GEORGIA INSTITUTE OF TECHNOLOGY — OFFICE OF CONTRACT ADMINISTRATION

PROJECT ADMINISTRATION DATA SHEET

[x] ORIGINAL [ ] REVISION NO. ______

Project No. E-25-606 GTRI/~~GIT~~ DATE 8 / 3 /84

Project Director: G. G. Eichholz School/~~Lab~~ ME-NE/HP

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: This Change / Total to Date

Estimated: $ ______ $ 49,957

Funded: $ ______ $ 49,957

Cost Sharing Amount: $ n/a Cost Sharing No: ______

Title: Transport Model for Radionuclide Migration in the SRP Lysimeters

ADMINISTRATIVE DATA

OCA Contact Dennis Farmer x4820

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

(or) Company/Industrial Proprietary: 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:

Sponsor I.D. #02.240.004.84.004

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FORM OCA 4:383

GEORGIA INSTITUTE OF TECHNOLOGY OFFICE OF CONTRACT ADMINISTRATION

SPONSORED PROJECT TERMINATION/CLOSEOUT SHEET

Date August 1, 1985

Project No. E-25-606 School/Lab ME

Includes Subproject No.(s)

Project Director(s) G.G. Eichholz GTRC / GIT

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
- [X] Final Invoice or Final Fiscal Report
- [X] Closing Documents
- [X] Final Report of Inventions
- [ ] Govt. Property Inventory & Related Certificate
- [ ] Classified Material Certificate
- [ ] Other

Continues Project No. Continued by Project No.

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FORM OCA 69.285

57 347 170

Georgia Institute of Technology

A UNIT OF THE UNIVERSITY SYSTEM OF GEORGIA

SCHOOL OF MECHANICAL ENGINEERING

August 9, 1984

Please reply to:

NUCLEAR ENGINEERING AND
HEALTH PHYSICS PROGRAM
CHERRY EMERSON BUILDING
GEORGIA INST. OF TECH.
ATLANTA, GEORGIA 30332 U.S.A.

Dr. S. B. Oblath
Waste Disposal Technology Division
Savannah River Laboratory
E.I. Du Pont de Nemours & Co.
Aiken, SC 29808

Monthly 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 mean time 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

GGE/swm

cc: O. H. Rodgers

Georgia Institute of Technology
A UNIT OF THE UNIVERSITY SYSTEM OF GEORGIA
SCHOOL OF MECHANICAL ENGINEERING

September 7, 1984

Please reply to:

NUCLEAR ENGINEERING AND
HEALTH PHYSICS PROGRAM
CHERRY EMERSON BUILDING
GEORGIA INST. OF TECH.
ATLANTA, GEORGIA 30332 U.S.A.

Dr. S.B. Oblath
Waste Disposal Technology Division
Savannah River Laboratory
E.I. Du Pont de Nemours & Co.
Aiken, SC 29808

Monthly Progress Report - Project E-25-606 (P.O. AX0654763)

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)

Georgia Institute of Technology
A UNIT OF THE UNIVERSITY SYSTEM OF GEORGIA
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October 10, 1984

Please reply to:

NUCLEAR ENGINEERING AND
HEALTH PHYSICS PROGRAM
CHERRY EMERSON BUILDING
GEORGIA INST. OF TECH.
ATLANTA, GEORGIA 30332 U.S.A.

Dr. S.B. Oblath
Waste Disposal Technology Division
Savannah River Laboratory
E.I. Du Pont de Nemours & Co.
Aiken, SC 29808

Monthly Progress Report - Project E-25-606 (P.O. AX0654763)

Dear Dr. Oblath:

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)

Telephone. 404-894-3720 Telex: 542507 GTRIOCAATL Fax: 404-894-3120 (Verify: 404-894-4850)

Georgia Institute of Technology

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November 8, 1984

Please reply to:

NUCLEAR ENGINEERING AND
HEALTH PHYSICS PROGRAM
CHERRY EMERSON BUILDING
GEORGIA INST. OF TECH.
ATLANTA, GEORGIA 30332 U.S.A.

Dr. S. B. Oblath
Waste Disposal Technology Division
Savannah River Laboratory
E.I. Du Pont de Nemours & Co.
Aiken, SC 29808

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

CGE/swm
cc: O.H. Rodgers (OCA)

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ATLANTA, GEORGIA 30332 U.S.A.

December 11, 1984

Dr. S.B. Oblath
Waste Disposal Technology Division
Savannah River Laboratory
E.I. Du Pont de Nemours & Co.
Aiken, SC 29808

Monthly Progress Report - Project E-25-606 (P.O. AX0654763)

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 G T 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

Georgia Institute of Technology
A UNIT OF THE UNIVERSITY SYSTEM OF GEORGIA
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February 7, 1985

Please reply to:

NUCLEAR ENGINEERING AND
HEALTH PHYSICS PROGRAM
CHERRY EMERSON BUILDING
GEORGIA INST. OF TECH.
ATLANTA, GEORGIA 30332 U.S.A.

Dr. S.B. Oblath
Waste Disposal Technology Division
Savannah River Laboratory
E.I. Du Pont de Nemours & Co.
Aiken, SC 29808

Monthly Progress Report - Project E-25-606 (P.O. AX0654763)

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

GGE/sm
cc: P. Heitmuller (OCA)

Georgia Institute of Technology
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March 11, 1985

Please reply to:
NUCLEAR ENGINEERING AND
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GEORGIA INST. OF TECH.
ATLANTA, GEORGIA 30332 U.S.A.

Dr. S. B. Oblath
Waste Disposal Technology Division
Savannah River Laboratory
E.I. Du Pont de Nemours & Co.
Aiken, SC 29808

Monthly Progress Report - Project E-25-606 (P.O. AX0654763)

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. Eichholz
Regents' Professor

GGE/swm

cc: P. Heitmuller

Telephone: 404-894-3720 Telex: 542507 GTRIOCAATL Fax: 404-894-3120 (Verify: 404-894-4850)

Georgia Institute of Technology
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April 10, 1985

Please reply to:
NUCLEAR ENGINEERING AND
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CHERRY EMERSON BUILDING
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ATLANTA, GEORGIA 30332 U.S.A.

Dr. S. B. Oblath
Waste Disposal Technology Division
Savannah River Laboratory
E. I. Du Pont de Nemours & Co.
Aiken, SC 29808

Monthly Progress Report - Project E-25-606 (P.O. AX0654763)

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. Eichholz
G.G. Eichholz
Regents' Professor

GGE/swm

cc: P. Heitmuller (OCA)

Telephone: 404-894-3720 Telex: 542507 GTRIOCAATL Fax: 404-894-3120 (Verify: 404-894-4850)

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May 10, 1985

Please reply to:
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ATLANTA, GEORGIA 30332 U.S.A.

Dr. S.B. Oblath
Waste Disposal Technology Division
Savannah River Laboratory
E.I. Du Pont de Nemours & Co.
Aiken, SC 29808

Monthly Progress Report - Project E-25-606 (P.O. AX0654763)

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

GGE/sm
cc: Pat Heitmuller (OCA)

Telephone: 404-894-3720 Telex: 542507 GTRIOCAATL Fax: 404-894-3120 (Verify: 404-894-4850)

Georgia Institute of Technology
A UNIT OF THE UNIVERSITY SYSTEM OF GEORGIA
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June 7, 1985

Please reply to:

NUCLEAR ENGINEERING AND
HEALTH PHYSICS PROGRAM
CHERRY EMERSON BUILDING
GEORGIA INST. OF TECH.
ATLANTA, GEORGIA 30332 U.S.A.

Dr. S.B. Oblath
Waste Disposal Technology Division
Savannah River Laboratory
E.I. Du Pont de Nemours & Co.
Aiken, SC 29808

Monthly Progress Report - Project E-25-606 (P.O. AX0654763)

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 wili be taken up with organizing our data and the preparation of the final report on this project.

Yours sincerely

Geoffrey G. Eichholz
Regents' Professor

cc: 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

CONTENTS

Project Personnel (All part-time)

Geoffrey G. Eichholz, Ph.D	Project Director
Fernando N. Carneiro de Sousa, MSHP	Graduate Research Assistant
Jooho Whang, MSHP	Graduate Research Assistant
M. Frank Petelka, MSHP	Graduate Research Assistant
M. Christine Daily, B.S.	Graduate Research Assistant
Harry K. Anderson, B.S.	Graduate Research Assistant
Bruce W. Patton, B.S.	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 than 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 propertional to the rate of water movement through the waste zone.

Direct comparison of the model with output date 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.

<u>FLOW MODEL</u>

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

$$L(\psi) = C^* \frac{\partial \psi}{\partial t} - \nabla \cdot (K \nabla \psi) + \frac{\partial K}{\partial z} = 0 \qquad (1)$$

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

$C^* = \partial\theta / \partial\psi$

ψ 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 θ 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.

$$\psi(t, r, z)\Big|_{t=0} = \psi_o(r, z) \qquad (2)$$

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

$$\psi(t, r, z) = \tilde{\psi}(t, r, z) \tag{3}$$

on Γ_1 ; or Neumann boundary, where the flux due to the gradient of the pressure head is constant,

$$\int_A \vec{q}(t, r, z)\,dA = \int_A (K\vec{\nabla}z + K\vec{\nabla}\psi(t, r, z)\,dA = \text{const.} \tag{4}$$

on Γ_2 where $\Gamma = \Gamma_1 + \Gamma_2$ 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.

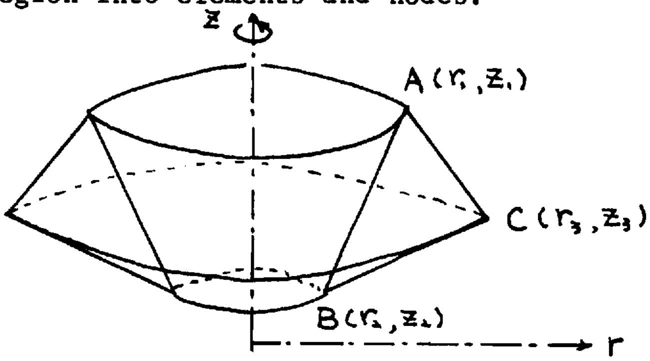


Fig. 1

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

$$N_i^e(r,z) = \frac{a_i^e + b_i^e r + c_i^e z}{2A^e} \tag{5}$$

where $2A^e = (r_1 z_2 - r_2 z_1) + (r_3 z_1 - r_1 z_3) + (r_2 z_3 - r_3 z_2)$

$$= 2 \cdot \det \begin{vmatrix} 1 & r_1 & z_1 \\ 1 & r_2 & z_2 \\ 1 & r_3 & z_3 \end{vmatrix} \tag{6}$$

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

$$\hat{\psi}(t,r,z) = \sum_{i=1}^{3} N_i^e(r,z)\,\psi_i(t) \tag{7}$$

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:

$$\hat{\psi} = \sum_{i=1}^{3} \psi_i N_i \tag{8}$$

$$\hat{K} = \sum_{L=1}^{3} K_L N_L \tag{9}$$

$$\hat{C}^* = \sum_{L=1}^{3} \hat{C}^*_L N_L \tag{10}$$

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:

$$\int_V C^*(\psi)\frac{\partial \psi}{\partial t} N_j \, dV = \int_V \vec{\nabla}\cdot\left\{K(\psi)\,(\vec{\nabla}\psi - \hat{k} Z)\right\} N_j \, dV \qquad (11)$$

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

$$\int_V C^*(\psi)\frac{\partial \psi}{\partial t} N_j \, dV = \int_V \vec{\nabla}\left[K(\psi)\,(\vec{\nabla}\psi - \hat{k} z)\, N_j\right] dV - \int_V \left[K(\psi)(\vec{\nabla}\psi - \hat{k} z)\cdot \nabla N_j\right] dV$$

$$= \int_{\Gamma_2} \vec{n}_{\Gamma_2}\cdot\left[K(\psi)(\vec{\nabla}\psi - \hat{k} z)\right] N_j \, d\Gamma_2 - \int_V K(\psi)\vec{\nabla}\psi \cdot \nabla N_j \, dV + \int_V K(\psi)\frac{\partial N_j}{\partial z}\, dV \qquad (12)$$

