\frac{(A(I,1)+B(I,1)*RC+C(I,1)*ZC)}{2./\text{AR}(I)}
\text{CN2}=\frac{(A(I,2)+B(I,2)*RC+C(I,2)*ZC)}{2./\text{AR}(I)}
\text{CN3}=\frac{(A(I,3)+B(I,3)*RC+C(I,3)*ZC)}{2./\text{AR}(I)}
\text{CNE}(I,1)=\text{CNE}(I,1)+\text{DV}*\text{CN1}**2
\text{CNE}(I,2)=\text{CNE}(I,2)+\text{DV}*\text{CN1}*\text{CN2}
\text{CNE}(I,3)=\text{CNE}(I,3)+\text{DV}*\text{CN1}*\text{CN3}
\text{CNE}(I,4)=\text{CNE}(I,4)+\text{DV}*\text{CN2}**2
\text{CNE}(I,5)=\text{CNE}(I,5)+\text{DV}*\text{CN2}*\text{CN3}
\text{CNE}(I,6)=\text{CNE}(I,6)+\text{DV}*\text{CN3}**2
\text{CNE}(I,7)=\text{CNE}(I,7)+\text{DV}*\text{CN1}
\text{CNE}(I,8)=\text{CNE}(I,8)+\text{DV}*\text{CN2}
\text{CNE}(I,9)=\text{CNE}(I,9)+\text{DV}*\text{CN3}
\text{CNEE}(I,1)=\text{CNEE}(I,1)+\text{DV}*\text{CN1}**3
\text{CNEE}(I,2)=\text{CNEE}(I,2)+\text{DV}*\text{CN1}**2*\text{CN2}
\text{CNEE}(I,3)=\text{CNEE}(I,3)+\text{DV}*\text{CN1}**2*\text{CN3}
\text{CNEE}(I,4)=\text{CNEE}(I,4)+\text{DV}*\text{CN1}**2*\text{CN2}
\text{CNEE}(I,5)=\text{CNEE}(I,5)+\text{DV}*\text{CN1}**2*\text{CN3}
\text{CNEE}(I,6)=\text{CNEE}(I,6)+\text{DV}*\text{CN1}*\text{CN2}**2
\text{CNEE}(I,7)=\text{CNEE}(I,7)+\text{DV}*\text{CN1}*\text{CN3}**2
\text{CNEE}(I,8)=\text{CNEE}(I,8)+\text{DV}*\text{CN2}**3
\text{CNEE}(I,9)=\text{CNEE}(I,9)+\text{DV}*\text{CN2}**2*\text{CN3}
\text{CNEE}(I,10)=\text{CNEE}(I,10)+\text{DV}*\text{CN3}**3
\text{CNEE}(I,11)=\text{CNEE}(I,11)+\text{DV}*\text{CN2}**2*\text{CN3}
\text{CNEE}(I,12)=\text{CNEE}(I,12)+\text{DV}*\text{CN3}**2
11 \text{CONTINUE}
\text{RETURN}
\text{END}
SUBROUTINE TMDT (TH, HD, NOD)
 PARAMETER (NE=20, ND=22, IH0=2, NDD=1)
 COMMON/CCK/CK(ND), CC(ND)
 COMMON/TMD/SER, SES, HES, CKS, RMM, APH, ITM
 DIMENSION TH(ND), HD(ND), NOD(NE,3)
   DO 10 I=1, ND
      ITM1=ITM+2
      GO TO (100, 200, 300, 400, 500) ITM1

100  TH(I)=SES
     CC(I)=0.
     CK(I)=CKS
     HD(I)=HES
     GO TO 10

200  CONTINUE
   PH=ABS(HD(I))
   IF(PH.LT.HES) GO TO 100
   IF(PH.GE.29.484) THEN
      TH(I)=.6829 -.09524*LOG(PH)
      CC(I)=.09524/PH
      CK(I)=19.34E5/PH**3.4095
   ELSE
      TH(I)=.4531 -.02732*LOG(PH)
      CC(I)=.02732/PH
      CK(I)=516.8/PH**.97814
   ENDIF
   GO TO 10

