**GEORGIA INSTITUTE OF TECHNOLOGY** **OFFICE OF CONTRACT ADMINISTRATION**

# PROJECT ADMINISTRATION DATA SHEET

[x] ORIGINAL [ ] REVISION NO. ______

Project No. E-26-627 GTRI/GIT DATE 7 / 21/ 83

Project Director: Dr. G. G. Eichholz School/Lab Nuclear Engr.

Sponsor: E. I. du Pont de Nemours & Company, Savannah River Plant, Aiken, SC

Type Agreement: P.O. No. AX-0598188 (Prime DOE AC09-76SR00001)

Award Period: From 6/27/83 To 7/1/84 (Performance) --- (Reports)

Sponsor Amount:

| | This Change | Total to Date |
|---|---|---|
| Estimated: | $ 49,861 | $ 49,861 |
| Funded: | $ 49,861 | $ 49,861 |

Cost Sharing Amount: $ None Cost Sharing No: N/A

Title: Develop Transport Model for Radionuclide Migration in the SRP Lysimeters

**ADMINISTRATIVE DATA** OCA Contact William F. Brown Ext. 4820

1) Sponsor Technical Contact:

S. B. Oblath
E.I. du Pont de Nemours & Co.
Savannah River Plant
Aiken, SC 29808-0001
(803) 725-2838

2) Sponsor Admin/Contractual Matters:

Francis Thomas Iwuc
E. I. du Pont de Nemours & Co.
Savannah River Plant
Aiken, SC 29808-0001
(803) 725-3866

Defense Priority Rating: None Military Security Classification: None
(or) Company/Industrial Proprietary: ______

**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:**



**COPIES TO:**

Project Director
Research Administrative Network
Research Property Management
Procurement/EES Supply Services
Research Security Services
Reports Coordinator (OCA)
GTRI
Library
Project File

GEORGIA INSTITUTE OF TECHNOLOGY | OFFICE OF CONTRACT ADMINISTRATION

SPONSORED PROJECT TERMINATION/CLOSEOUT SHEET

Date 11/16/84

Project No. ~~E-25-655~~ (Formerly E-26-627) School/XXX/ ME (Formerly NE)
P.O. No. AX-0598188 (Prime DOE AC09-76SR00001)

Includes Subproject No.(s) None

Project Director(s) Dr. G. G. Eichholz GTRI / XXX

Sponsor E. I. Dupont De Nemours & Co., Savannah River Plant, Aiken, S.C.

Title Develop Transport Model for Radionuclide Migration in the SRP Lysimeters

Effective Completion Date: 7/1/84 (Performance) 7/1/84 (Reports)

Grant/Contract Closeout Actions Remaining:

- [ ] None
- [x] Final Invoice or Final Fiscal Report
- [ ] Closing Documents
- [x] Final Report of Inventions (DOE)
- [ ] Govt. Property Inventory & Related Certificate
- [ ] Classified Material Certificate
- [ ] Other ______

Continues Project No. ______ Continued by Project No. ______

COPIES TO:

Project Director
Research Administrative Network
Research Property Management
Accounting
Procurement/EES Supply Services
Research Security Services
Reports Coordinator (OCA)
Legal Services

Library
GTRI
Research Communications (2)
Project File
Other Heyser, Jones

Georgia Institute of Technology
A UNIT OF THE UNIVERSITY SYSTEM OF GEORGIA
SCHOOL OF NUCLEAR ENGINEERING AND HEALTH PHYSICS
ATLANTA, GEORGIA 30332
(404) 894-3720

August 11, 1983

Dr. S. B. Oblath
Savannah River Plant
E. I. DuPont de Nemours & Co.
Aiken, SC 29808

First Monthly Progress Letter
Project AX-0598188 - Our Project E-26-627

Dear Dr. Oblath:

The above project got under way at the beginning of July, 1983. Mr. John C. Oliver, a Ph.D. candidate in our School at this point is the only research assistant working on this problem. As other areas of work are identified additional staff will be involved, probably starting next month.

For mutual information purposes Mr. Oliver and I visited SRP on July 8 to discuss the present status of the lysimeter tests, which were inspected, and to gather information on currently available data on the tests and previous work on modeling.

Since then the applicability of using a one-dimensional transport equation for modeling soil columns was checked and verified. The solution to the convective - dispersive transport equation used in DP-1591 was verified and implementation of the appropriate subroutines in the code MODEL 2, used to generate the data in DP-1591, was accomplished. Further work to verify these data is in progress.

Independently we are looking at flow paths around waste packages and leaching conditions under unsaturated flow conditions. This work is expected to be related to the lysimeter model in the coming months.

Yours sincerely,

Geoffrey G. Eichholz
Project Director

GGE/vw

cc. W. F. Brown (OCA)

Georgia Institute of Technology
A UNIT OF THE UNIVERSITY SYSTEM OF GEORGIA
SCHOOL OF NUCLEAR ENGINEERING AND HEALTH PHYSICS
ATLANTA, GEORGIA 30332
(404) 894-3720

October 14, 1983

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

Monthly Progress Report - Project E26-627

Dear Dr. Oblath:

In confirmation of our discussion at yesterday's meeting with you and Dr. Stone, I want to summarize the status of the project at this stage. We feel that the existing saturated flow model has been checked adequately and the necessary corrections have been made. Further work on that model is probably unprofitable at this stage.

Other models have been reviewed, primarily, those developed under ONWI auspices. These models will be further evaluated and tablulated with respect to their suitability to describe unsaturated flow under near-surface conditions. Ultimately the model will have to be formulated as a one-dimensional, two-region cylindrical system.

Additional information needs to be obtained particularly on two subjects:

a. The nature of the flow through or around the waste package.

b. The effective leach rate that occurs when water movement is unsaturated or cyclic.

We are trying to address the second aspect already in conjunction with some other work we are doing and expect to correlate results. With regard to the first one, we hope to run some small-scale tests to look at the effect of comparing crushed and uncrushed laboratory waste and to get a general idea of the hydraulic conductivity changes introduced by the waste package. We would appreciate it if you would send us a package of clean but equivalent lab trash.

Please call me if there are any additional questions.

Yours truly,

Geoffrey G. Eichholz
Regents' Professor

GGE/vw

cc: W. F. Brown (OCA)

Georgia Institute of Technology
A UNIT OF THE UNIVERSITY SYSTEM OF GEORGIA
SCHOOL OF NUCLEAR ENGINEERING AND HEALTH PHYSICS
ATLANTA, GEORGIA 30332
(404) 894-3720

November 11, 1983

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

Monthly Progress Report - Project E26-627

Dear Dr. Oblath:

During the past month, work has been concentrated in two areas: the adaptation of an unsaturated model to lysimeter conditions and flow conditions around an inhomogeneous waste package. We hope to have an unsaturated one-dimensional model working early in the new year. Extension to the two-dimensional case may be relatively simple. In view of John Oliver's impending departure, we are trying to maintain continuity in effort through Messers. Harry K. Anderson and F. N. deSousa. We are also documenting the final version of the saturated model for the record.

We have started putting together a simulated waste package containing miscellaneous waste materials in an ice cream container. This will be tested for permeability and flow patterns in air and water at various stages of compaction.

Leach tests have been started on TVA waste resin samples using slowly circulating soil-equilibrated water. It is planned to run four loops in parallel to establish baseline leach conditions in saturated flow. Since the activity levels are low, this is expected to be a relatively long-range test.

Please call me if there are any additional questions.

Yours truly,

Geoffrey G. Eichholz
Regents' Professor

GGE/ctm

cc: W. F. Brown (OCA)

Georgia Institute of Technology
A UNIT OF THE UNIVERSITY SYSTEM OF GEORGIA
SCHOOL OF NUCLEAR ENGINEERING AND HEALTH PHYSICS
ATLANTA, GEORGIA 30332
(404) 894-3720


February 8, 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-26-627

Dear Dr. Oblath:

During the past month work has continued on the development of a two-dimensional flow model to describe flow in the lysimeter through and around the waste layer. Mr. D. Y. Suh has been added to the team to provide additional programming expertise for this work.