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

$$[M]\left\{\frac{\partial \psi}{\partial t}\right\} = [Q] - [S]\{\psi\} + [P] \qquad (13)$$

where $[M]$, $[Q]$, $[S]$, $[P]$ 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:

$$m_j = \sum_{L=1}^{3} \int_V C_L^* N_L N_j \, dV = \sum_{L=1}^{3} C_L^* \int_V N_L N_j \, dV \tag{14}$$

$$S_{ji} = \sum_{L=1}^{3} \int_V K_L N_L \nabla N_i \cdot \nabla N_j \, dV = \nabla N_i \cdot \nabla N_j \sum_{L=1}^{3} K_L \int_V N_L \, dV \tag{15}$$

$$P_i = \sum_{L=1}^{3} \int_V K_L N_L \frac{\partial N_j}{\partial Z} \, dV = \frac{\partial N_j}{\partial Z} \sum_{L=1}^{3} K_L \int_V N_L \, dV \tag{16}$$

$$q_i = - \int_{\Gamma_2} \vec{n}_{\Gamma_2} \cdot q \, d\Gamma_2 \tag{17}$$

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.

$$[M]\frac{\phi^{K+1}-\phi^{K}}{\Delta t} = [Q] - [S]\frac{\phi^{K+1}+\phi^{K}}{2} + [P] \tag{18}$$

Equation (18) can be written as,

$$\left\{\frac{[M]}{\Delta t} + \frac{[S]}{2}\right\}\phi^{K+1} = \left\{\frac{[M]}{\Delta t} - \frac{[S]}{2}\right\}\phi^{K} + [Q] + [P] \tag{19}$$

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 accomodated 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.

$$\theta = \begin{cases} 0.6829 - 0.09524 \ln|\psi| & \psi \leq -29.484 \text{ (Cm of Water)} \\ 0.4531 - 0.02732 \ln|\psi| & -29.484 \leq \psi \leq -14.495 \end{cases}$$

$$K = \begin{cases} 19.34 \times 10^{5} |\psi|^{-3.4095} & \psi \leq -29.484 \\ 516.8 \; |\psi|^{-0.97814} & -29.484 \leq \psi \leq -14.495 \end{cases}$$

$$C^{*} = \begin{cases} 0.09524 \, / \, |\psi| & \psi \leq -29.484 \\ 0.02732 \, / \, |\psi| & -29.484 \leq \psi \leq -14.495 \end{cases}$$

VAN GENUCHTEN MODEL

It can be used by assigning iTM=1.

$$\theta = \theta_r + (n - \theta_r) \left(\frac{1}{1 + (\alpha\psi)^{\lambda}} \right)^{m}$$

$$C^{*} = m (n - \theta_r) \lambda \frac{(\alpha\psi)^{\lambda}}{\psi} \left(\frac{1}{1 + (\alpha\psi)^{\lambda}} \right)^{m+1}$$

$$K = K_s \sqrt{\Theta} \left\{ 1 - (1 - \Theta^{\frac{1}{m}})^{m} \right\}^{2}$$

where θ_r is the residual water content,

n is the porosity,

K_s is the saturation hydraulic conductivity,

$M = 1 - \frac{1}{\lambda}$, and

$Ⓗ = (\theta - \theta_r) / (n - \theta_r)$.

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 ψ_s is the air-entry value

HAVERKAMP MODEL

It can be used by assigning iTM =3.

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

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

$$K = K_s \left(\frac{\beta}{\beta + \psi^{\lambda}}\right)$$

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:

iTM	SER	SES	HES	CKS	RMM	APH
−1		n	ψ_s	K_s		
0		n	ψ_s	K_s		
1	θ_r	n	ψ_s	K_s	λ	a
2	θ_r	n	ψ_s	K_s	λ	
3	θ_r	n	β	K_s	λ	a

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

$$\frac{\partial(\theta C)}{\partial t} + \rho K_d \frac{\partial C}{\partial t} = \vec{\nabla} \cdot (\theta \vec{\vec{D}} \cdot \vec{\nabla} C - \vec{q} C) + \lambda \theta C + \beta \rho K_d C + \gamma \theta \tag{20}$$

where θ is the volumetric water content,

C is the concentration of solute in solution,

ρ is the soil bulk density,

K_d is the distribution coefficient,

D is the hydrodynamic dispersion coefficient,

q is the volumetric flux

λ is the first-order rate constant (liquid phase),

β is the first-order rate constant (solid phase), and

γ 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

$$S = K_d C \tag{21}$$

where S is the adsorbed concentration.

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

$$\frac{\partial(\theta R C)}{\partial t} = \vec{\nabla}\cdot(\theta D \cdot \nabla C - \vec{q} C) + \alpha\theta C + \beta\rho K_d C + \gamma\theta \tag{22}$$

where R is the retardation factor representing

$$R = 1 + \rho K_d / \theta \tag{23}$$

If the reactions of the solute with soil are only adsorption and radioactive decay, coefficients α and β become both equivalent to a decay constant of the radionuclide in question, and γ 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

$$\theta R \frac{\partial c}{\partial t} = \vec{\nabla} \cdot (\theta \vec{\vec{D}} \cdot \vec{\nabla} C - \vec{q} C) + \alpha' C \tag{24}$$

where

$$\alpha' = \left(\alpha\theta + \beta \rho K_d - \frac{\partial \theta}{\partial t} \right) \tag{25}$$

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

$$\int_V \theta R N_j \frac{\partial c}{\partial t} dV = \int_{\Gamma_2} (\theta \vec{\vec{D}} \cdot \vec{\nabla} C - \vec{q} C) \cdot \vec{n}_{\Gamma_2} d\Gamma_2 - \int_V \theta \vec{\vec{D}} \cdot \vec{\nabla} C \cdot \vec{\nabla} N_j dV + \int_V \vec{q} C \cdot \vec{\nabla} N_j dV + \int_V \alpha' C N_j dV \tag{26}$$

which results in the following form:

$$[M]\left\{\frac{\partial c}{\partial t}\right\} = [Q] - [A]\{c\} + [B]\{c\} + [F]\{c\} \tag{27}$$

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

$$m_{ii} = \sum_{L=1}^{3} (\theta R)_L \int_V N_L N_i \, dV \tag{28}$$

$$q_{bi} = \int_{\Gamma_2} (\theta \vec{D} \cdot \vec{\nabla} C - \vec{q} C) \cdot \vec{n}_{\Gamma_2} d\Gamma_2 = - q''_{b0} C_0 \int_{\Gamma_2} d\Gamma_2 \tag{29}$$

where q''_{b0} is the surface flux of water and C_o is the concentration of solute.

$$b_{ji} = \int_V K \left(-\frac{\partial \psi}{\partial r}, 1 - \frac{\partial \psi}{\partial z}\right) \begin{pmatrix} \partial N_j / \partial r \\ \partial N_j / \partial z \end{pmatrix} N_i \, dV \tag{30}$$

$$= \int_V K(0, 1) \begin{pmatrix} \partial N_j / \partial r \\ \partial N_j / \partial z \end{pmatrix} N_i \, dv - \int_V K \left(\frac{\partial \psi}{\partial r}, \frac{\partial \psi}{\partial z}\right) \begin{pmatrix} \partial N_j / \partial r \\ \partial N_j / \partial z \end{pmatrix} N_i \, dV \tag{31}$$

$$= \sum_{L=1}^{3} K_L \int_V N_L N_i \, dv \left\{ \frac{\partial N_j}{\partial z} - \sum_k \psi_k \nabla N_k \cdot \nabla N_j \right\} \tag{32}$$

$$f_{ji} = \sum_{L=1}^{3} \left(\partial\theta + \beta \rho K_d - \frac{\partial \theta}{\partial t} \right)_L \int_V N_i N_j N_L \, dV \tag{33}$$

The second term of the right-hand side of equation (26) can be expressed as follows:

$$\vec{\nabla}\cdot(\theta\vec{\vec{D}}\cdot\vec{\nabla}C) = \left(\frac{\partial}{\partial r}, \frac{\partial}{\partial z}\right)\begin{pmatrix}\theta D_{rr} & \theta D_{rz} \\ \theta D_{zr} & \theta D_{zz}\end{pmatrix}\begin{pmatrix}\partial C/\partial r \\ \partial C/\partial z\end{pmatrix} \tag{34}$$

where the hydrodynamic coefficients are

$$D_{rr} = D_d^* + (\alpha_L V_r^2 + \alpha_T V_z^2) / V \tag{35}$$

$$D_{rz} = D_{zr} = (\alpha_L - \alpha_T) V_r V_z / V \tag{36}$$

$$D_{zz} = D_d^* + (\alpha_L V_z^2 + \alpha_T V_r^2) / V \tag{37}$$

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

$$\vec{V} = \vec{q} / \theta \tag{38}$$

is the velocity of water

$$|V| = \sqrt{V_r^2 + V_z^2} \tag{39}$$

and flux is given by

$$\vec{q} = K\vec{\nabla}(z - \psi) \tag{40}$$

where, for each direction

$$\vec{q}_z = K(1 - \partial\psi/\partial z) \tag{41}$$

$$\vec{q}_r = -K\,\partial\psi/\partial r \tag{42}$$

Thus, the water velocity for each direction is

$$\vec{V}_r = K(r, z)(-\partial\psi/\partial r)/\theta(r, z) \tag{43}$$

$$\vec{V}_z = K(r, z)(1 - \partial\psi/\partial z)/\theta(r, z) \tag{44}$$

Substituting equation (43), (44), and (39) into equation (35), (36), and (37) and multiplying them by θ, we have

$$\theta D_{rr} = D_d^* \theta(r,z) + K(r,z) \frac{\left[\alpha_L \left(-\frac{\partial \psi}{\partial r}\right)^2 + \alpha_T \left(1 - \frac{\partial \psi}{\partial z}\right)^2\right]}{\sqrt{\left(-\frac{\partial \psi}{\partial r}\right)^2 + \left(1 - \frac{\partial \psi}{\partial z}\right)^2}} \tag{45}$$

$$\theta D_{rz} = \theta D_{zr} = K(r,z) \frac{(\alpha_L - \alpha_T)\left[\left(-\frac{\partial \psi}{\partial r}\right)\left(1 - \frac{\partial \psi}{\partial z}\right)\right]}{\sqrt{\left(-\frac{\partial \psi}{\partial r}\right)^2 + \left(1 - \frac{\partial \psi}{\partial z}\right)^2}} \tag{46}$$

$$\theta D_{zz} = D_d^* \theta(r,z) + K(r,z) \frac{\left[\alpha_L \left(1 - \frac{\partial \psi}{\partial z}\right)^2 + \alpha_T \left(-\frac{\partial \psi}{\partial r}\right)^2\right]}{\sqrt{\left(-\frac{\partial \psi}{\partial r}\right)^2 + \left(1 - \frac{\partial \psi}{\partial z}\right)^2}} \tag{47}$$

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

$$D^- = D - q^2 \Delta t / 6 \theta^2 R \tag{48}$$

$$D^+ = D + q^2 \Delta t / 6 \theta^2 R \tag{49}$$

Thus, equations (35), (36), and (37) are given by

$$D_{rr}^{\pm} = D_{rr} \pm q_{rr}^{2} \Delta t / 6\theta^{2} R \tag{50}$$

$$D_{rz}^{\pm} = D_{rz}^{\pm} = D_{rz} = D_{zr} \tag{51}$$

$$D_{zz}^{\pm} = D_{zz} \pm q_{zz}^{2} \Delta t / 6\theta^{2} R \tag{52}$$

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 $\left[A \right]$ in equation (27) becomes as follows:

$$C_i \left[\begin{pmatrix} \Theta D_{rr}^{\pm} & \Theta D_{rz}^{\pm} \\ \Theta D_{zr}^{\pm} & \Theta D_{zz}^{\pm} \end{pmatrix}_L \begin{pmatrix} \partial N_i/\partial r \\ \partial N_i/\partial z \end{pmatrix} \right]^T \begin{pmatrix} \partial N_j/\partial r \\ \partial N_j/\partial z \end{pmatrix}$$

$$= \frac{C_i}{2A^2} \left[\begin{pmatrix} \Theta D_{rr}^{\pm} & \Theta D_{rz}^{\pm} \\ \Theta D_{zr}^{\pm} & \Theta D_{zz}^{\pm} \end{pmatrix}_L \begin{pmatrix} b_i \\ c_i \end{pmatrix} \right]^T \begin{pmatrix} b_j \\ c_j \end{pmatrix}$$

$$= \frac{C_i}{2A^2} \begin{pmatrix} \Theta_L D_{rr_L}^{\pm} b_i + \Theta_L D_{rz_L}^{\pm} c_i \\ \Theta_L D_{zr_L}^{\pm} b_i + \Theta_L D_{zz_L}^{\pm} c_i \end{pmatrix}^T \begin{pmatrix} b_j \\ c_j \end{pmatrix} \tag{53}$$