300  CONTINUE
   PH=ABS(HD(I))
   IF(PH.LE.HES) GO TO 100
   OMN=1.-1./RMM
   AHN=(APH*PH)**RMM
   AHN1=(1+AHN)**(-OMN)
   TH(I)=SER+(SES-SER)*AHN1
   CC(I)=OMN*(SES-SER)*RMM*AHN/PH*(AHN1/(1+AHN))
   BIGT=(TH(I)-SER)/(SES-SER)
   CK(I)=CKS*SQRT(BIGT)*(1-(1.-BIGT**(1./OMN))**OMN)**2
   GO TO 10

400  CONTINUE
   PH=ABS(HD(I))
   IF(PH.LE.HES) GO TO 100
   TH(I)=SER+(SES-SER)*(HES/PH)**RMM
   CC(I)=(SES-SER)**(HES)**RMM*PH**(RMM+1)
   CK(I)=CKS*((TH(I)-SER)/(SES-SER))**RMM
   GO TO 10

500  CONTINUE
   PH=ABS(HD(I))
   TH(I)=SER+APH*(SES-SER)/(APH+PH**RMM)
   CC(I)=RMM*APH*(SES-SER)*PH*(RMM-1)/(APH+PH**RMM)**2
   CK(I)=CKS*HES/(HES+PH**RMM)
   GO TO 10

10  CONTINUE
   RETURN
END

******************************************************************************

SUBROUTINE TMDPD(TH,HD)
PARAMETER(NE=20,ND=22,IHO=2,NDD=1)
COMMON/CCKD/CK(NDD),CC(NDD),NODD(NDD),NBE,NEE
COMMON/TMDD/SER,SES,HES,CKS,RMM,APH,ITM
DIMENSION TH(NDD),HD(ND)
DO 10 I=1,NDD
II=NODD(I)
ITM1=ITM+2
GO TO (100,200,300,400,500)ITM1

*------------------------- SATURET MODEL -------------------------------*
100 TH(I)=SES
CC(I)=0.
CK(I)=CKS
HD(II)=HES
GO TO 10

*------------------------- WARRICK MODEL -------------------------------*
200 CONTINUE
PH=ABS(HD(NODD(I)))
IF(PH.LT.HES)GO TO 100
 IF(PH.GE.29.484)THEN
   TH(I)=.6829-.09524*LOG(PH)
   CC(I)=.09524/PH
   CK(I)=19.34E5/PH**3.4095
 ELSE
   TH(I)=.4531-.02732*LOG(PH)
   CC(I)=.02732/PH
   CK(I)=516.8/PH**.97814
ENDIF
GO TO 10

*------------------------- VAN GENUCHTEN MODEL ---------------------------*
300 CONTINUE
PH=ABS(HD(NODD(I)))
IF(PH.LE.HES)GO TO 100
 OMN=1.-1./RMM
 AHN=(APH*PH)**RMM
 AHN1=(1+AHN)**(-OMN)
 TH(I)=SER+(SES-SER)*AHN1
 CC(I)=OMN*(SES-SER)*RMM*AHN/PH*AHN1/(1+AHN)
 BIGT=(TH(I)-SER)/(SES-SER)
 CK(I)=CKS*SQT(BIGT)*(1-(1.-BIGT**(1./OMN))**OMN)**2
GO TO 10

*------------------------- BROOKS AND COLEY MODEL ------------------------*
400 CONTINUE
PH=ABS(HD(NODD(I)))
IF(PH.LE.HES)GO TO 100
 TH(I)=SER+(SES-SER)*(HES/PH)**RMM
 CC(I)=(SES-SER)*(HES)**RMM*RMM/PH**(RMM+1)
 CK(I)=CKS*((TH(I)-SER)/(SES-SER))**RMM
GO TO 10

*------------------------- HAUERKAMP MODEL -------------------------------*
500 CONTINUE
PH=ABS(HD(NODD(I)))
 TH(I)=SER+APH*(SES-SER)/(APH+PH**RMM)
 CC(I)=RMM*APH*(SES-SER)*PH*(RMM-1)/(APH+PH**RMM)**2
 CK(I)=CKS*HES/(HES+PH**RMM)