Several crushing tests have been conducted on simulated waste materials, resembling those in the lysimeters, to measure the change in permeability, compared with surrounding soil, the waste layer has introduced. At this time it looks as if the compacted layer may short-circuit some surrounding soil and serve as a water-reservoir; this would be expected to accelerate leaching. It is proposed to insert the crushed waste layer into a short soil test bed to determine this effect.

Further tests have been conducted to measure the residual soil moisture in drained columns. For sand the residual water content seems to be fairly independent of pore size. Tests are continuing on Savannah River soil samples.

Please call me if there are additional questions.

Yours truly,

Geoffrey G. Eichholz
Regents' Professor

GGE/vw

cc: W. F. Brown (OCA)

Georgia Institute of Technology
A UNIT OF THE UNIVERSITY SYSTEM OF GEORGIA
SCHOOL OF NUCLEAR ENGINEERING AND HEALTH PHYSICS
ATLANTA, GEORGIA 30332

(404) 894-3720

March 8, 1984

Dr. S. B. Oblath
Waste Disposal Technology Division
Savannah River Laboratory
E.I. DuPont deNemours & Company, Inc.
Aiken, SC 29808

Monthly Progress Report - Project E-26-627

Dear Dr. Oblath:

During the past month considerable progress has been made on the development of a new computer model to simulate the movement of waste materials in the lysimeters under unsaturated conditions. The model will be a two-dimensional finite element model, solving the transport and flow equations simultaneously. A computer program for unsteady unsaturated flow has been completed, using a one-dimensional finite-element method for space and an explicit finite difference method for time. Work is in progress to make the program an implicit one to verify stability and accuracy of the method.

A very simple program has been written to study the two-dimensional finite-element method. It is proposed next to complete the program for the implicit method and to combine this with an explicit one into a predictor-corrector method.

Measurements have continued to determine drying rates on soil columns and the residual water content. As expected, higher clay-content soils have higher water retention, but conductivity measurements indicate that little of that retained water may contribute to migration effects. It is planned to design experiments to determine whether the clay-retained water contributes to waste leaching.

Further crushing tests have been conducted on simulated waste with interesting results. It is evident that not all the waste would be fully crushed by the overlying soil at 10 ft depth. Even when further compacted, the waste layer remains relatively open and permeable. This raises the question whether water flow would be diverted into waste volume and stored there, increasing the leach rate. We are starting some simple tests using a sand bed in a large barrel to study the flow into and around such a simulated waste layer.

We would welcome a visit from you to discuss this work. Please call me if there are any questions.

Yours sincerely,

G.G. Eichholz
Regents' Professor

cc: W.F. Brown (OCA)

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

May 11, 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-26-627

Dear Dr. Oblath:

During the past month we have continued work in two areas: The 1-D and 2-D flow models have been corrected and it is expected to introduce the transport model by the end of the month. The code will then be compared with the experimental results which you sent with your letter of April 13.

On the experimental side, work has progressed on a small cylindrical system in a drainable drum to simulate the flow and moisture distribution. Two lysimeter systems are being designed; in one water infiltration into the cylindrical waste volume can occur from above only; in the other, lateral flow is possible as well. (See attached sketch) A number of nickel-plated electrodes have been made up, to be embedded in various regions in the lysimeter to monitor moisture conditions. This should help indicate whether the compacted waste region attracts water, causes perching, or speeds up drainage through that region.

Though we expect to continue this work under a renewed contract we will prepare an annual report as a final report on the present contract before June 30, 1984.

Yours Sincerely,

G.G. Eichholz
Regents' Professor

cc: O.H. Rodgers (OCA)

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

June 11, 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-26-627

Dear Dr. Oblath:

During the past month work has proceeded steadily on all three fronts. Improvements have been made in the calculational model and we hope to be able, next month, to compare it with the latest lysimeter results.

A simulated waste pellet has been inserted into a cylindrical soil-filled drum and we are monitoring water flow to establish the flow regime into, through, or around the waste material.

Additional tests are proceeding to obtain drainage coefficients for SRP soil and to predict unsaturated flow conditions. These tests will, hopefully, provide a correlation between soil type, permeability, drainage rates, and residual moisture content.

A final project report is being written to summarize the year's results. Many of these are still only preliminary in nature and it is expected to complete the work under the renewal contract being negotiated at present.

Yours sincerely,

G. G. Eichholz,
Regents' Professor

GGE/swm

cc: O. H. Rodgers

# RADIONUCLIDE MIGRATION IN THE SRP LYSIMETERS

Final Report

Project E26-627 (SRP Purchase Order AX0598188)

edited by

Geoffrey G. Eichholz
Project Director

Submitted to

Waste Disposal Technology Division
Savannah River Laboratory
EI Du Pont de Nemours & Co.
Aiken, S. C. 29808

June 1984

CONTENTS

## SUMMARY

The project described in this report was undertaken in support of the current studies conducted by the Savannah River Laboratory on the migration of radionuclides from on-site disposal trenches. These studies center on a series of lysimeters which have been installed to simulate various waste forms and flow conditions in local SRP soil and under local climatic conditions.

The work described here, which is being continued, addresses three separate but related tasks:

1. The development of an improved transport model to describe and predict waste flow observations in the lysimeters;
2. Experimental tests to characterize the flow characteristics of unsaturated SRP soil; and
3. Leach tests on simulated waste material in a configuration resembling that of the lysimeters to provide guidance to the model development in describing the modification in flow pattern and source term introduced by the waste volume.

Project Personnel (all part-time)

| | |
|---|---|
| Geoffrey G. Eichholz, Ph.D. | Project Director |
| T. F. Craft Ph.D. | Senior Research Scientist |
| John C. Oliver, M.S. | Graduate Research Assistant |
| Fernando N. de Sousa, M.S.H.P. | Graduate Research Assistant |
| Harry K. Anderson, B.S. | Graduate Research Assistant |
| Suzanne G. Chervitz, B.S.H.P. | Graduate Research Assistant |
| Denise D. Hardy, B.S. | Graduate Research Assistant |
| Ann A. Mizner, M.S.H.P. | Graduate Research Assistant |
| Deog Y Suh, B.S.N.E. | Graduate Research Assistant |

# INTRODUCTION

Solid radioactive wastes have been stored at the Savannah River Plant (SRP) since the early days of operation and low-level wastes have been buried there in shallow trenches. In order to assess any potential environmental impact, extensive tests have been conducted at various times to study the characteristics of the underlying soil, the hydrology and the meteorological factors affecting water flow through potential disposal sites (1,2,3). In addition, extensive studies have been conducted to assess the suitability of the SRP site as a permanent disposal site for high-level wastes (4,5,6). Reference 6, in particular, contains much of the relevant literature. The impact calculations in that Statement are more thoroughly developed for the airborne pathway than the liquid one, which is primarily based on the AQUAMAN code (7) and the ORNL methodology (8). These models typically assume a uniform geological medium surrounding the waste, saturated flow conditions, and do not readily accommodate the special conditions associated with a back-filled near-surface trench in a humid climate, such as is found at SRP.

To obtain some experimental evidence regarding the specific leaching and migration conditions in SRP soil, an extensive field study was initiated there in 1981, which uses a large number of lysimeters to define leaching and migration rates from "typical" buried wastes(9). These lysimeters, shown diagrammatically in Fig. 1, were constructed of corrugated aluminum pipe sections that were coated with asphalt. They are 6 or 10 ft. in diameter and 10 ft. deep. The bottom of the lysimeter rests on a gravel bed and percolated water can be pumped out and sampled. Ordinarily, only natural precipitation provides the water flow through the lysimeter, which therefore, varies considerably with the seasons. The principal difference between lysimeters was the nature of the waste buried, some of which is shown in Fig. 2 (9). Most of the waste contained either fission products or plutonium traces on a rather heterogeneous mixture of laboratory materials, such as beakers, wipers, containers, gloves and metallic objects, that were poorly or not all consolidated . Initial observations have been reported by Oblath, Stone and Wiley (10) and showed the appearance of cobalt-60 and some cesium-137 in the porous cup samplers beneath the waste form. These tests have supplemented other observations on waste migration at the SRP waste disposal area. (11).