Finally $[A]$ in equation (26) has an array of

$$a_{ji}^{\pm} = \sum_{L=1}^{3} \left[\begin{pmatrix} \Theta D_{rr}^{\pm} & \Theta D_{rz}^{\pm} \\ \Theta D_{zr}^{\pm} & \Theta D_{zz} \end{pmatrix}_L \begin{pmatrix} \partial N_i/\partial r \\ \partial N_i/\partial z \end{pmatrix} \right]^T \begin{pmatrix} \partial N_j/\partial r \\ \partial N_j/\partial z \end{pmatrix} \tag{54}$$

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

$$[A^{\pm}] = [A] \pm [AD] \tag{55}$$

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

$$\left[A^{\pm} \right] \left\{ C \right\} = \left[A^{+} \right] \left\{ \frac{C^{t}}{2} \right\} + \left[A^{-} \right] \left\{ \frac{C^{t+\Delta t}}{2} \right\} \tag{56}$$

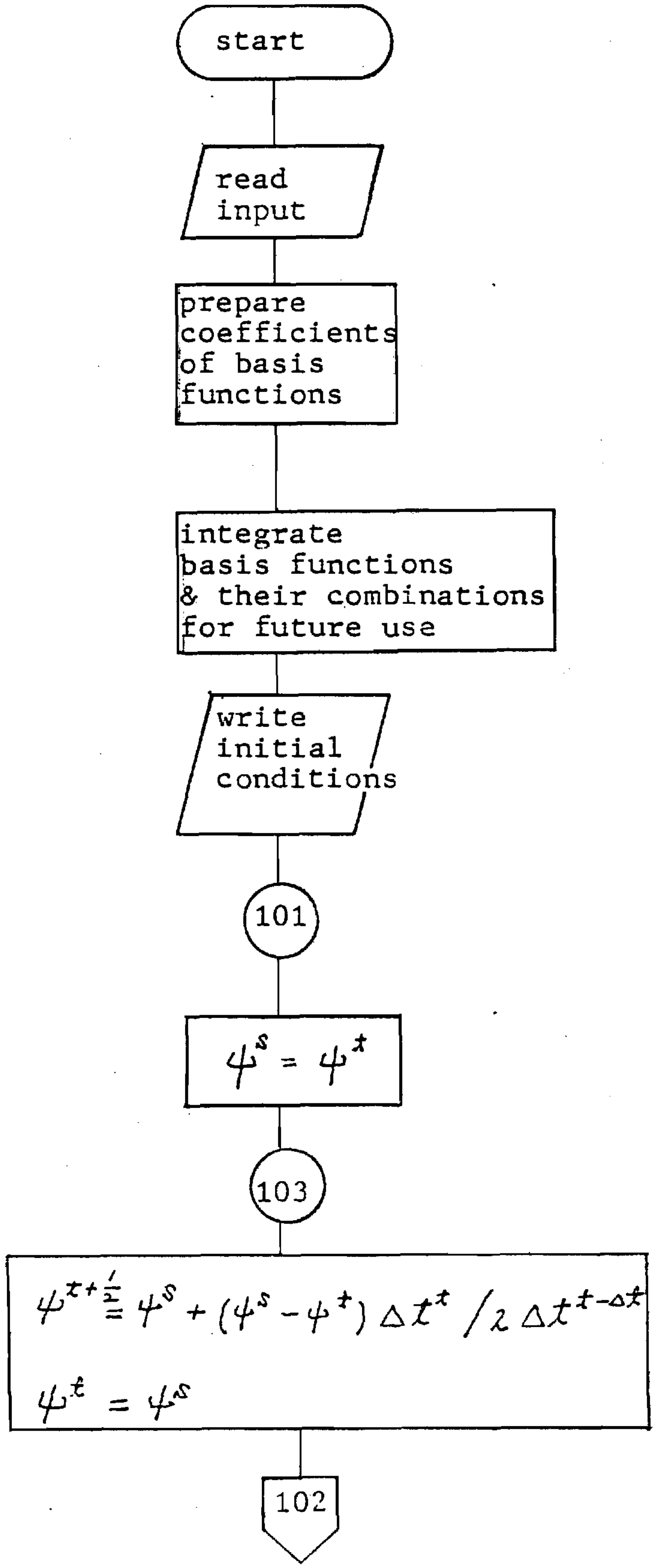
Equation (27), with the Crank-Nicolson time step, becomes

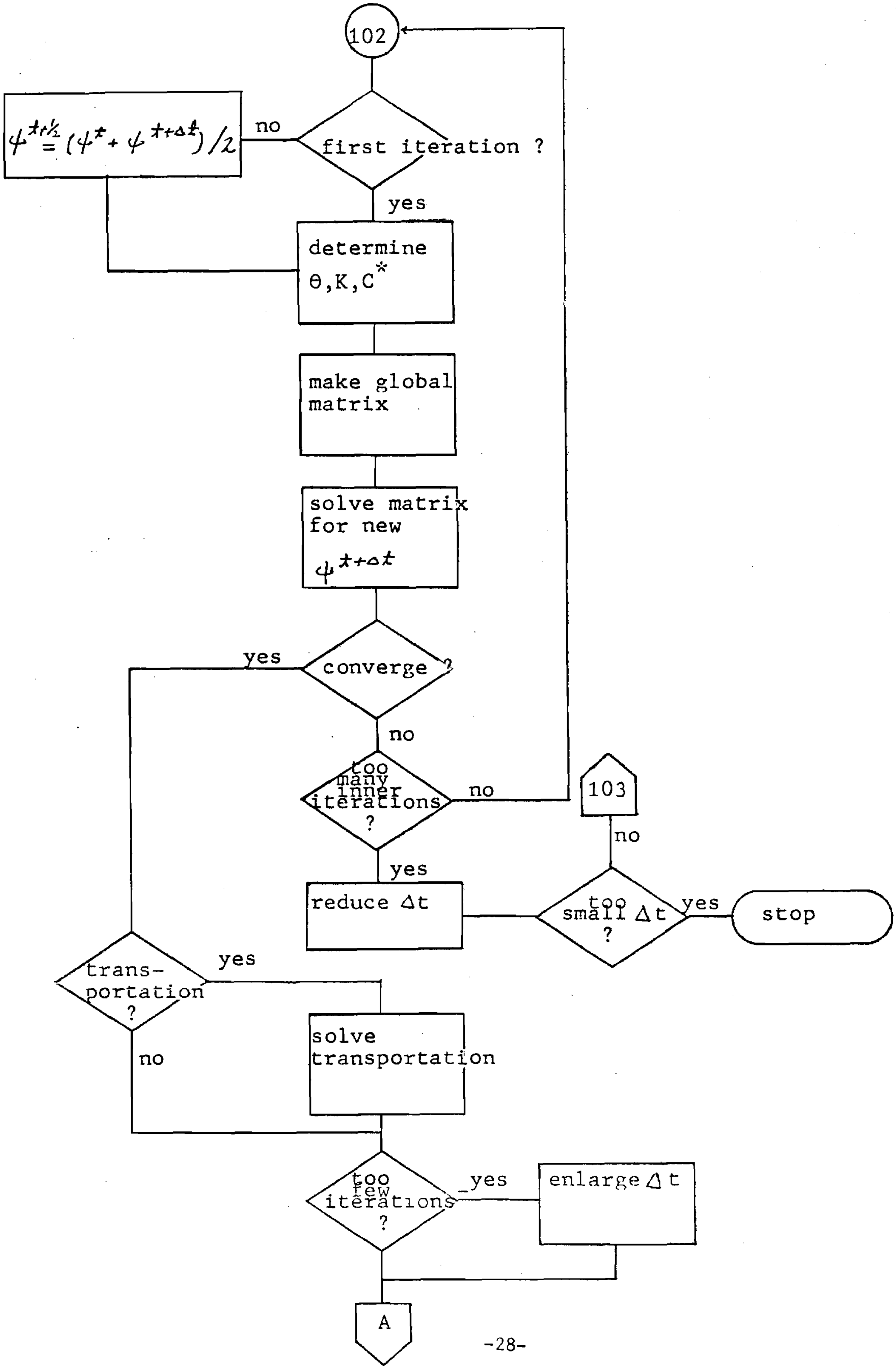
$$\left[\frac{[M]}{\Delta t} \quad \frac{[A]-[B]-[F]-[AD]}{2} \right] \left\{ C^{t+\Delta t} \right\} = \left[\frac{[M]}{\Delta t} + \frac{-[A]-[AD]+[B]+[F]}{2} \right] \left\{ C^{t} \right\} + \left[Q \right] \tag{57}$$

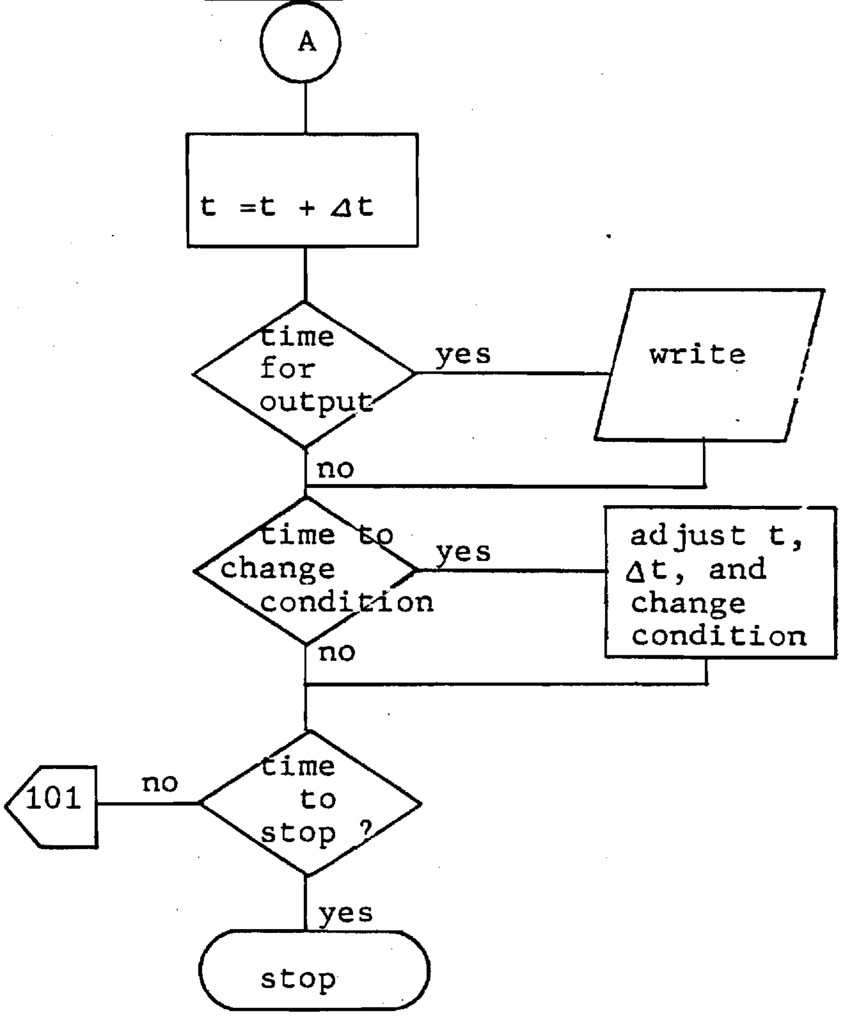
Other steps toward solving equation (57) are the same as were done for equation (19).