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SUBROUTINE SYS(IQ,AL,DT,NOD,HDL,QM,BDC,HDBT,IDFF)
  PARAMETER(NE=20,ND=22,IHO=2,NDD=1)
  REAL LHS
  COMMON/RZA/R(ND),Z(ND),A(NE,3),B(NE,3),C(NE,3),AR(NE),ISF(IHO)
  COMMON/CCKD/CKD(NDD),CCD(NDD),NODD(NDD),NBE,NEE
  COMMON/EEE/CNE(NE,9),CSE(NE,3,3)
  COMMON/CCK/CK (ND) , CC (ND)
  COMMON/LR/LHS(ND,ND),RHS(ND)
  DIMENSION NOD(NE,3),HDL(ND),BDC(IHO),CM(ND),CS(ND,ND),CP(ND)
  DO 9 I=1,ND
    CP(I)=0.
    DO 9 J=1,ND
      CS(I,J)=0.
    9 CONTINUE
  DO 10 I=1,NE
    I1=NOD(I,1)
    I2=NOD(I,2)
    I3=NOD(I,3)
    IF(IDFF.EQ.0)GO TO 19
    IF(I.LT.NBE.OR.I.GT.NEE)GO TO 19
    DO 18 K=1,NDD
      IF(I1.EQ.NODD(K)) 31-K
      IF(I2.EQ.NODD(K))J2=K
      IF(I3.EQ.NODD(K))33=K
    18 CONTINUE
    C1=CCD(J1)
    C2=CCD(J2)
    C3=CCD(J3)
    CK1=CKD(J1)
    CK2=CKD(J2)
    CK3=CKD(J3)
  19 CONTINUE
  DO 21 I=1,NE
    I1=NOD(I,1)
    I2=NOD(I,2)
    I3=NOD(I,3)
    CM(I)=0.
    CM(I1)=CM(I1)+C1*CNE(I,1)+C2*CNE(I,2)+C3*CNE(I,3)
    CM(I2)=CM(I2)+C1*CNE(I,2)+C2*CNE(I,4)+C3*CNE(I,5)
    CM(I3)=CM(I3)+C1*CNE(I,3)+C2*CNE(I,5)+C3*CNE(I,6)
    CSK=CK1*CNE(I,7)+CK2*CNE(I,8)+CK3*CNE(I,9)
    CS(I1,I1)=CS(I1,I1)+CSE(I,1,1)*CSK
    CS(I2,I2)=CS(I2,I2)+CSE(I,1,2)*CSK
    CS(I3,I3)=CS(I3,I3)+CSE(I,1,3)*CSK
    CS(I2,I1)=CS(I1,I2)+CSE(I,2,1)*CSK
    CS(I1,I2)=CS(I2,I1)
  21 CONTINUE
  * (M)
  CM(I1)=CM(I1)+C1*CNE(I,1)+C2*CNE(I,2)+C3*CNE(I,3)
  CM(I2)=CM(I2)+C1*CNE(I,2)+C2*CNE(I,4)+C3*CNE(I,5)
  CM(I3)=CM(I3)+C1*CNE(I,3)+C2*CNE(I,5)+C3*CNE(I,6)
  * (S)
  CSK=CK1*CNE(I,7)+CK2*CNE(I,8)+CK3*CNE(I,9)
  CS(I1,I1)=CS(I1,I1)+CSE(I,1,1)*CSK
  CS(I2,I2)=CS(I2,I2)+CSE(I,1,2)*CSK
  CS(I3,I3)=CS(I3,I3)+CSE(I,1,3)*CSK
  CS(I2,I1)=CS(I1,I2)+CSE(I,2,1)*CSK
  CS(I1,I2)=CS(I2,I1)
** (P)

CPK=CSK/2./AR(I)
CP((I))=CP((I))+CPK*C(I,1)
CP((I))=CP((I))+CPK*C(I,2)
CP((I))=CP((I))+CPK*C(I,3)
10 CONTINUE

* RHS = SOMETHING - (F)
DO 14 I=1,ND
RHS(I)=CP(I)

*-------- constamt water flux BC at the top
IF(I.LE.IHO.AND.IQ.EQ.1)RHS(I)=RHS(I)-CP(I)*QM/CK(I)