The lysimeter tests are intended to be of a long-term nature and planned to be conducted over several years into the future. However, to be useful it is important to be able to explain any observations and to correlate them with the site characteristics, waste characteristics and rainfall in a way that permits extrapolation to the actual disposal area. This requires the development of an adequate calculational model and this is the major objective of the present project.

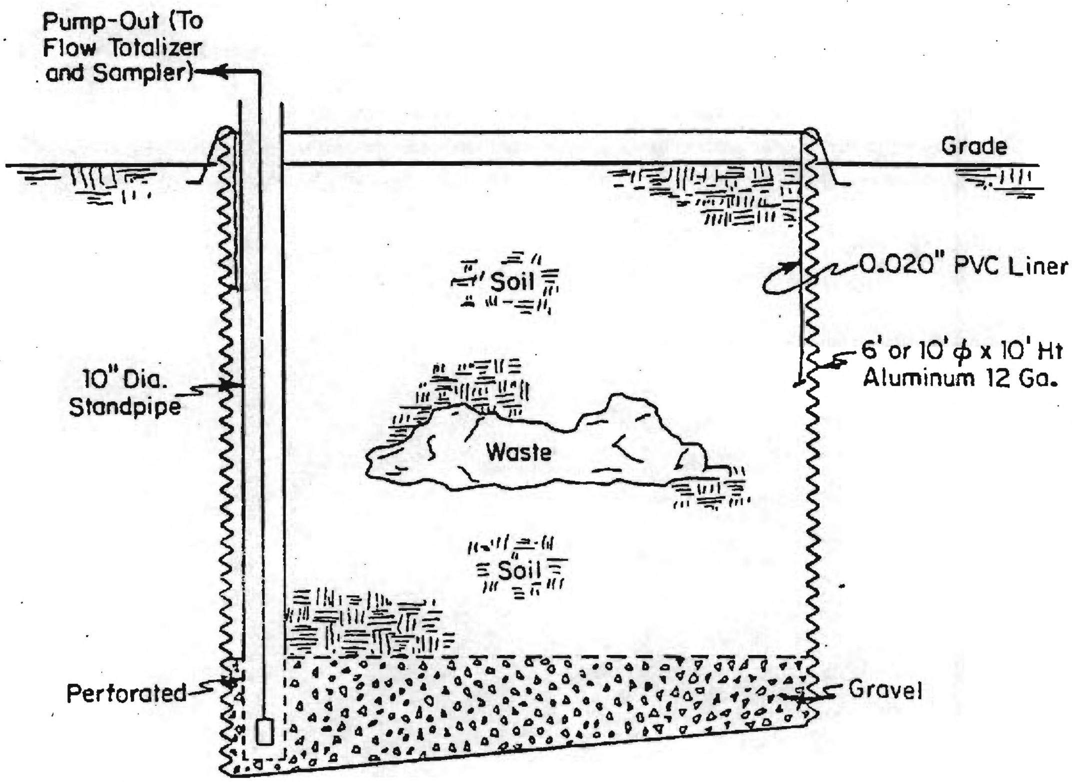



FIGURE 1. Lysimeter Cross Section (Ref. 9)

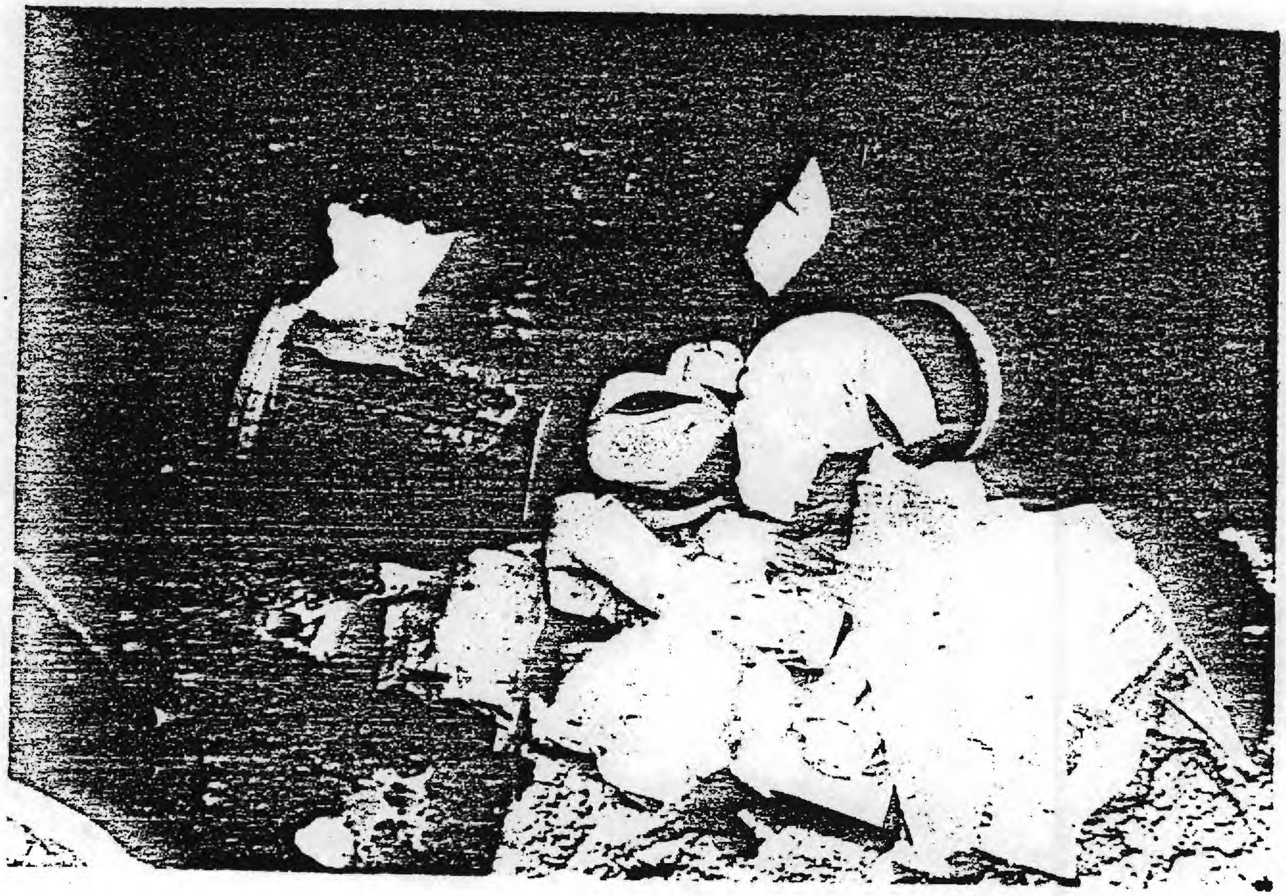


FIGURE 2. Separations Laboratory Glove Box Waste in Lysimeter (Ref. 9)

## MODEL DEVELOPMENT

To describe the migration of waste material through the backfill and soil underlying the waste trench, it is important to identify the various processes involved. Figure 3 diagrammatically indicates the main stages which in one form or other underlie all models. These are the rate of water infiltration, the leaching of radionuclides from the waste form, the subsequent movement of the dissolved or absorbed radionuclides with the ground water, the selective removal or retardation of the radioactive material on rock or soil surfaces, and the emergence of the potentially contaminated water into the accessible environment.

The basic procedure for choosing a suitable model has been indicated recently by Simmons and Cole (12), who list a number of current programs. There are a fair number of transport models in the literature that simulate mass transport processes, using typically the same transport equations which are solved through finite-element or finite-difference methods. Among these are the models of Duguid and Reeves (13), Papadopoulos and Winograd (14), Lu (15), Oztunali and Aikens (16), Silvieira et al. (17), Cleary and Ungs (18) and Burkholder and Rosinger (19). For unsaturated conditions, Yeh and Luxmoore (20) have described a model and a literature review has been done at Georgia Tech. by de Sousa (21).