A flowchart of the main program follows.

FLOW-CHART OF MAIN PROGRAM.




102
first iteration ?
no
$\psi^{t+1/2} = (\psi^{t} + \psi^{t+\Delta t})/2$
yes
determine
θ,K,C*
make global matrix
solve matrix for new
$\psi^{t+\Delta t}$
converge ?
yes
no
too many inner iterations ?
no
103
yes
reduce Δt
no
too small Δt ?
yes
stop
trans-portation ?
yes
solve transportation
no
too few iterations ?
yes
enlarge Δt
A


A
t =t + Δt
time for output
yes
write
no
time to change condition
yes
adjust t, Δt, and change condition
no
101
no
time to stop ?
yes
stop

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

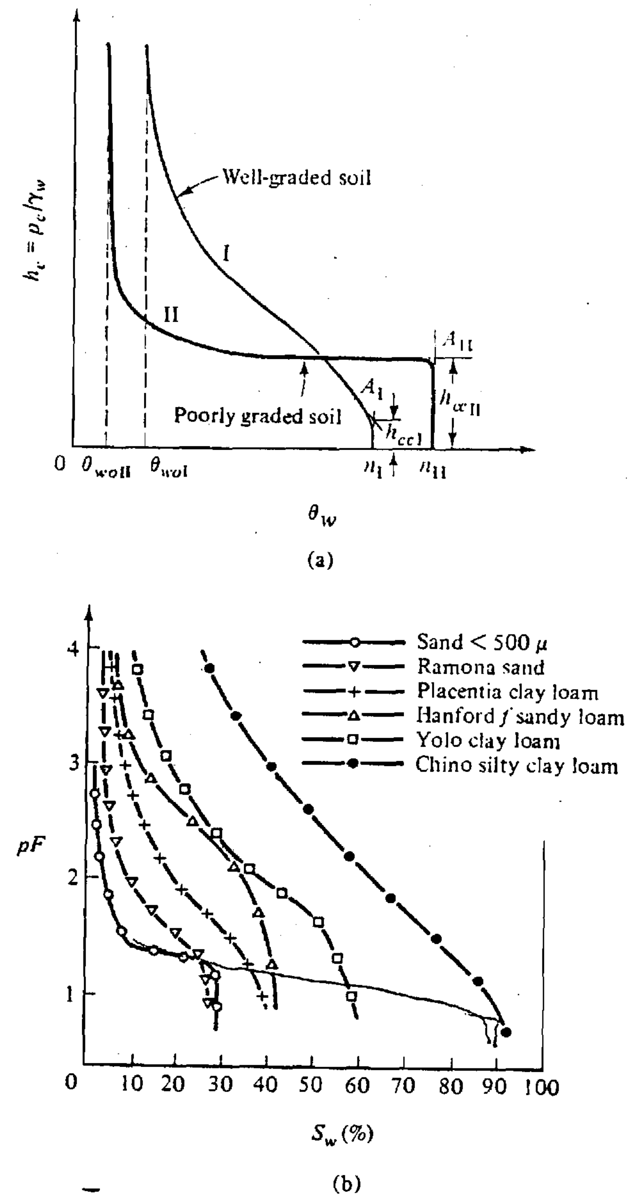


Figure I Typical retention curves in soil during drainage. (a) Schematic curves. (b) Curves obtained during desaturation (after Richards and Weaver, 1944).

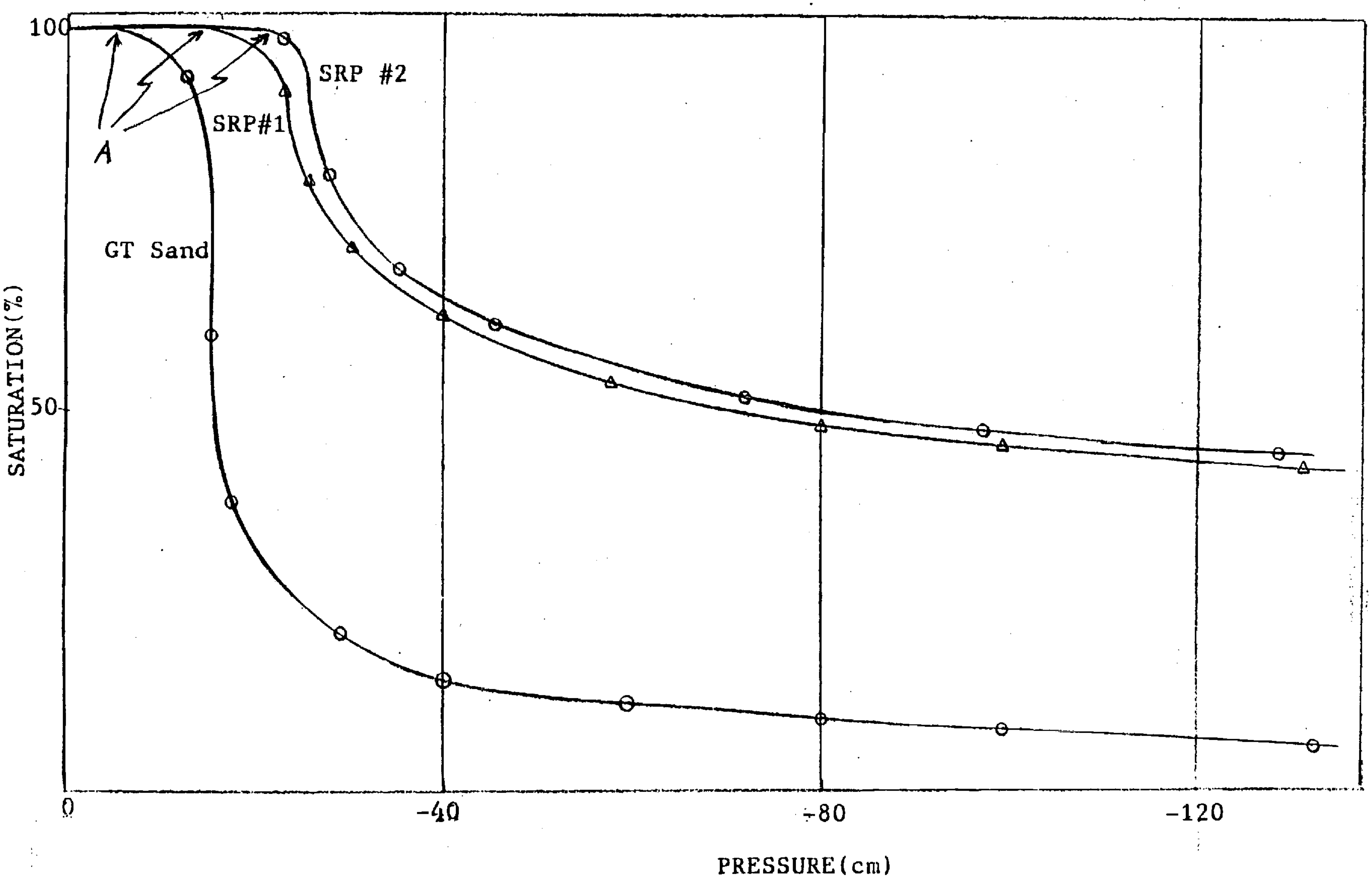


Figure 2 - Soil-Water Characteristics

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 θ , 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 Poulovassilis 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 glassbead plate and several Buchner funnels are employed to produce different negative pressures.

(Because of the strength of the fritted glassbead 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.

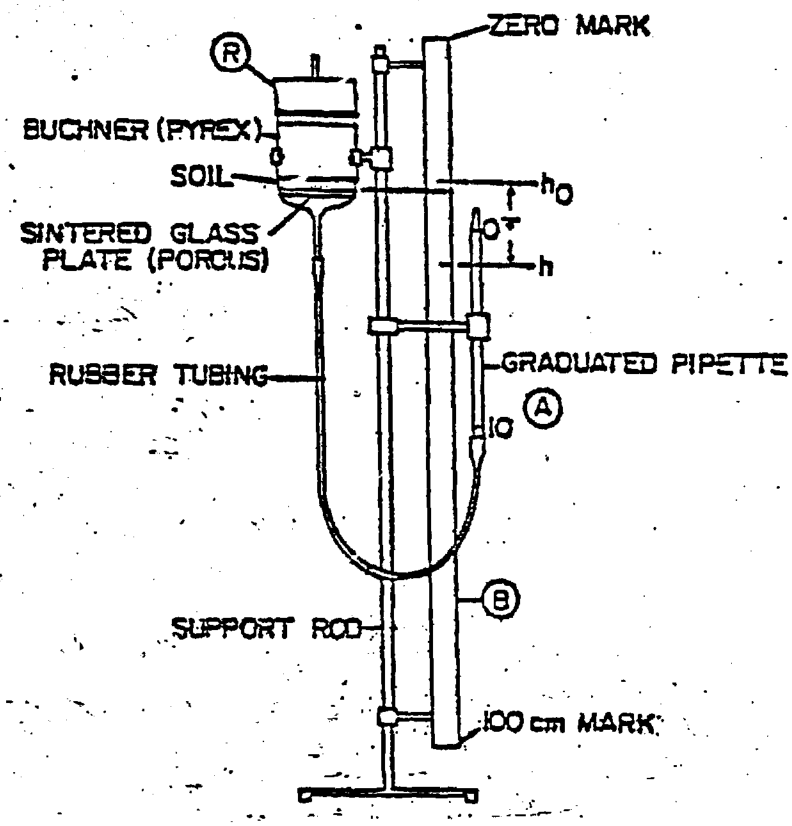


Figure 3 - Hanging Column (Wilson,1980)

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 glassbead 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.

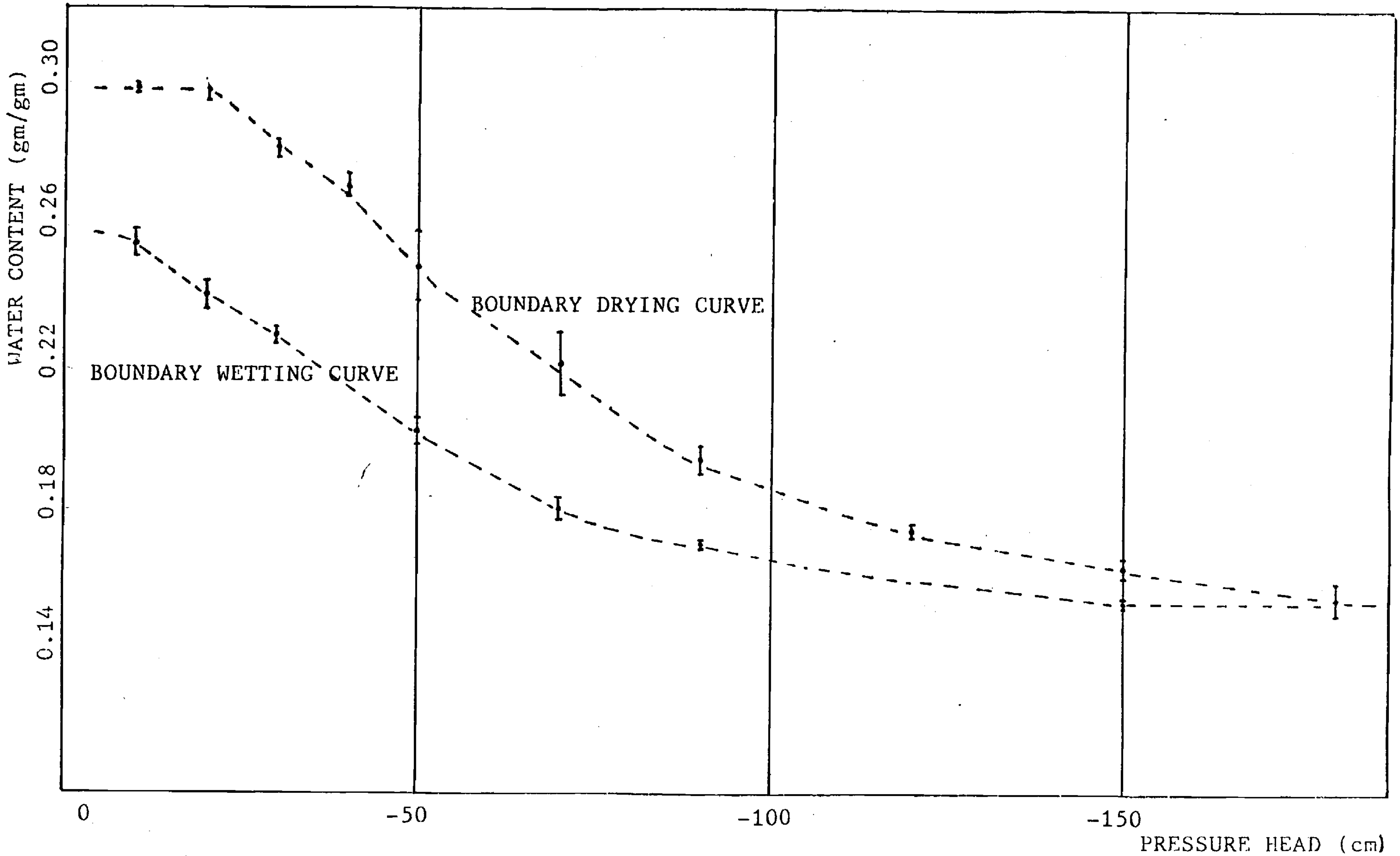


FIGURE 4 - HYSTERETIC SOIL-WATER CHARACTERISTICS OF SRP #1.