*-------- NEXT TWO LINES FOR TOP BC OF TRANSPORT EQ.
IF(I.LE.IHO.AND.IQ.EQ.1)BDC(I)=ABS(CP(I)*QM/CK(I))
IF(I.LE.IHO.AND.IQ.EQ.0)BDC(I)=ABS(CP(I))

*-------- MAKE GLOBAL MATRIX
DO 141 J=1,ND
RHS(I)=RHS(I)-CS(I,J)*(1.-AL)*HDL(J)
141 LHS(I,J)=AL*CS(I,J)
RHS(I)=RHS(I)+CM(I)/DT*HDL(I)
14 LHS(I,I)=LHS(I,I)+CM(I)/DT

*-------- constant head BC at bottom and/or top
DO 15 J=1,IHO
DO 16 I=1,ND
IF(IQ.EQ.0)RHS(J)=QM
RHS(ND-J+1)=HDBT
IF(IQ.EQ.0)LHS(J,J)=1.
15 LHS(ND-J+1,ND-J+1)=1.
RETURN
END

**************************************************************************
*    **************************************************************************
SUBROUTINE TRANSP(HD,HDL,THH,THL,NDL,DTL,CQ,CON,IQC,BDC,HDH,V,CBT,IDP,THHD,THLD)
PARAMETER(NE=20,ND=22,IHO=2,NDD=1)
INTEGER E
REAL LHS
EXTERNAL CZ
COMMON/RZA/R(ND),Z(ND),A(NE,3),B(NE,3),C(NE,3),AR(NE),ISF(IHO)
COMMON/LR/LHS(ND,ND),RHS(ND)
COMMON/CK/CCK(ND),CC(ND)
COMMON/CKD/CCKD(NDD),CCD(NDD),NODD(NDD),NBE,NEE
COMMON/OPTION/AAM,BBM,CCM,DDM,IWRI
COMMON/EEE/CNE(NE,9),CSE(NE,3,3)
DIMENSION DM(ND),DT(ND,ND),V(NE),DRR(ND),DZZ(ND),DRZ(ND),
1 DRRD(ND),DZZD(ND),DRZD(ND),DADD(ND,ND),1
1 DB(IHO),BDC(IHO),CON(IHO),R1(3),
2 TH(ND),THL(ND),HD(ND),HDL(ND),N(3),CN(3,3),
3 NOD(NE,3),HDH(ND),THH(ND),DA(ND,ND),DDB(ND,ND),DF(ND,ND)
1 ,DRD(ND),DZD(ND),DXD(ND),DRDD(NDD),DZDD(NDD),DXDD(NDD)
1 ,DRE(3),DZE(3),DZE(3),DRDE(3),DZDE(3),DXDE(3)
1 ,THD(NDD),THLD(NDD),THHD(NDD),THE(3),THLE(3),THHE(3)
1 ,CKE(3)

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COMMON/TRA/RH,DK,DOT,AFL,AFT,GAM,ALF,BET
COMMON/TRA/RH,DK,DOT,AFL,AFT,GAM,ALF,BET

DO 10 I=1,ND
   HDH(I)=(HD(I)+HDL(I))/2.
   DM(I)=0.
   RHS(I)=0.
   IF(I.LE.IHO)DB(I)=0.
DO 10 J=1,ND
   LHS(I,J)=0.
   DA(I,J)=0.
   DAD(I,J)=0.
   DDB(I,J)=0.
   DF(I,J)=0.
10   DT(I,J)=0.

*------- CALCULATE WATER CONTENT, K AND C -----------------------------*
   CALL TMDP(TH,HD,NOD)
   CALL TMDP(THH,HDH,NOD)
   IF(IDFF.EQ.1)THEN
      CALL TMDPD(THD,HD)
      CALL TMDPD(THHD,HDH)
   ENDIF