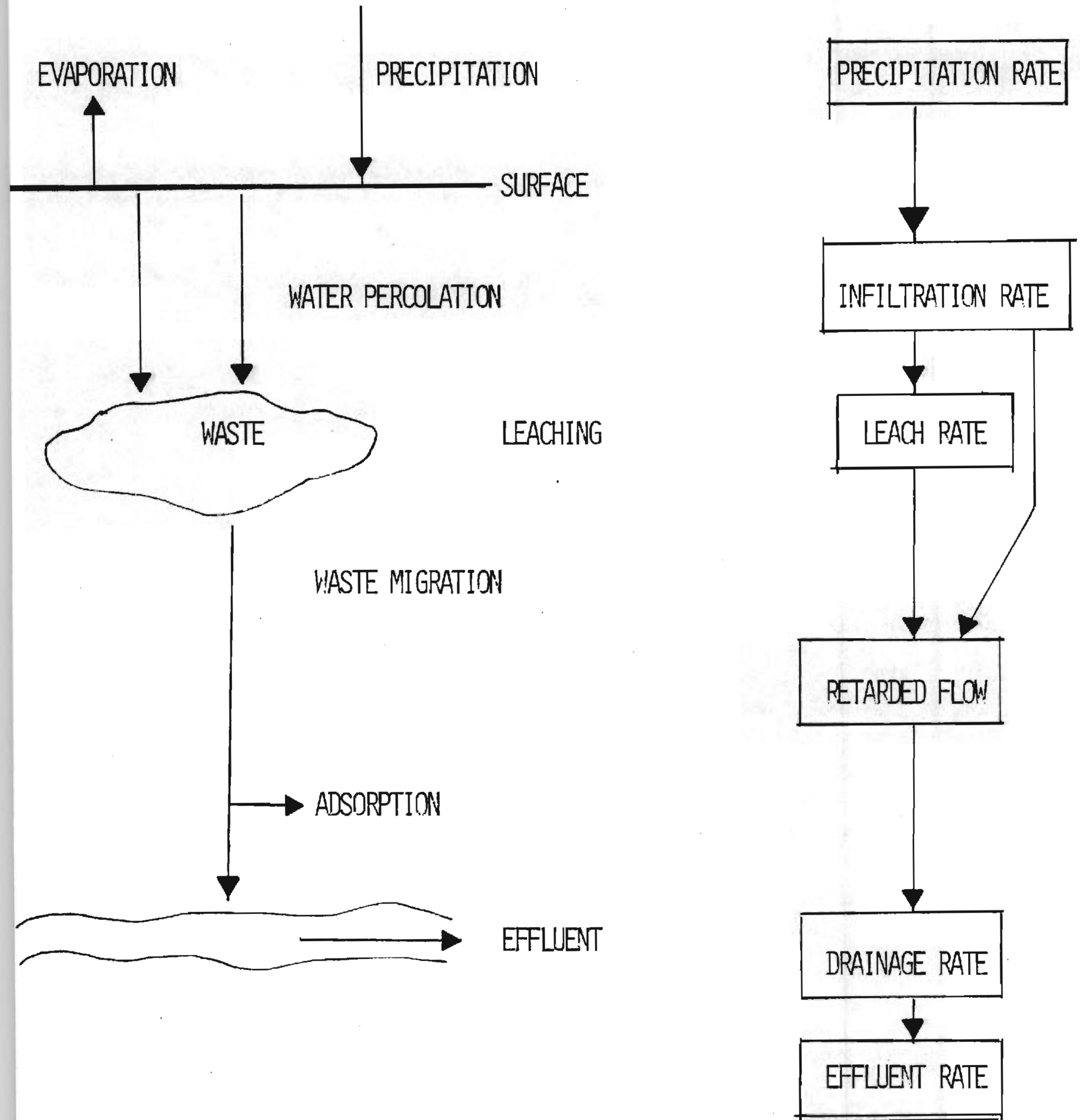



FIG. 3 MIGRATION MODEL DIAGRAM

For simplicity most models have been based on a one-dimensional description, with vertical flow through a homogeneous saturated medium whose characteristics could be described simply in terms of the hydraulic conductivity or porosity and the surface absorption capacity, $K_d$. Hooker and Root (9), in their description of the SRP lysimeter tests, adopted Cleary's model (18) in a preliminary form to analyze flow behavior.

One of the motivations of the present project was the realization that the lysimeters in practice do not satisfy the assumptions of the saturated models. Relying as they do on rather spasmodic rainfall, and 1983 was a very dry summer, the soil is not normally saturated and this was recognized early and reported by Horton (22). In addition, the rather large obstruction posed by the waste material in the lysimeters makes it unlikely that the flow will percolate smoothly, solely in a vertical direction. For that reason another objective of the present work is to develop a 2-dimensional model, that can take into account the diversion of water flow owing to the presence of the waste material.

As a starting point, the applicability of using a one-dimensional saturated transport equation was checked. The solution to the convective dispersive transport equation in Ref (9) was verified and the appropriate subroutines in the code MODEL 2 used to generate the data in Ref. 9 were implemented. It was found that some corrections had to be made in that code. Adequate agreement was obtained for the corrected code with computations done independently at Georgia Tech and SRP.

To deal adequately with actual conditions in the lysimeters it was decided to develop a new program that would be two-dimensional and capable of dealing with unsaturated flow conditions. In preparation for this, the parameters involved were identified and are listed in Table 1.

As Table 1 shows, the principal factors affected in moving from a saturated to an unsaturated flow model are the hydraulic conductivity, the time integration and the variable water content, as well as the major transition to a finite-element solution. Table 2 compares several of the unsaturated models that have been described in the literature. Each of them has some obvious advantages and disadvantages. FEMWASTE probably comes closest to the proposed approaches described in Table 1.

The principal difference between the models listed in Table 2 and the situation encountered in the SRP lysimeters is imposed by the cylindrical geometry of the lysimeters. This is illustrated in Fig.4 which compares the one-dimensional geometry assumed by the Cleary model (9) with a configuration that allows for the diversion of water flow into or around the waste volume. This gives rise to the need to develop a two-dimensional model in cylindrical coordinates. This work is still in progress and the present description should be considered only preliminary in nature.

TABLE I

MODEL COMPARISON

TRANSPORT EQUATION:

| PARAMETER | SATURATED | UNSATURATED | FUTURE |
|---|---|---|---|
| DIMENSION | 1 | 1-2 | 1-2 |
| HOMOGENEITY | HOMOGENEOUS | HOMOGENEOUS | HETEROGENEOUS |
| ISOTROPY | ISOTROPIC | ISOTROPIC | ANISOTROPIC |
| TIME ANALYSIS | UNSTEADY | UNSTEADY | UNSTEADY |
| DISPERSION COEFFICIENT(D) | CONSTANT | $D(\theta)$ | $D(\theta,z)$ |
| WATER CONTENT ($\theta$) | CONSTANT | VARIABLE | VARIABLE |
| WATER FLUX (q) | CONSTANT | VARIABLE | VARIABLE |
| FIRST ORDER DECAY (LIQ)($\alpha$) | YES | YES | YES |
| FIRST ORDER DECAY(SOL)($\beta$) | NO | YES | YES |
| ZERO ORDER DECAY(LIQ)($\gamma$) | NO | NO | YES |
| HYDRAULIC CONDUCTIVITY(K) | CONSTANT | $K(\theta)$ | $K(\theta,z)$ |
| $K(\theta)$ | CONSTANT | BROOKS-COREY | DIFFERENT MODELS |
| $\theta(h)$ | CONSTANT | GARDNER | DIFFERENT MODELS |
| SORPTION | LINEAR | LINEAR | DIFFERENT MODELS |
| BOUNDARY CONDITION | EXPON. DECAY | CONSTANT | SEVERAL |
| SOLUTION | ANALYTICAL | FEM | FEM |
| TIME INTEGRAL | ANALYTICAL | IMPLICIT FD | IMPLICIT,EXPLICIT CRANK-NICOLSON |
| FEM SOLUTION | NO | LINEAR | LINEAR,HERMITIAN |
| COMPRESSIBILITY($\alpha'$) | NO | NO | YES |