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 ψ_s 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)

SOIL	BROOKS AND COREY				VAN GENUCHTEN		
	n	θ_r	ψ_s	λ	θ_r	α	m
G. T. SAND	0.44	0.035	11.2	1.52	0.035	0.049	8.00
SRP #1	0.47	0.17	26.0	1.42	0.17	0.027	2.60
SRP #2	0.52	0.22	30.0	1.71	0.22	0.024	3.85

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.

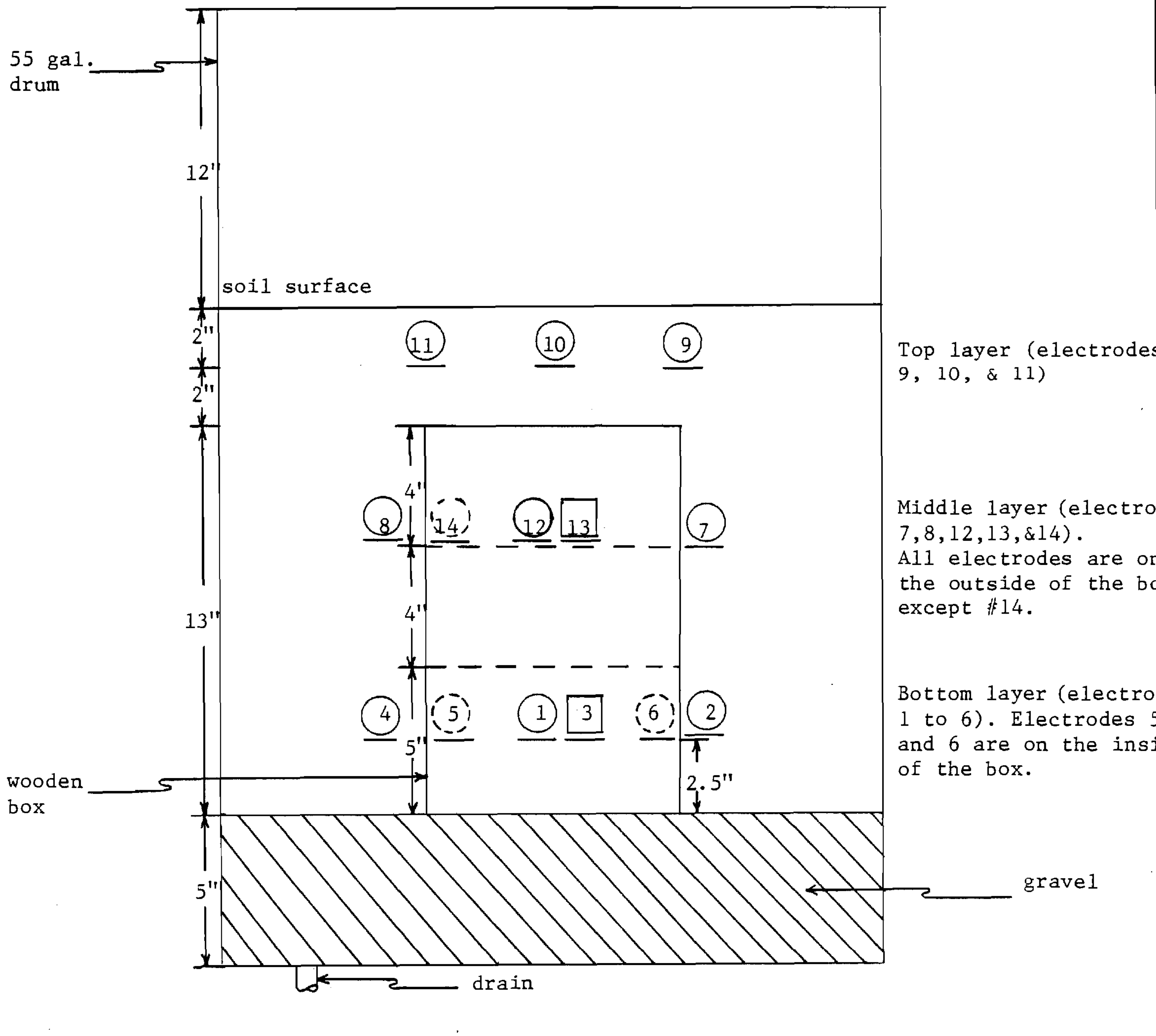


Figure 5. Configuration for Test No. 3

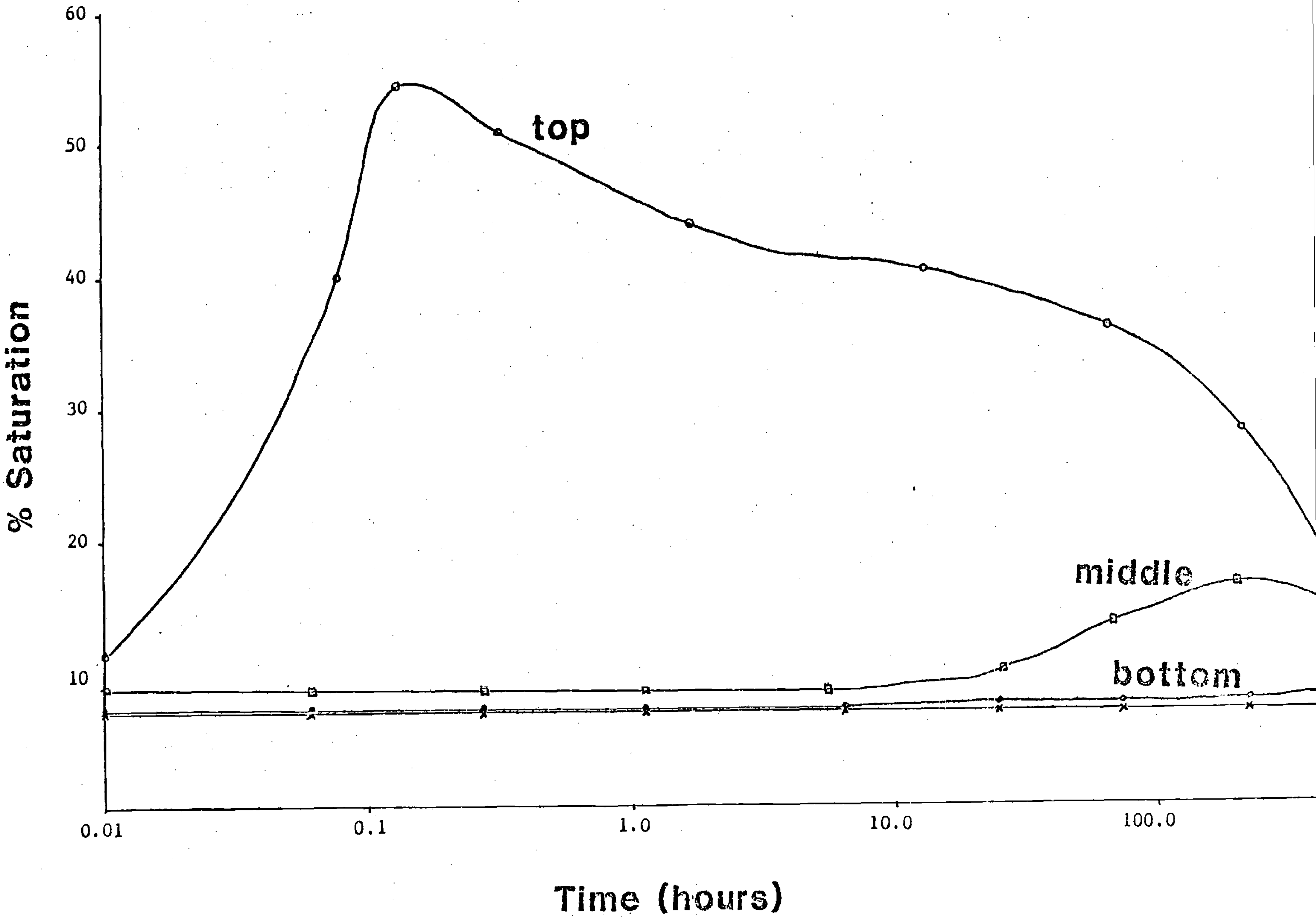