*------- CALCULATE DISPERSION COEFFICIENT TENSOR -----------------------*
   CALL QQ(HDH,NOD,V,THH,DRR,DRZ,DZZ,DRRD,DRZD,DZZD,
   THHD,DRD,DXD,DZD,DRDD,DXDD,DZDD,IDFF)
   DO 12 E=1,NE
      I1=NOD(E,1)
      I2=NOD(E,2)
      I3=NOD(E,3)
      CN(1,1)=CNE(E,1)
      CN(1,2)=CNE(E,2)
      CN(1,3)=CNE(E,3)
      CN(2,2)=CNE(E,4)
      CN(2,3)=CNE(E,5)
      CN(3,3)=CNE(E,6)
      CN(2,1)=CN(1,2)
      CN(3,1)=CN(1,3)
      CN(3,2)=CN(2,3)
   IF(IDFF.EQ.0)GO TO 19
   IF(I.LT.NBE.OR.I.GT.NEE)GO TO 19
   DO 18 R=1,NDD
      IF(I1.EQ.NODD(R))N(1)=K
      IF(I2.EQ.NODD(K))N(2)=K
      IF(I3.EQ.NODD(K))N(3)=K
   18  CONTINUE
   RHE=RHD
   DKE=DKD
   ALFE=ALFD
   BETE=BETD
   DO 22 L=1,3
      THE(L)=THD(N(L))
      THHE(L)=THHD(N(L))
      THLE(L)=THLD(N(L))
      DRE(L)=DRD(N(L))
      DXE(L)=DXD(N(L))
      DZE(L)=DZD(N(L))
      DRDE(L)=DRDD(N(L))
      DXDE(L)=DXDD(N(L))
      DZDE(L)=DZDD(N(L))
      CKE(L)=CKD(N(I))
   22  CONTINUE
GO TO 21
19 CONTINUE
DO 23 L=1,3
23 N(L)=NOD(E,L)
RHE=RH
DKE=DK
ALFE=ALF
BETE=BET
DO 24 L=1,3
THE(L)=TH(N(L))
THHE(L)=THH(N(L))
THLE(L)=THL(N(L))
DRE(L)=DRR(N(L))
DXE(L)=DRZ(N(L))
DZE(L)=DZZ(N(L))
DRDE(L)=DRRD(N(L))
DXDE(L)=DRZD(N(L))
DZDE(L)=DZZD(N(L))
CKE(L)=CK(N(L))
24 CONTINUE
21 CONTINUE
DO 15 II=1,3
N(II)=NOD(E,II)
*----------- CALCULATE RETARDATION FACTOR -------------------------------*
R1(II)=1.+RHE*DKE/THHE(II)
15 CONTINUE
DO 12 J=1,3
NJ=N(J)
B1=C(E,J)/2./AR(E)
DO 17 M=1,3
NM=N(M)
DM(NJ)=DM(NJ)+THHE(M)*R1(M)*CN(J,M)
B1=B1+ABS(HDH(NM))*CSE(E,J,M)
17 DO 12 I=1,3
NI=N(I)
DO 12 L=1,3
DA(NJ,NI)=DA(NJ,NI)+THHE(L)*((DRE(L)*B(E,I)+DXE(L))
1 *C(E,I))*B(E,J)+(DZE(L)*C(E,I)+DXE(L)*
1 B(E,I))*C(E,J)+((THLE(L)-THE(L))/DTL+
1 ALFE+RHE*BETE*DKE)*CZ(E,L,I,J)
12 CONTINUE
IF(IQC.EQ.0)GO TO 113
*------------- TOP BC : CONSTANT FLUX -----------------------------------*
DO 144 I=1,IHO
144 RHS(I)=BDC(I)*CQ
113 CONTINUE
*--------------- GENERATE GLOBAL MATRIX -------------------------------*
DO 20 I=1,ND
LHS(I,I)=DM(I)/DTL
DO 30 J=1,ND
LT(I,J)=DA(I,J)+DDB(I,J)+DF(I,J)-DAD(I,J)
LHS(I,J)=LHS(I,J)-LT(I,J)/2.
RHS(I)=RHS(I)+(LHS(I,J)+LT(I,J)+DAD(I,J))*CON(J)
30 CONTINUE
**BC : CONSTANT CONCENTRATION AT THE TOP AND BOTTOM**