SATURATED - PREVIOUS MODEL

UNSATURATED - MODEL BEING DEVELOPED

FUTURE - OPTIONS THAT CAN BE INCLUDED IN THE FUTURE

TABLE 2

UNSATURATED MODELS

| PARAMETER | SEGOL | SUMATRA-1 | TARGET | FEMWASTE | MLTRAN |
|---|---|---|---|---|---|
| DIMENSION | 2-3 | 1 | 3 | 2 | 2 |
| COMPRESSIBILITY ($\alpha'$) | YES | NO | NO | YES | YES |
| DISPERSION COEFFICIENT(D) | D(O) | D(O) | D(O) | D(O) | NO |
| FIRST ORDER DECAY(LIQ)($\alpha$) | NO | YES | YES | YES | NO |
| FIRST ORDER DECAY(SOL)($\beta$) | NO | YES | YES | YES | NO |
| ZERO ORDER DECAY(LIQ)($\gamma$) | YES | YES | NO | NO | NO |
| HYSTERESIS | NO | NO | NO | NO | NO |
| SORPTION | NO | LINEAR | FREUNDLICH | LINEAR | LINEAR |
| SOLUTION | FEM | FEM | IFD | FEM | IFD |
| FEM SOLUTION | HEXAHEDRAL | HERMITIAL CUBIC | | QUADRIL. | |

FEM - FINITE ELEMENTS

IFD - INTEGRATED FINITE DIFFERENCES

SEGOL - GENEVIEVE SEGOL (32)

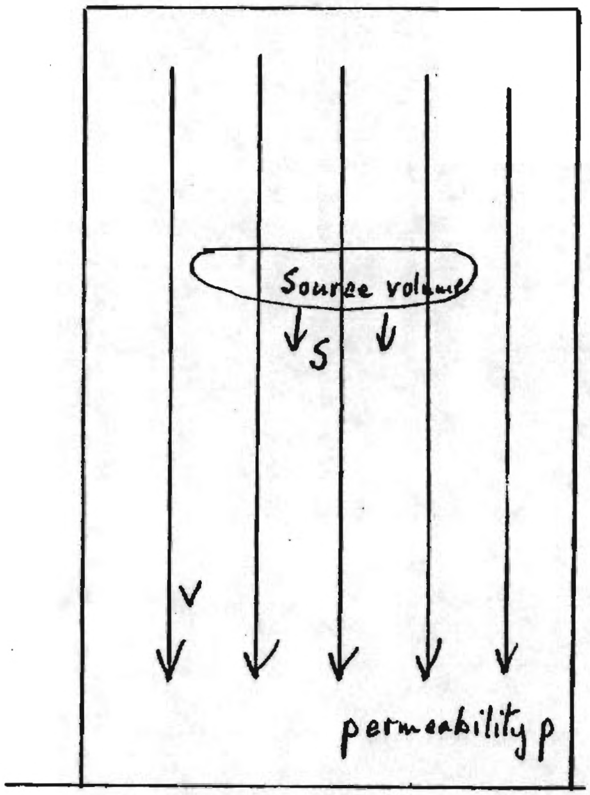
SUMATRA-1 - M. Th. VAN GENUCHTEN (28)

TARGET - DAMES & MOORE (31)

FEMWASTE - G. T. YEH & D. S. WARD (29)

MULTRAN - A. E. REISENAUER (33)

DP - 1091 MODEL



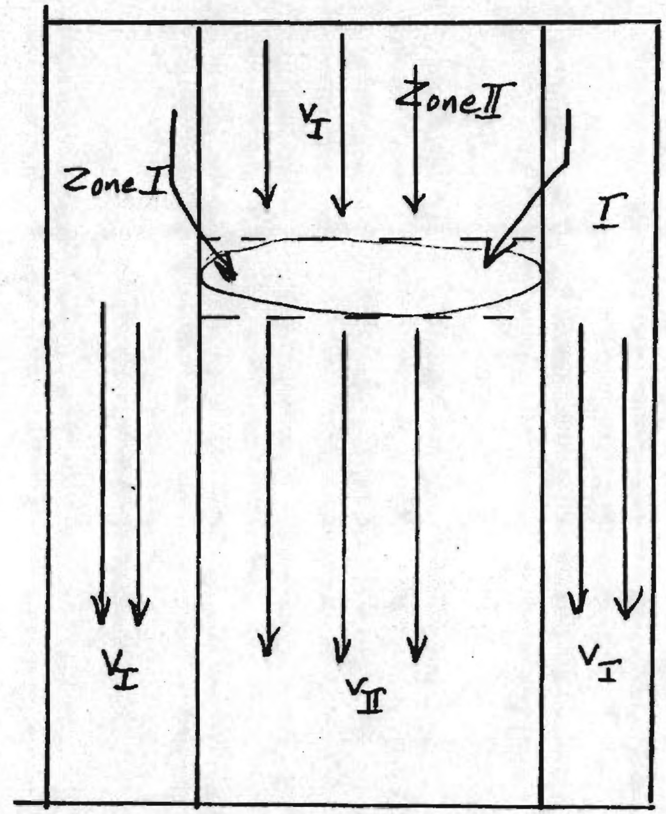

V CONSTANT

P UNIFORM

SOIL SATURATED

S SOURCE INJECTION RATE

GA. TECH. MODEL




$V_I \neq V_{II}$

SOIL UNSATURATED

SOURCE INJECTION PERIODIC AND REDUCED

LITTLE LEACHING IF $V_{II} << V_I$

Fig. 4 Comparison of Flow Regimes

# THE UNSATURATED FLOW AND TRANSPORT MODEL

## INTRODUCTION

The current waste disposal practices often place undesirable materials in environments in which the movement of the pollutants occurs under variably unsaturated conditions. The transport processes are, in general, described by a set of partial differential equations which are a function of the state variables of pressure and concentration.

What makes the unsaturated flow and transport equations difficult to solve is the fact that the hydraulic conductivity and the water content are a function of the pressure head. This implies that the resulting equations are non-linear, and consequently the approximating algebraic equations will also be non-linear. To handle this non-linearity, further assumptions are made in order to linearize the algebraic equations, or the solution is reached by iterative methods.

This report presents the efforts done in developing a 1-dimensional and a 2-dimensional finite element model that can be used to simulate the water flow and solute transport through unsaturated soils. A description of the model, as it is now, is presented, as well as the steps that are going to be taken in the near future. Also, a brief description of the capabilities that the model may have in the future is presented.

## II-FLOW AND TRANSPORT EQUATIONS

### 1-FLOW EQUATION

The water flow equation comes from the combination of the Darcy's law with the continuity equation. The Darcy's law is .

$$q = -K(h)\nabla H \tag{1}$$

Where $q$ is the volumetric flux, K is the hydraulic conductivity, h is the pressure head, and H is the hydraulic head. The continuity equation can be written as

$$\frac{\partial \theta}{\partial t} = -\nabla . q \tag{2}$$

Where $\theta$ is the volumetric water content and t is time.
Combining eq. 1 and 2.

$$\frac{\partial \theta}{\partial t} = \nabla . (K(h)\nabla H) \tag{3}$$

The hydraulic head, H, is given by

$$H = z + h \tag{4}$$

where z is the elevation head. Introducing eq. 4 into eq. 3.

$$\frac{\partial \theta}{\partial t} = \nabla . (K(h)\nabla (z+h)) \tag{5}$$

For simplicity, writing eq. 5 in one dimension

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left(K(h)\frac{\partial h}{\partial z}\right) + \frac{\partial K(h)}{\partial z} \tag{6}$$

But

$$\frac{\partial h}{\partial z} = \frac{\partial h}{\partial \theta}\frac{\partial \theta}{\partial z}$$

Hence

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left(K(h)\frac{\partial h}{\partial \theta}\frac{\partial \theta}{\partial z}\right) + \frac{\partial K(h)}{\partial z} \tag{7}$$

The quantity $\frac{\partial \theta}{\partial h}$ is called specific water capacity.