Figure 6. Test No. 3 Run 1

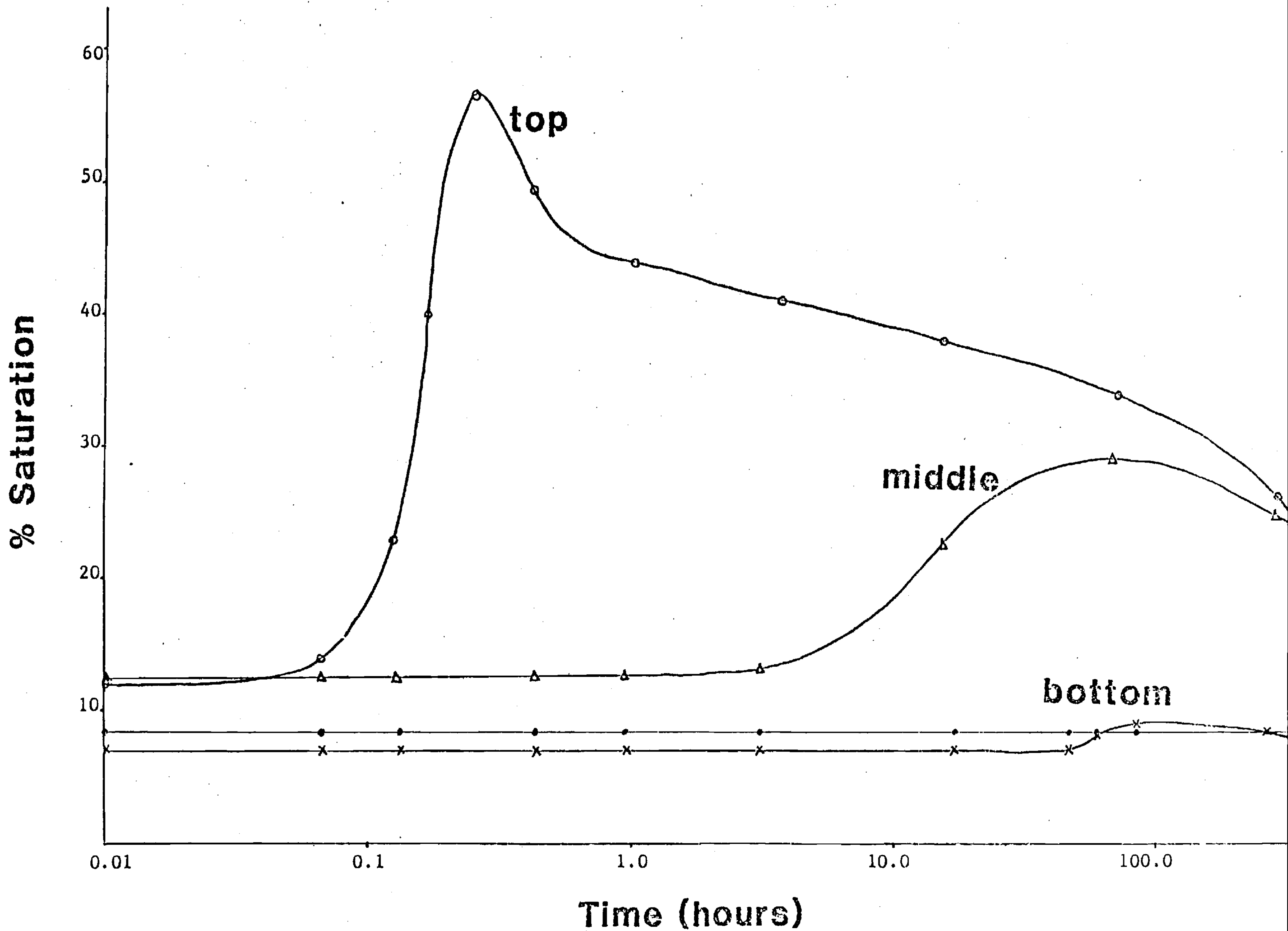
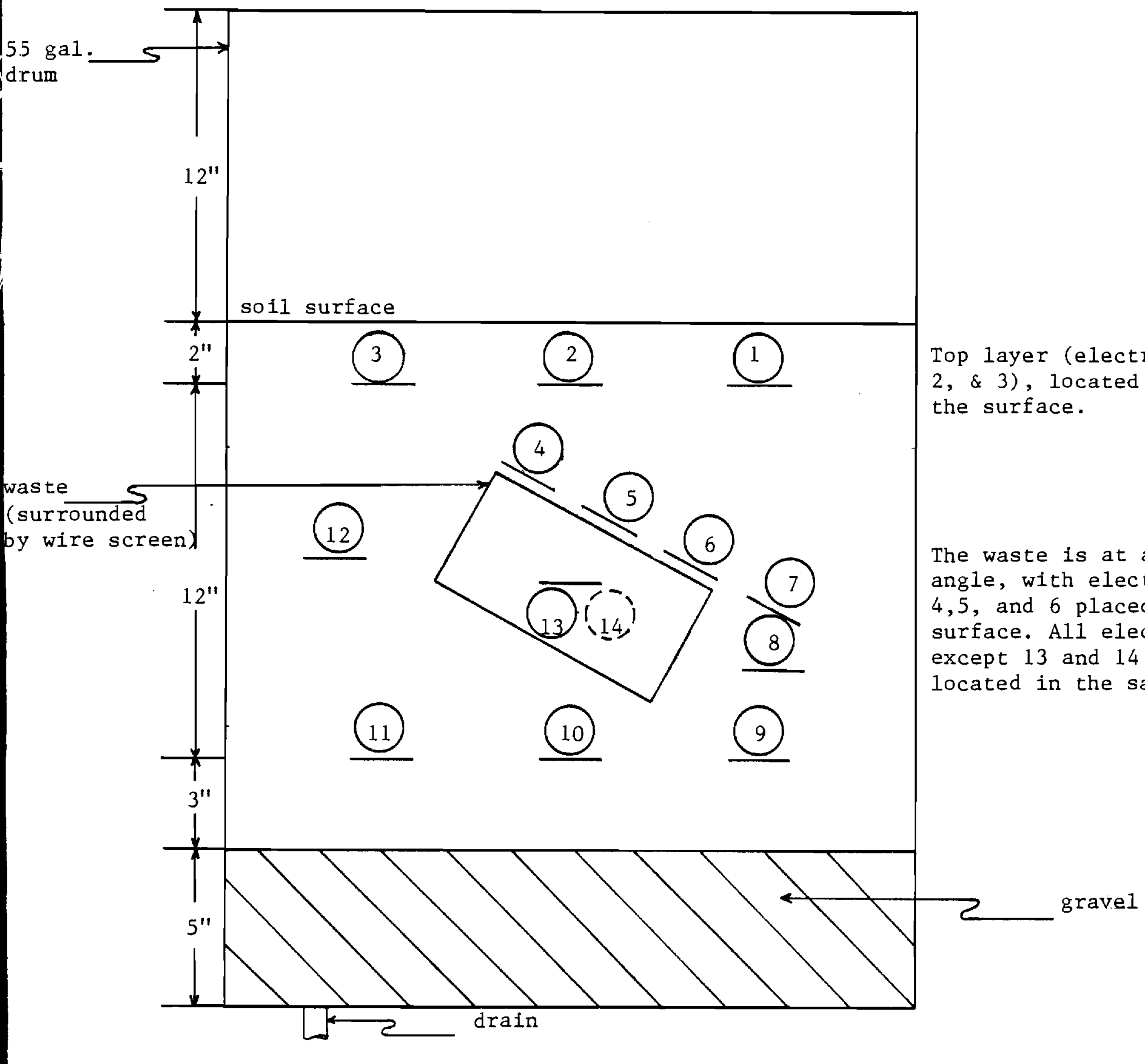


Figure 7. Test No. 3 Run 2



Top layer (electrodes 1, 2, & 3), located 2" belo[w] 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 plan[e]

Figure 8. Configuration for Test No. 4

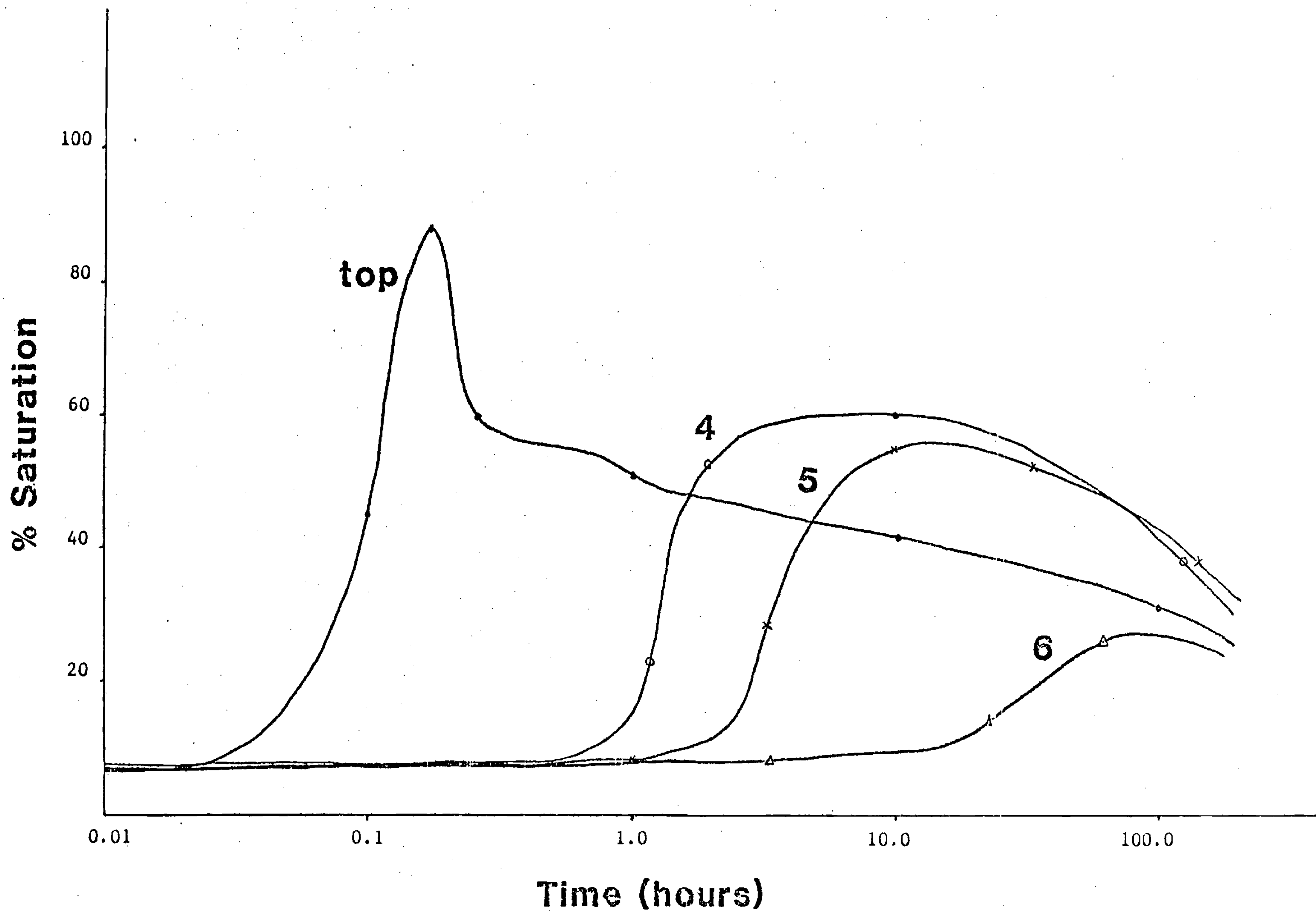


Figure 9.   Test No. 4   Run 1

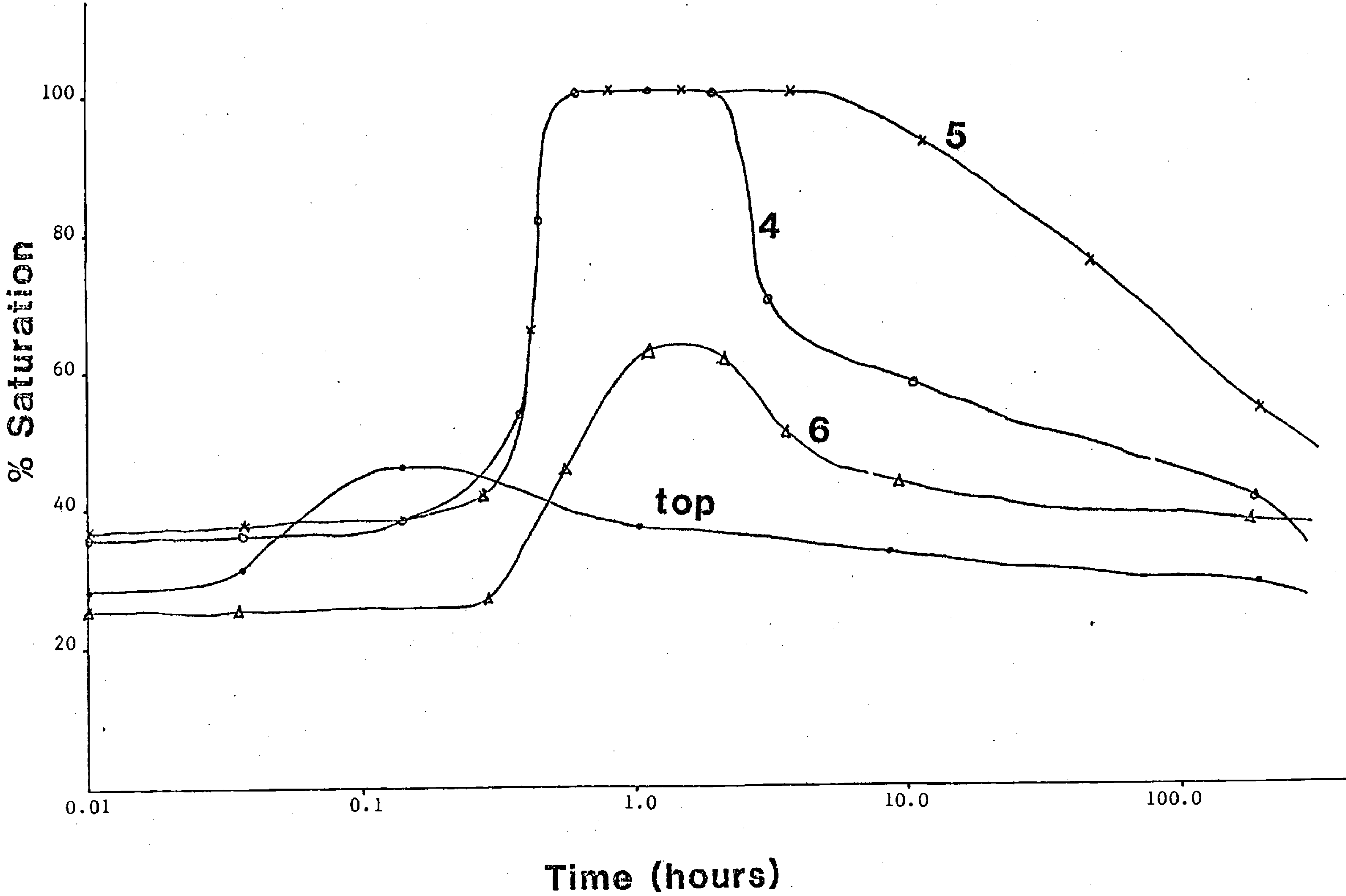


Figure 10. Test No. 4 Run 2

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.