DO 51 J=1,IHO
DO 16 I=1,ND
IF(IQC.EQ.0)LHS(J,I)=0.
16     LHS(ND-J+1,I)=0.
IF(IQC.EQ.0)RHS(J)=CQ
RHS(ND-J+1)=CBT
IF(IQC.EQ.0)LHS(J,J)=1.
51     LHS(ND-J+1,ND-J+1)=1.
RETURN
END

*****************************************************************************
* * * *
*****************************************************************************
SUBROUTINE QQ(HDH,NOD,V,THH,DRR,DRZ,DZZ,DRRD,DRZD,DZZD,
1 THHD,DRD,DXD,DZD,DRDD,DXDD,DZDD,IDFF)
PARAMETER(NE=20,ND=22,IHO=2,NDD=1)
COMMON/TRA/RH,DK,DOT,AFL,AFT,GAM,ALF,BET
COMMON/TRAD/RHD,DKD,DOTD,AFLD,AFTD,ALFD,BETD
COMMON/CCKD/CKD(NDD),CCD(NDD),NODD(NDD),NBE,NEE
COMMON/OPTION/AAM,BBM,CCM,DDM,IWRI
COMMON/CCK/CK(ND),CC(ND)
COMMON/EEE/CNE(NE,9),CSE(NE,3,3)
COMMON/RZA/R(ND),Z(ND),A(NE,3),B(NE,3),C(NE,3),AR(NE),ISF(IHO)
INTEGER E
DIMENSION QR(ND),QZ(ND),QA(ND),HDH(ND),NOD(NE,3),V(NE)
1 ,THH(ND),DRR(ND),DZZ(ND),DRZ(ND)
2 ,DRRD(ND),DRZD(ND),DZZD(ND)
1 ,THHD(NDD),DRD(NDD),DZD(NDD),DXD(NDD),CKE(3)
2 ,DRDD(NDD),DXDD(NDD),DZDD(NDD)
DO 10 I=1,ND
QR(I)=0.
QZ(I)=0.
10 CONTINUE
**------------------- CALCULATE RADIAL AND AXIAL FLUX --------------------**
DO 20 E=1,NE
BUFF=0.
IF(IDFF.EQ.0)GO TO 13
IF(E.LT.NBE.OR.E.GT.NEE)GO TO 13
DO 18 K=1,NDD
IF(NOD(E,1).EQ.NODD(K))CKE(1)=CKD(K)
IF(NOD(E,2).EQ.NODD(K))CKE(2)=CKD(K)
IF(NOD(E,3).EQ.NODD(K))CKE(3)=CKD(K)
18 CONTINUE
GO TO 14
13 CONTINUE
DO 15 L=1,3
CKE(L)=CK(NOD(E,L))
14 CONTINUE
DO 30 L=1,3
NL=NOD(E,L)
30     BUFF=BUFF+CKE(L)*CNE(E,6+L)
BUFF=BUFF/V(E)/AR(E)/2
DO 40 J=1,3
NJ=NOD(E,J)
QZ(NJ)=QZ(NJ)+B(E,J)*BUFF*HDH(NJ)
40     QZ(NJ)=QZ(NJ)+(C(E,J)*HDH(NJ)+2.*AR(E))*BUFF
20 CONTINUE
*--------- CALCULATE DISPERSION TENSOR IN NORMAL REGION ---------------*
DO 35 I=1,ND
QA(I)=SQRT(QR(I)**2+QZ(I)**2)
IF(QA(I).EQ.0.)THEN
  DRR(I)=DOT
  DZZ(I)=DOT
  DRZ(I)=0.
GO TO 35
ENDIF
DRR(I)=DOT+(AFL*QR(I)**2+AFT*QZ(I)**2)/QA(I)/THH(I)
DZZ(I)=DOT+(AFL*QZ(I)**2+AFT*QR(I)**2)/QA(I)/THH(I)
DRZ(I)=(AFL-AFT)*QR(I)*QZ(I)/QA(I)/THH(I)
DRRD(I)=(QR(I)/THH(I))**2/6.
DZZD(I)=(QZ(I)/THH(I))**2/6.
DRZD(I)=(QR(I)*QZ(I)/QA(I)/THH(I))**2/6.
35 CONTINUE