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left(\frac{K(\theta)}{C(\theta)}\frac{\partial \theta}{\partial z}\right) + \frac{\partial K(\theta)}{\partial z} \tag{8}$$

The hydraulic diffusivity is defined as the ratio $K(\theta)/C(\theta)$. Consequently

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left(D(\theta)\frac{\partial \theta}{\partial z}\right) + \frac{\partial K(\theta)}{\partial z} \tag{9}$$

It is seen that eq. 9 is written in terms of the water content, $\theta$; the same derivation is applied if the chosen variable is the pressure head, h. In this case, the equation is given by:

$$C^* \frac{\partial h}{\partial t} = \frac{\partial}{\partial z}\left(K(h)\frac{\partial h}{\partial z}\right) + \frac{\partial K(h)}{\partial z} \tag{10}$$

The term $C^*$ is equal to $C(\theta)$ for unsaturated soils, but for saturation it is given by:

$$C^* = \frac{\theta}{n} + n\frac{\partial S_w}{\partial h} \tag{11}$$

where n is the porosity, $S_s$ is the specific storage efficient and $S_w$ is the degree of saturation. The second term on the right-hand side of eq. 11 is zero for a saturated medium.

The other term, on the other hand, is insignificantly small compared to the second term when the soil becomes unsaturated; in this case, C* is equal to $\partial\theta/\partial h$, which is the value of $C(\theta)$ in eq. 8. The reason for having introduced $C(\theta)$ as $\partial\theta/\partial h$ instead of eq.11 is because eq. 8 cannot be applied to a saturated soil, since $C(\theta) \rightarrow 0$.

As is pointed out by Raudkivi and Callander (27), the equation using $\theta$ as the variable is better for numerical solutions of unsaturated flow because changes in $\theta$ and D are two or three or ders of magnitude smaller than corresponding changes in h and $\partial\theta/\partial h$. However, as $\theta$ approaches saturation the driving potential becomes independent of moisture content and $D(\theta)$ tends to infinity. Consequently, solutions involving saturation and unsaturation have to use the equation using pressure head.

## 2. Transport Equation

The governing partial differential equation is based on the following principle of mass conservation (Yeh, 1982 and Van Genuchten, 1978):

Rate of change of mass = (advection in - advection out)
+(Dispersion in - Dispersion out)
-Decay

(12)

Equation 12 is transformed from a verbal description into the following mathematical equation:

$$\frac{\partial}{\partial t}(\theta C+\rho S) = \nabla\cdot(\theta D\nabla C - q C) + \alpha\theta C + \beta\rho S + \gamma\theta + \alpha'\frac{\partial h}{\partial t}(\theta C+\rho S) \quad (13)$$

where:

C is the solution concentration ($ML^{-3}$)
D is the dispersion coefficient ($L^2T^{-1}$)
S is the absorbed concentration
$q$ is the volumetric flux ($LT^{-1}$)
$\alpha$ is a first-order rate constant (liquid phase) ($T^{-1}$)
$\beta$ is a first-order rate constant (solid phase) ($T^{-1}$)
$\gamma$ is a zero-order rate constant (liquid phase) ($ML^{-3}T^{-1}$)
$\rho$ is the bulk density ($ML^{-3}$)
$\alpha'$ is the compressibility of the medium ($L^{-1}$)
$\theta$ is the volumetric moisture content
h is the pressure head (L)

In order to solve eq. (13), it is necessary to determine the moisture content ($\theta$) and the volumetric flux ($q$). In general, most of the available models assume the moisture content to be a unique function of the pressure head (h), and use equation 10 (the flow equation) to determine $\theta$. The volumetric flux is also obtained from eq.(10) by making use of Darcy's law (eq.1). However, the relation between $\theta$ and h is an hysteretic one; this is due to the fact that air is entrapped in the pore spaces during wetting of the soil. Consequently, for a given pressure head the water content values are generally smaller during wetting than drying. Hysteresis will be included in the model, probably by using the procedure given by Gilham et al. (26).

The dispersion coefficient (D) represents the effects of both molecular diffusion and mechancial dispersion. It is a tensor given by

$$\theta D_{ij} = a_T |\bar{U}| \delta_{ij} + (a_L - a_T) U_i U_j / |\bar{U}| + a_m T \delta_{ij} \theta \tag{14}$$

where:

$a_T$ is the transverse dispersivity (L)
$a_L$ is the longigudinal dispersivity (L)
$\delta_{ij}$ is the Kronecker delta
$a_m$ is the molecular diffusion coefficient ($L^2/T$)
$T$ is the tortuosity
U is the magnitude of the velocity vector
$U_i$ is the i-th component of velocity vector
$U_j$ is the j-th component of velocity vector

One also needs an expression relating the absorbed concentration (s) with the solution concentration C(c). Many models are available to describe absorption or ion exchange, such as equilibrium and kinetic models. In general, the available models use the linear absorption isotherm

$$S=KC \tag{15}$$

where K is the distribution coefficient; the model being developed will incorporate several different sorption models.

## 3-Initial and Boundary Conditions

In order to completely describe the transport of radioactive materials through unsaturated soils, it is necessary to specify the initial and boundary conditions. In general, it is assumed that the initial conditions are given by:

$$h_{(x,z,o)} = h_{o(x,z)}$$
$$C_{(x,z,o)} = C_{o(x,z)} \tag{16}$$

The specification of boundary conditions is the most difficult task in groundwater flow and transport modeling (29). The boundary conditions may be one of the following: Dirichlet boundary, for which the functional value is prescribed, Neumann boundary, for which the flux due to the gradient of the function is known, or Cauchy boundary, for which the total flux is given. A more difficult problem arises when the boundary condition is not known a priori; either one of the three boundary conditions may prevail and change with time. These boundary conditions are given by:

$$
\begin{aligned}
&\text{Dirichlet:} && C_{(x,z,t)} = C_d(x_b, z_b, t) \\
&\text{Cauchy:} && \bar{n} \cdot (\bar{V} C - \theta D \cdot \nabla C) = q_c(x_b, z_b, t) \qquad (17) \\
&\text{Neumann:} && -\bar{n} \cdot \theta D \cdot \nabla C = q_n
\end{aligned}
$$

The conditions imposed on the variable boundary, which is normally the soil-air or soil-water interface, are either Neumann with zero concentration gradient or Cauchy with the total flux given.

## III - MODEL DESCRIPTION

### 1. INTRODUCTION

The model that is being developed is a 1-D and 2-D finite element model. From section II, it was shown that in order to completely describe the movement of radioactive materials through unsaturated soils, it is necessary to simultaneously solve the flow and transport equations (Eq. 10 and Eq. 13.). In this first step, the flow equation is being studied and the description of the present model is given in the next section. Section III.3 presents the steps that will be taken in the near future in order to completely characterize the transport of radionuclides through unsaturated soils.

### 2. Water Flow Model

In this initial stage, a finite-element model was developed to solve the water flow equation, which is written as a function of the water content (Eq. 9). Since the z direction was chosen to be in the downward direction, the resultant equation is

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial Z}\left(D(\theta)\frac{\partial \theta}{\partial Z}\right) - \frac{\partial K(\theta)}{\partial Z} \qquad (18)$$

In general, when the finite element method is used to solve a differential equation, the following steps are followed (29):

(1) Divide the region into elements and nodes,
(2) Define base functions for each node.
(3) Define weighting functions for each node.
(4) Approximate the function in terms of basis functions and node values.
(5) Define the residual as the difference between true solution and approximate solution.
(6) Set weighed residual to zero,
(7) Derive the matrix equation,
(8) Incorporate boundary conditions to the matrix equation,
(9) Use initial conditions to advance the solution through time.

The following description is applied to the 1-dimensional model; the 2-dimensional model has a similar derivation.

In this initial simulation, the model was kept as simple as possible because the idea was to check if the formulation of the finite element method was working properly.