ACKNOWLEDGMENTS

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.

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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

$$ER > MAX\left(\left|\frac{\psi_i^K - \psi_i^{K+1}}{\psi_i^{K+1}}\right|\right) \quad \text{where } i=1,2\cdots ND$$

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	ρ, The bulk density of fluid(g/cm)
DOT	$D_o\tau$, where D_o is the molecular diffusion coefficient(cm/day) and τ is the tortuodity factor.
AFL	α_L,Longitudial dispersivity of the porous medium
AFT	α_T,Trasversal dispersivity of the porous medium
DK	K_d',The empirical coefficient for absorbed concentration(cm/g) absorbed concentration $S = K_d'C$ total concentration $=\theta C+\rho K_d'C$ $=\theta RC$ where $R=1+\rho K_d'/\theta$

ALF α,a First order rate constant(liquid phase)(day)
BET β,a First order rate constant(solid phase)(day)
GAM γ,a zeroth order rate constant(liquid phase)(g/cm /day)
CBT   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 ρ, $D_0\tau$, α_L, α_T, K_d', α and β in the different region.

The (8+ITRSP+NS+NE+ND+IDFF*2)th Line ,ITM
The option for the relationships of θ ,K and C to ψ 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 θ ,K and C to ψ in different region.

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

MODEL	ITM	SER	SES	APH	RMM	CKS	HES
Saturation	-1		n			K_s	ψ_s
Warrick Sand	0		n			K_s	ψ_s
Van Genuchten	1	θ_r	n	α	λ	K_s	ψ_s
Brooks and Corey	2	θ_r	n		λ	K_s	ψ_s
Haverkamp	3	θ_r	n	α	λ	K_s	β

HES $= |\psi_s| > 0$

Symbolic Constants

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

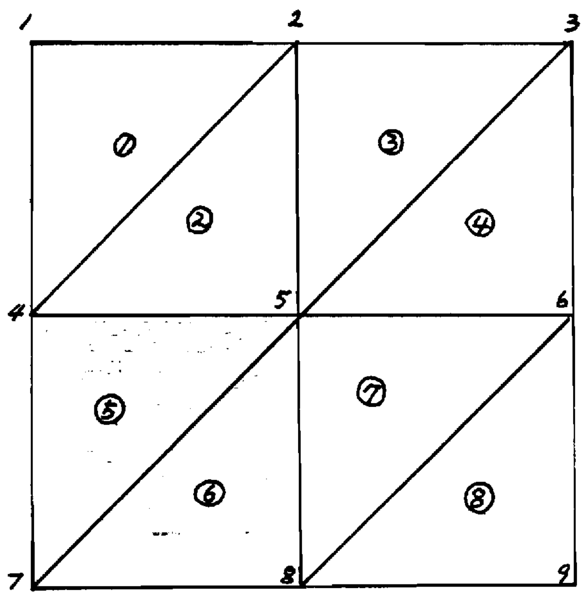
NE : number of elements

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)



NE = 8

ND = 9

iHO = 3 (1, 2, 3)

NOD = 4 (4, 5, 7, 8)

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

Variables in Main Program

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

A (NE,3) : ai^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: α_L , the longitudinal dispersivity $[L]$

AFT, AFTD: α_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: α , 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_i^e 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_i^e 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) iBC(i) = 0, Q (i) is constant hydraulic head on the top $[L]$, i.e., B.C. of constant head.

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

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

C_i (NS) iBCC (i) = 1, C_i (i) 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

$R = 1 + \rho k_d/\theta$ where ρ is the bulk density $[M/L^3]$ of porous medium, and θ is the volumetric water content $[L^3/L^3]$

DT: Δt, the current time interval

DTL: Δt, the previous time interval

DTLL: Δt, the buffler 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: ERROR = $\left| \dfrac{\psi_j^{i+1} - \psi_j^{i}}{\psi_j^{i+1}} \right|$ where ψ_j^{i} is the pressure head at the j-th node at the i-th iteration.

ERR: The maximum value of ERROR among j nodes.

It is used as follows:

ERR $>$ ER: Do more interation

ERR $<$ 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 $t + \Delta t/2$

$\psi^{t+\Delta t/2} = \psi^{t} + (\psi^{t} - \psi^{t-\Delta t'})\,\Delta t/2\,\Delta t'$ at the beginning of inner iteration (extrapolation)

$\psi^{t+\Delta t/2} = (\psi^{t+\Delta t} - \psi^{t})/2$ during inner iteration (interpolation)

HDL (ND): ψ^{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 ψ^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

- IFLAG = 0 .... good matrix to have as many roots as its order.
- IFLAG = i .... bad matrix, to have i indefinite roots
- IFLAG = 100 .. singular matrix

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.

- IPPP = 0 .... normal case
- IPPP = 1 .... they are defined by CKTiME.

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, K, C* of ψ.

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.

$[A]\{X\} = \{B\}$

$[A]$ = LHS (nxn)

$\{X\}$ = unknown (nx1) which can either be ψ or C

$\{B\}$ = 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 $[L^3]$

$$V(i) = \int_r \int_z 2\pi r \, dr \, dz$$

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.

$$CNE(E,i) = \int_{v^e} N_k^e \, N_\ell^e \, dv, \ldots\ldots\ldots\ldots (a)$$

$$CNE\ (E,i) = \int_{v^e} N_k^e \, dv \ldots\ldots\ldots\ldots\ldots\ldots (b) \quad , \text{ or}$$

$$CNE\ (E,i) = \int_{v^e} N_k^e \, N_\ell^e \, N_\mu^e \, dv \ldots\ldots\ldots\ldots (c)$$

k, 1, and μ are 1, 2, or 3, respectively, and

i = 1 ~ 6 for (a), i= 7 ~ 9 for (b), and

i = 1 ~ 10 for (c)

$$CSE(E,j,K) = \int_{v^e} \nabla N_j \cdot \nabla N_k \, dv$$

<u>SUBROUTINE TMDP:</u> 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).

<u>SUBROUTINE TMDPD:</u> 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.

<u>SUBROUTINE SYS:</u> The global matrix is generated to calculate hydraulic head at next time step.

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

Important variables are:

$$CM(I) = \sum^{e} \sum_{j=1}^{3} C^{*e}_{j} \int_{V^e} N^e_j N^e_i \, dV$$

$$CS(I,J) = \sum^{e} \nabla N^e_i \cdot \nabla N^e_j \sum_{K=1}^{3} K^e_K \int N^e_K \, dV$$

$$CP(I) = \sum^{e} \frac{\partial N_i}{\partial Z} \sum_{K=1}^{3} K^e_K \int N^e_K \, dV$$

$$LHS(I,J) = AL * CS(I,J) + CM(I)/DT$$

$$RHS(I) = CP(I) + CM(I)/DT * HDL(I) - \sum_{j=1}^{ND} CS(I,J) * (1-AL) * HDL(J)$$

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

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

Important variables are:

$$DM(I) = \sum^{e} \sum_{j=1}^{3} \theta^e_j R^e_j \int_{V^e} N_j N_i \, dV$$

$$DA(J,I) = \sum^{e} \sum_{K=1}^{3} \theta^e_K (\vec{D}^e_K \cdot \nabla N^e_i) \cdot \nabla N^e_j \int_{V^e} N_K \, dV$$

$$DAD(J,I) = \sum^{e} \sum_{K=1}^{3} \frac{\theta^e_K}{R^e_K} (\vec{D}'^e_K \cdot \nabla N^e_i) \cdot \nabla N^e_j \int_{V^e} N_K \, dV$$

$$DDB(J,I) = \sum^{e} \sum_{l=1}^{3} \sum_{K=1}^{3} \psi^e_l (\nabla N_l \cdot \nabla N_j) K^e_K \int_{V^e} N_K \, dV$$

$$DF(J,I) = \sum^{e} \sum_{K=1}^{3} \left(-\frac{\partial \theta^e_K}{\partial t} + \lambda \theta^e_K + \rho\beta K_d\right) \int_{V^e} N_i N_j N_K \, dV$$

where D is the dispersion coefficient tensor and D is the corrected dispersion coefficient tensor.

LHS(I,J)=DM(I)/DTL -(DDB(I,J)-DA(I,J)+DF(I,J)-DAD(I,J))/2

RHS(I) =DM(I)/DTL*CON(I) +(DDB(I,J)-DA(I,J)+DF(I,J)+DAD(I,J)) /2

SUBROUTINE Q Q: It generates dispersion coefficient tensors.

OUTPUT:

DRR (ND), DRZ (ND), and DZZ (ND) are the dispersion coefficient tensors in normal region, which represent Drr, Drz = Dzr and Dzz respectively.

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

DRD (NDD), DZD (NDD), DXD (NDD) are the dispersion coefficient tensors in different region, which represents Drr, Dzz, and Drz = Dzr, respectively.

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

Important variables are:

QR (ND) which is $\vec{q}_r$, radial flux, at a node,

QZ (ND) which is $\vec{q}_z$ axial flux, at a node,

$$QR(I) = \sum^{e} \sum_{k=1}^{3} K_k^e \psi_i^e \frac{\partial N_i}{\partial r} \int_{V^e} N_k \, dV \, / V^e$$

$$QZ(I) = \sum^{e} \sum_{k=1}^{3} \left(1 + \psi_i^e \frac{\partial N_i}{\partial z}\right) K_k^e \int_{V^e} N_k \, dV \, / V^e$$

$$QA(I) = \sqrt{QR^2(I) + QZ^2(I)}$$

<u>SUBROUTINE GAUSSE:</u> It solves ND-th order matrix equation of which the form is $\left[A\right]\left\{X\right\} = \left[B\right]$.

INPUT: LHS (ND,ND)..... $\left[A\right]$

RHS (ND) .... $\left[B\right]$

OUTPUT LHS (ND,ND)... unit matrix

RHS (ND) .... X, unknown matrix.