*--------- CALCULATE DISPERSION TENSOR IN DIFFERENT REGION ---------------*
DO 36 I=1,NDD
II=NODD(I)
IF(QA(II).EQ.0.)THEN
  DRD(I)=DOTD
  DZD(I)=DOTD
  DXD(I)=0.
GO TO 36
ENDIF
DRD(I)=DOTD+(AFLD*QR(II)**2+AFTD*QZ(II)**2)/QA(II)/THHD(I)
DZD(I)=DOTD+(AFLD*QZ(II)**2+AFTD*QR(II)**2)/QA(II)/THHD(I)
DXD(I)=(AFLD-AFTD)*QR(II)*QZ(II)/QA(II)/THHD(I)
DRDD(I)=(QR(II)/THHD(I))**2/6.
DZDD(I)=(QZ(II)/THHD(I))**2/6.
DXDD(I)=(QR(II)*QZ(II)/QA(II)/THHD(I))**2/6.
36 CONTINUE
RETURN
END

FUNCTION CZ(IP, I, J, K)
  PARAMETER (NE=20, ND=22, IHO=2, NDD=1)
  COMMON/CNEE/CNEE(NE,10)
  DIMENSION IK(3)
  IK(1)=I
  IK(2)=J
  IK(3)=K
  DO 10 M=2,3
    IF(IK(1).GE.IK(J))THEN
      IB=IK(1)
      IK(1)=IK(M)
      IK(M)=IB
    ENDIF
  10  CONTINUE
  IF(IK(2).GE.IK(3))THEN
    IB=IK(2)
    IK(2)=IK(3)
    IK(3)=IB
  ENDIF
  L=IK(1)
  M=IK(2)
N=IK(3)
IF(L.EQ.1.AND.M.EQ.1.AND.N.EQ.1)CZ=CNEE(IP,1)
IF(L.EQ.1.AND.M.EQ.1.AND.N.EQ.2)CZ=CNEE(IP,2)
IF(L.EQ.1.AND.M.EQ.1.AND.N.EQ.3)CZ=CNEE(IP,3)
IF(L.EQ.1.AND.M.EQ.2.AND.N.EQ.2)CZ=CNEE(IP,4)
IF(L.EQ.1.AND.M.EQ.2.AND.N.EQ.3)CZ=CNEE(IP,5)
IF(L.EQ.1.AND.M.EQ.3.AND.N.EQ.3)CZ=CNEE(IP,6)
IF(L.EQ.2.AND.M.EQ.2.AND.N.EQ.2)CZ=CNEE(IP,7)
IF(L.EQ.2.AND.M.EQ.2.AND.N.EQ.3)CZ=CNEE(IP,8)
IF(L.EQ.2.AND.M.EQ.3.AND.N.EQ.3)CZ=CNEE(IP,9)
IF(L.EQ.3.AND.M.EQ.3.AND.N.EQ.3)CZ=CNEE(IP,10)

RETURN
END

***************************************************************************
*--------------------------------------------------------------------------*
**SUBROUTINE GAUSSE(IFLAG)**
*--------------------------------------------------------------------------*
REAL LHS
PARAMETER(NE=20,ND=22,IHO=2,NDD=1)
COMMON/LR/LHS(ND,ND),RHS(ND)

N=ND
IFLAG=0
DO 100 I=1,N
J=I+1
10 IF(LHS(I,I).EQ.0.)THEN
IFLAG=IFLAG+1
IF(J.LT.N)THEN
B=RHS(J)
RHS(J)=RHS(I)
RHS(I)=B
DO 200 K=1,N
A=LHS(J,K)
LHS(J,K)=LHS(I,K)
LHS(I,K)=A
200 CONTINUE
ELSE
IFLAG=100
RETURN
ENDIF
J=J+1
GO TO 10
ENDIF
AI=LHS(I,I)
DO 50 II=1,N
LHS(I,II)=LHS(I,II)/AI
RHS(I)=RHS(I)/AI
DO 300 K=1,N
IF(K.EQ.I)GO TO 300
AK=LHS(K,I)
RHS(K)=RHS(K)-RHS(I)*AK
DO 400 L=1,N
LHS(K,L)=LHS(K,L)-LHS(I,L)*AK
400 CONTINUE
300 CONTINUE
100 CONTINUE
RETURN
END