In the finite element approach the dependent variable is approximated by

$$h(z,t) \cong \hat{h}(z,t) = \sum_{j=1}^{m} \phi_j(z)\, a_j(t) \tag{19}$$

where the $\phi_j(z)$ are the selected basis functions and the aj(t) are the associated, unknown, time-dependent coefficients which represent the solutions of eq. 18 at specified nodes. Because only a finite number of basis functions are used in the expansion, eq. 19, the residual obtained when eq. 19 is substituted in eq. 18 is not zero; however, this residual may be minimized by requiring that L(h) be orthogonal to a set of mutually independent weighting functions. In the Galerkin method, these functions are equal to the basis functions.

The equation can be written as

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left[\frac{K(\theta)}{C(\theta)}\frac{\partial \theta}{\partial Z}\right] - \frac{\partial K(\theta)}{\partial \theta}\frac{\partial \theta}{\partial Z}$$

1-D Model
Distance = L
Number of nodes = $\frac{L}{m} + 1$ $\quad$ n = no. of elements

Galerkin Form: $\quad i \overset{\ell}{\text{————————}} j \quad$ 2 node element

$$A = \frac{K(\theta)}{C(\theta)} \quad \therefore \quad B = \frac{\partial K(\theta)}{\partial \theta}$$

(assumed constant in each element for simplicity)

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial Z}\left[A \frac{\partial \theta}{\partial Z}\right] - B \frac{\partial \theta}{\partial Z}$$

Basis functions: $\quad \bar{\theta} = N_i \, \theta_i + N_j \, \theta_j \quad$ (linear approximation)

$$I = \int_\ell N_k \left[\frac{\partial}{\partial t}(N_i \theta_i) - \frac{\partial}{\partial Z}\left(A \frac{\partial}{\partial Z}(N_i \theta_i)\right) + B \frac{\partial}{\partial Z}(N_i \theta_i)\right] dz = 0 \qquad (21)$$

$$N_i = a_i + b_i \, z = \xi_i$$

$$\xi_1 = 1 - \frac{z}{\ell} \quad \therefore \quad \xi_2 = \frac{z}{\ell}$$

At each interaction, A and B are constant.

$$I = \int_\ell N_k \left\{\left[\underbrace{\frac{\partial}{\partial t}(N_i \theta_i)}_{③} - \underbrace{\frac{\partial}{\partial Z}\left(A \frac{\partial}{\partial Z}(N_i \theta_i)\right)}_{①} + \underbrace{B \frac{\partial}{\partial Z}(N_i \theta_i)}_{②}\right]\right\} dz = 0 \qquad (22)$$

Term <u>1</u> in eq. 22

$$\int_\ell - N_k \frac{\partial}{\partial Z}\left(A \frac{\partial}{\partial Z}(N_i \, \theta_i)\right) dz$$

Integrating by parts: $\int_a^b U\,dV = -\int_a^b V\,dU + UV\Big|_a^b$

$$U = N_K \qquad dV = \frac{\partial}{\partial Z} A \left(\frac{\partial}{\partial Z}(N_i\,\theta_i)\right)$$

$$dU = \frac{\partial}{\partial Z} N_K \qquad V = A\frac{\partial}{\partial Z}(N_i\,\theta_i)$$

Term 1 in eq. 22

$$\int_0^\ell A\frac{\partial}{\partial Z}(N_i\theta_i)\frac{\partial}{\partial Z}N_K\,dz + \underbrace{N_K A\frac{\partial}{\partial Z}(N_i\,\theta_i)\Big|_0^\ell}_{④} \tag{23}$$

$$\int_0^\ell A\frac{\partial}{\partial Z}(N_i\,\theta_i)\frac{\partial}{\partial Z}N_K\,dZ$$

$$\theta = N_i\,\theta_i + N_j\,\theta_j \qquad N_i = 1 - \frac{Z}{\ell} \qquad N_j = \frac{Z}{\ell}$$

$$\frac{\partial\theta}{\partial Z} = \frac{\partial N_i}{\partial Z}\theta_i + \frac{\partial N_j}{\partial Z}\theta_j \qquad \frac{\partial N_i}{\partial Z} = -\frac{1}{\ell} \qquad \frac{\partial N_j}{\partial Z} = \frac{1}{\ell}$$

$$\frac{\partial\theta}{\partial Z} = -\frac{1}{\ell}\theta_i + \frac{1}{\ell}\theta_j$$

If $N_k = N_i$

$$\int_0^\ell A\left(-\frac{1}{\ell}\theta_i + \frac{1}{\ell}\theta_j\right)\left(-\frac{1}{\ell}\right)dZ = \frac{A}{\ell}(\theta_i - \theta_j)$$

If $N_k = N_j$

$$\int_0^\ell A\left(-\frac{1}{\ell}\theta_i + \frac{1}{\ell}\theta_j\right)\left(\frac{1}{\ell}\right)dZ = \frac{A}{\ell}(-\theta_i + \theta_j)$$

In matrix form:

Term 1 $\quad \underbrace{\frac{A}{\ell}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}}_{S} \begin{Bmatrix} \theta_i \\ \theta_j \end{Bmatrix}$

Term $\underline{2}$ in eq. 22 $\int_\ell N_K B \frac{\partial}{\partial z}(N_i \theta_i)\, dz$

$$\int_\ell N_K B \left(-\frac{1}{\ell}\theta_i + \frac{1}{\ell}\theta_j\right) dz$$

If $N_k = N_i = 1 - \frac{z}{\ell}$

Term 2 becomes

$$\int_\ell \left(1-\frac{z}{\ell}\right) B \left(-\frac{1}{\ell}\theta_i + \frac{1}{\ell}\theta_j\right) dz = B\left(-\frac{\theta_i}{\ell} + \frac{\theta_j}{\ell}\right)\int_0^\ell \left(1-\frac{z}{\ell}\right) dz$$

$$= \frac{B}{2}\left(-\theta_i + \theta_j\right)$$

If $N_k = N_j$, Term 2 becomes

$$\int_\ell \frac{z}{\ell} B\left(-\frac{1}{\ell}\theta_i + \frac{1}{\ell}\theta_j\right) dz = B\left(-\frac{\theta_i}{\ell} + \frac{\theta_j}{\ell}\right)\int_0^\ell \frac{z}{\ell}\, dz$$

$$= \frac{B}{2}\left(-\theta_i + \theta_j\right)$$

Using natural coordinates

$$\int_\ell \xi_1 B\left(-\frac{\theta_i}{\ell} + \frac{\theta_j}{\ell}\right) dz = \therefore \quad \int_\ell g\, \xi_1\, d\ell = g\,\frac{\ell}{2}$$

$$= B\left(-\frac{\theta_i}{\ell} + \frac{\theta_j}{\ell}\right)\frac{\ell}{2} = \frac{B}{2}\left(-\theta_i + \theta_j\right)$$

Same thing for $\xi_2$

In matrix form: Term 2

$$\frac{B}{2}\begin{bmatrix} -1 & 1 \\ -1 & 1 \end{bmatrix}\begin{Bmatrix} \theta_i \\ \theta_j \end{Bmatrix}$$

Term 3 in eq. 22

$$\int_0^\ell N_k \left(\frac{\partial}{\partial t}(N_i \theta_i)\right) dz = \int_0^\ell N_k \left(N_i \frac{\partial \theta_i}{\partial t}\right) dz$$

$$= \int_0^\ell \xi_i \left(\xi_j \frac{\partial \theta_i}{\partial t}\right) dz \quad \therefore \quad \int_0^\ell \xi_1^p \, \xi_2^q \, d\ell = \frac{p!\,q!}{(p+q+1)!}\,\ell$$

$$\xi_i = \xi_j \quad \therefore \quad p=2,\ q=0 \quad \therefore \quad \frac{2!\,0!}{3!}\,\ell = \frac{\ell}{3}$$

$$\xi_i \neq \xi_j \quad \therefore \quad p=1,\ q=1 \quad \therefore \quad \frac{1!\,1!}{3!} = \frac{\ell}{6}$$