<u>FUNCTION CZ (IP, I, J, K):</u> It assigns a value to

$$\int_{v^e} N_i^e\, N_j^e\, N_k^e\, dv$$

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/CCK/CK(ND),CC(ND)
    COMMON/CCKD/CKD(NDD),CCD(NDD),NODD(NDD),NBE,NEE
      COMMON/TMD/SER,SES,HES,CKS,RMM,APH,ITM
      COMMON/TMDD/SERD,SESD,HESD,CKSD,RMMD,APHD,ITMD
   COMMON/CNEEE/CNEE(NE,10)
      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)
   DIMENSION NOD(NE,3),HD(ND),HDL(ND),TH(ND),HDH(ND),HDS(ND),HDLL(ND)
  1 ,Q(20),TB(20),IBC(20),IBCC(20),CI(20)
  1 ,THL(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(///5X,12A5,///)
**********************************************************************
*     AL :  0 FORWARD  1 BACKWARD 1/2 CRANK-NICOLSON                 *
*     IL :  MAX. NUMBER OF INNER ITERATIONS                          *
*     ER :  ERROR BOUND OF INNER ITERATION                           *
*  DTMAX :  MAX. TIME INTERVAL IN HOUR                               *
*  DTMIN :  MIN. TIME INTERVAL IN HOUR                               *
*     DT :  INITIAL TIME INTERVAL IN HOUR                            *
**********************************************************************
      READ(5,*)AL,IL,ER,DTMAX,DTMIN,DT
             DTMAX=DTMAX/24.
             DTMIN=DTMIN/24.
             DT=DT/24.
**********************************************************************
*      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                           *
*   CBT      : 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 CONCEN.      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)
    1                            ,CI(I),I=1,NS)
          READ(5,*)(ISF(I),I=1,IHO-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
```

```
      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.OR.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.OR.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)
*------------ CALCULATE COEFFICIENTS OF BASIC FUCTIONS ---------------------*
        CALL ABC(NOD)
*--------- INTEGRATED COMBINATIONS OF BASIC FUCTIONS OVER EACH ELEMENT ---*
        CALL ITGL(NOD,V)
*------------ PREPARATION FOR THE FIRST TIME STEP -------------------------*
        DTL=DT
         TIME=DT
         TIMEL=0.
*---------------- PRINT INITIAL STATE -------------------------------------*
     HOUR=24.*TIMEL
     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)
        IF(IDFF.EQ.0)GO TO 345
        WRITE(6,542)
        DO 145 I=1,NDD
        NN=NODD(I)
        WRITE(6,540)NN,R(NN),Z(NN),THLD(I),CON(NN)
 145    CONTINUE
 345    CONTINUE
*****************************************************************************
*------------------ BEGINNING OF OUTER LOOP(NEXT TIME STEP) --------------*
```

```
***********************************************************************
 101     CONTINUE
            DO 31 I=1,ND
 31         HDS(I)=HD(I)
*------------ BEGINNING OF INNER LOOP(NEW TIME INTERVAL) ----------------*
 103     DO 30 I=1,ND
         HDH(I)=HDS(I)+(HDS(I)-HDL(I))/DTL*DT/2.
         HDL(I)=HDS(I)
 30      CONTINUE
*------------- BEGINNING OF INNER ITERATION(INCREMENT OF IT) -------------*
         IT=0
 102     CONTINUE
                  IF(IT.NE.0)THEN
             DO 17 I=1,ND
 17      HDH(I)=(HD(I)+HDL(I))*.5
                 ENDIF
         CALL TMDP(TH,HDH,NOD)
         IF(IDFF.EQ.1)CALL TMDPD(THD,HDH)
             ENDIF
         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
         IF(ERR.GE.ER)THEN
         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 --------------------*
         GO TO 103
          ENDIF
*------- RESUME INNER ITERATION FOR CONVERGENCE -------------------------*
          GO TO 102
         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,CON,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) --*
*--------- FOR APPROXIMATE CHECK OF BALANCE.                       --*
            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)
 130         SUM2=SUM2+CON(I)*TH(I)
             HOUR=TIME*24.
              WRITE(6,239)HOUR,SUM1,SUM2
 239         FORMAT(/'      AT ',F7.2,' HOUR',2X,
    1  ' W.C. SUM = ',F7.3,2X,'CON. SUM = ',F7.2,/)
 90         CONTINUE
*-------------- PREPARE NEXT TIME STEP ---------------------------------*
       TIMEL=TIME
          DTL=DT
        IF(IT.LE.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
 122      WRITE(6,540)I,R(I),Z(I),TH(I),CON(I)
        IF(IDFF.EQ.0)GO TO 543
        WRITE(6,542)
 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,I4,' 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
```

```
        TIME=CKTIME
        DT=CKTIME-TIMEL
        IPPP=1
        ENDIF
 277   FORMAT(//'    IQ=',I3,'  Q0 = ',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)
      DIMENSION ZE(3),R2(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/CNEEE/CNEE(NE,10)
         COMMON/EEE/CNE(NE,9),CSE(NE,3,3)
           DIMENSION NOD(NE,3),V(NE)
                  P=3.141592
         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
         IF(R3.LE.R(NOD(I,J)))THEN
```

```
      R3=R(NOD(I,J))
       ISM=J
      ENDIF
10    CONTINUE
       Z1=Z(NOD(I,ILG))
       Z3=Z(NOD(I,ISM))
       IM=6-ISM-ILG
       R2=R(NOD(I,IM))
       Z2=Z(NOD(I,IM))
      DR=(R3-R1)/10.0000000001
        DZ=DR
      DO 12 J=1,9
    CNEE(I,J)=0.
12    CNE(I,J)=0.
     CNEE(I,10)=0.
      DO 13 RC=R1,R3,DR
       IF(RC.LT.R2)THEN
        Z11=(Z2-Z1)/(R2-R1)*(RC-R1)+Z1
       ELSE
        Z11=(Z2-Z3)/(R2-R3)*(RC-R3)+Z3
      ENDIF
        Z22=(Z3-Z1)/(R3-R1)*(RC-R1)+Z1
      IF(Z11.GE.Z22)THEN
      BUFF=Z11
      Z11=Z22
      Z22=BUFF
      ENDIF
       DO 13 ZC=Z11,Z22,DZ
       DV=2*P*RC*DR*DZ
     V(I)=V(I)+DV
      CN1=(A(I,1)+B(I,1)*RC+C(I,1)*ZC)/2./AR(I)
      CN2=(A(I,2)+B(I,2)*RC+C(I,2)*ZC)/2./AR(I)
      CN3=(A(I,3)+B(I,3)*RC+C(I,3)*ZC)/2./AR(I)
      CNE(I,1)=CNE(I,1)+DV*CN1**2
      CNE(I,2)=CNE(I,2)+DV*CN1*CN2
      CNE(I,3)=CNE(I,3)+DV*CN1*CN3
      CNE(I,4)=CNE(I,4)+DV*CN2**2
      CNE(I,5)=CNE(I,5)+DV*CN2*CN3
      CNE(I,6)=CNE(I,6)+DV*CN3**2
      CNE(I,7)=CNE(I,7)+DV*CN1
      CNE(I,8)=CNE(I,8)+DV*CN2
      CNE(I,9)=CNE(I,9)+DV*CN3
      CNEE(I,1)=CNEE(I,1)+DV*CN1**3
      CNEE(I,2)=CNEE(I,2)+DV*CN1**2*CN2
      CNEE(I,3)=CNEE(I,3)+DV*CN1**2*CN3
      CNEE(I,4)=CNEE(I,4)+DV*CN1*CN2**2
      CNEE(I,6)=CNEE(I,6)+DV*CN1*CN3**2
      CNEE(I,5)=CNEE(I,5)+DV*CN1*CN2*CN3
      CNEE(I,7)=CNEE(I,7)+DV*CN2**3
      CNEE(I,10)=CNEE(I,10)+DV*CN3**3
      CNEE(I,8)=CNEE(I,8)+DV*CN2**2*CN3
      CNEE(I,9)=CNEE(I,9)+DV*CN2*CN3**2
13    CONTINUE
      DO 14 J=1,3
      DO 14 K=1,3
14    CSE(I,J,K)=(B(I,J)*B(I,K)+C(I,J)*C(I,K))/AR(I)**2/4.
11    CONTINUE
      RETURN
      END
***************************************************************************
```

```
*-----------------------------------------------------------------------*
*-----------------------------------------------------------------------*
*************************************************************************
        SUBROUTINE TMDP(TH,HD,NOD)
                 PARAMETER(NE=20,ND=22,IHO=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
*------------------ SATURATED MODEL ------------------------------------*
 100    TH(I)=SES
        CC(I)=0.
        CK(I)=CKS
        HD(I)=-HES
        GO TO 10
*------------------ WARRICK MODEL --------------------------------------*
 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
*------------------ VAN GENUCHTEN MODEL --------------------------------*
 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
*------------------ BROOKS AND COLEY MODEL -----------------------------*
 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*RMM/PH**(RMM+1)
        CK(I)=CKS*((TH(I)-SER)/(SES-SER))**RMM
        GO TO 10
*---------------- HAUERKAMP MODEL --------------------------------------*
 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
*------------------ SATURATED 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*SQRT(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)
```

```
        GO TO 10
 10     CONTINUE
        RETURN
        END
***************************************************************************
*-------------------------------------------------------------------------*
*-------------------------------------------------------------------------*
***************************************************************************
        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
             CM(I)=0.
             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))J1=K
      IF(I2.EQ.NODD(K))J2=K
      IF(I3.EQ.NODD(K))J3=K
 18   CONTINUE
      C1=CCD(J1)
      C2=CCD(J2)
      C3=CCD(J3)
      CK1=CKD(J1)
      CK2=CKD(J2)
      CK3=CKD(J3)
      GO TO 21
 19   CONTINUE
      C1=CC(I1)
      C2=CC(I2)
      C3=CC(I3)
      CK1=CK(I1)
      CK2=CK(I2)
      CK3=CK(I3)
 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,2,2)*CSK
        CS(I3,I3)=CS(I3,I3)+CSE(I,3,3)*CSK
        CS(I2,I1)=CS(I2,I1)+CSE(I,2,1)*CSK
        CS(I1,I2)=CS(I2,I1)
```

```
        CS(I2,I3)=CS(I2,I3)+CSE(I,2,3)*CSK
        CS(I3,I2)=CS(I2,I3)
        CS(I3,I1)=CS(I3,I1)+CSE(I,3,1)*CSK
        CS(I1,I3)=CS(I3,I1)
*  (P)
        CPK=CSK/2./AR(I)
        CP(I1)=CP(I1)+CPK*C(I,1)
        CP(I2)=CP(I2)+CPK*C(I,2)
        CP(I3)=CP(I3)+CPK*C(I,3)
 10     CONTINUE
*  RHS = SOMETHING - (F)
        DO 14 I=1,ND
         RHS(I)=CP(I)
*---------- CONSTANT 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)LHS(J,I)=0.
 16     LHS(ND-J+1,I)=0.
        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,NOD,DTL,CQ,CON,IQC,
     1 BDC,HDH,V,CBT,IDFF,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/CCK/CK(ND),CC(ND)
       COMMON/CCKD/CKD(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),DAD(ND,ND),
     1       DB(IHO),BDC(IHO),CON(ND),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(NDD),DZD(NDD),DXD(NDD),DRDD(NDD),DZDD(NDD),DXDD(NDD)
     1 ,DRE(3),DZE(3),DXE(3),DRDE(3),DZDE(3),DXDE(3)
     1 ,THD(NDD),THLD(NDD),THHD(NDD),THE(3),THLE(3),THHE(3)
     1 ,CKE(3)
```

```
      COMMON/TRA/RH,DK,DOT,AFL,AFT,GAM,ALF,BET
      COMMON/TRAD/RHD,DKD,DOTD,AFLD,AFTD,ALFD,BETD
     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,
    1 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 K=1,NDD
      IF(I1.EQ.NODD(K))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)
 17        B1=B1+ABS(HDH(NM))*CSE(E,J,M)
      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))*CNE(E,L+6)/4./AR(E)**2
         DAD(NJ,NI)=DAD(NJ,NI)+THHE(L)*((DRDE(L)*B(E,I)+DXDE(L)
     1            *C(E,I))*B(E,J)+(DZDE(L)*C(E,I)+DXDE(L)*
     1          B(E,I))*C(E,J))*CNE(E,L+6)/4./AR(E)**2*DTL/R1(L)
*13      CONTINUE
         DDB(NJ,NI)=DDB(NJ,NI)+B1*CKE(L)*CN(L,I)
         DF(NJ,NI)=DF(NJ,NI)+((THLE(L)-THE(L))/DTL+
     1      THHE(L)*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
         DT(I,J)=-DA(I,J)+DDB(I,J)+DF(I,J)-DAD(I,J)
         LHS(I,J)=LHS(I,J)-DT(I,J)/2.
         RHS(I)=RHS(I)+(LHS(I,J)+DT(I,J)+DAD(I,J))*CON(J)
 30   CONTINUE
```

```
 20   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
 15     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)
       QR(NJ)=QR(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
      IF(IDFF.EQ.0)RETURN
*------- 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/CNEEE/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)
                PARAMETER(NE=20,ND=22,IHO=2,NDD=1)
        REAL LHS
      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.O.)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
 50 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
```