In matrix form

Term 3

$$\underbrace{\ell\begin{bmatrix} \frac{1}{3} & \frac{1}{6} \\ \frac{1}{6} & \frac{1}{3} \end{bmatrix}}_{M}\begin{Bmatrix} \frac{d\theta_i}{dt} \\ \frac{d\theta_j}{dt} \end{Bmatrix}$$

Without using natural coordinates: $N_k = N_i$

$$\int_0^\ell N_k \left(N_i \frac{\partial \theta_i}{\partial t}\right) dz = \int_0^\ell \left(1-\frac{z}{\ell}\right)\left(1-\frac{z}{\ell}\right)\frac{\partial \theta_i}{\partial t}\, dz$$

$$= \frac{\partial \theta_i}{\partial t}\int_0^\ell \left(1-\frac{2z}{\ell}+\frac{z^2}{\ell^2}\right) dz = \frac{\ell}{3}\,\frac{\partial \theta_i}{\partial t}$$

$$\int_0^\ell N_k \left(N_j \frac{\partial \theta_j}{\partial t}\right) dz = \int_0^\ell \left(1-\frac{z}{\ell}\right)\left(\frac{z}{\ell}\right)\frac{\partial \theta_j}{\partial t}\, dz$$

$$= \frac{\partial \theta_j}{\partial t}\int_0^\ell \left(\frac{z}{\ell}-\frac{z^2}{\ell^2}\right) dz = \frac{\ell}{6}\,\frac{\partial \theta_j}{\partial t}$$

If $N_k = N_j$

$$\int_0^{\ell} \left(\frac{z}{\ell}\right)\left(\frac{z}{\ell}\right)\frac{\partial \theta_j}{\partial t}\, dz = \frac{\partial \theta_j}{\partial t}\left(\frac{z^3}{3\ell^2}\right) = \frac{\ell}{3}\,\frac{\partial \theta_j}{\partial t}$$

$$\int_0^{\ell} \left(1-\frac{z}{\ell}\right)\left(\frac{z}{\ell}\right)\frac{\partial \theta_i}{\partial t}\, dz = \frac{\ell}{6}\,\frac{\partial \theta_i}{\partial t}$$

The equation is then:

$$\left[M\right]\left\{\frac{\partial \theta}{\partial t}\right\} + \left[B\right]\left\{\theta\right\} + \left[S\right]\left\{\theta\right\} = 0$$

$$\left[B\right] + \left[S\right] = \left[A\right]$$

$$\left[M\right]\left\{\frac{\partial \theta}{\partial t}\right\} + \left[A\right]\left\{\theta\right\} = 0$$

<u>Boundary Conditions:</u>

The boundary condition is only applied to the first element (infiltration rate).

The boundary condition is: $q = -D(\theta)\frac{\partial \theta}{\partial Z} + K(\theta)$

where q is given

$$\frac{\partial \theta}{\partial Z} = -\frac{q}{D(\theta)} + \frac{K(\theta)}{D(\theta)}$$

For each interaction, $\frac{q}{D(\theta)}$ and $\frac{K(\theta)}{D(\theta)}$ are assumed constant

$$D(\theta)\frac{\partial\theta}{\partial z} - K(\theta) = -q$$ mixed Neumann boundary condition.

It will be assumed, at first, that the column of soil is infinite (no boundary condition at the end of the column is applied; no flux is then assumed at the extremity).

In order to introduce this boundary condition, we have to analyze the boundary term:
Term 4 in eq. 23 becomes

$$-N_k \, D(\theta) \frac{\partial}{\partial z} (N_i \, \theta_i) \Big|_0^{\ell}$$

From the boundary conditions $\frac{\partial\theta}{\partial z} = -\frac{q}{D(\theta)} + \frac{K(\theta)}{D(\theta)}$
Term 4

$$-N_K \, (-q + K(\theta)) \Big|_0^{\ell} = N_K \, (q - K(\theta)) \Big|_0^{\ell}$$

In $\ell$ (2nd node of first element) we do not have a boundary condition.
In 0, $N_k = 1$ and:
Term 4

$$-q + K(\theta)$$

In matrix form:

$$-\left\{ P \right\} = \left\{ \begin{matrix} -q + K(\theta) \\ 0 \\ \vdots \\ 0 \end{matrix} \right\}$$

The equation is then:

$$\left[ M \right] \left\{ \frac{\partial \theta}{\partial t} \right\} + \left[ A \right] \left\{ \theta \right\} = \left\{ P \right\}$$

Now it is necessary to solve the partial differential equations

The first approximation is

$$\left( \frac{d\theta}{dt} \right)_t = \frac{\left\{ \theta \right\}_{t+\Delta t} - \left\{ \theta \right\}_t}{\Delta t}$$

substituting

$$\left[ M \right] \left\{ \theta \right\}_{t+\Delta t} = \Delta t \left\{ P \right\} - \Delta t \left[ A \right] \left\{ \theta \right\}_t + \left[ M \right] \left\{ \theta \right\}_t \qquad (24)$$

Which eq. 19 we determine $\left\{ \theta \right\}_{t+\Delta t}$ using the initial conditions. Once $\left\{ \theta \right\}_{t+\Delta t}$ is obtained, then a better solution is used (implicit finite difference).

Expanding $\left\{ \theta \right\}_{t+\frac{1}{2}\Delta t}$ in Taylor series:

$$\left\{ \theta \right\}_{t+\frac{1}{2}\Delta t} = \left\{ \theta \right\}_t + \frac{\Delta t}{2} \left\{ \frac{d\theta}{dt} \right\}_t + \left( \frac{\Delta t}{2} \right)^2 \frac{1}{2!} \left\{ \frac{d^2\theta}{dt^2} \right\}_t + R(\Delta t^3)$$

$$\left\{ \theta \right\}_{t+\frac{1}{2}\Delta t} = \left\{ \theta \right\}_{t+\Delta t} - \frac{\Delta t}{2} \left\{ \frac{d\theta}{dt} \right\}_{t+\Delta t} + \left( \frac{\Delta t}{2} \right)^2 \frac{1}{2!} \left\{ \frac{d^2\theta}{dt^2} \right\}_{t+\Delta t} + R(\Delta t^3)$$

Subtracting

$$\left\{ \theta \right\}_{t+\Delta t} = \left\{ \theta \right\}_t + \frac{\Delta t}{2} \left( \left\{ \frac{d\theta}{dt} \right\}_t + \left\{ \frac{d\theta}{dt} \right\}_{t+\Delta t} + R \qquad (25)$$

$$\left\{\frac{d\theta}{dt}\right\}_t = [M]^{-1}\{P\}_t - [M]^{-1}[A]_t\{\theta\}_t$$

$$\left\{\frac{d\theta}{dt}\right\}_{t+\Delta t} = [M]^{-1}\{P\}_{t+\Delta t} - [M]^{-1}[A]_{t+\Delta t}\{\theta\}_{t+\Delta t}$$

Substituting

$$\{\theta\}_{t+\Delta t} = \{\theta\}_t + \frac{\Delta t}{2}\left([M]^{-1}\{P\}_t - [M]^{-1}[A]_t\{\theta\}_t + [M]^{-1}\{P\}_{t+\Delta t} - [M]^{-1}[A]_{t+\Delta t}\{\theta\}_{t+\Delta t}\right)$$

The final equation is then

$$\left(\frac{2}{\Delta t}[M] + [A]_{t+\Delta t}\right)\{\theta\}_{t+\Delta t} = \left(\frac{2}{\Delta t}[M] - [A]_t\right)\{\theta\}_t + \left(\{P\}_t + \{P\}_{t+\Delta t}\right) \qquad (26)$$

Equation 24 is used to determine $\{\theta\}_{t+\Delta t}$ in a first approximation using the initial condition. With $\{\theta\}_{t+\Delta t}$, $\{P\}_{t+\Delta t}$ and $[A]_{t+\Delta t}$ can be evaluated; and eq. 26 is then used until $\{\theta\}_{t+\Delta t}$ is determined with the desired precision. Then the boundary condition is changed and the process is repeated until convergence is obtained. Then a new time step can be started.

Figure 5 shows the flow diagram used to implement the model.

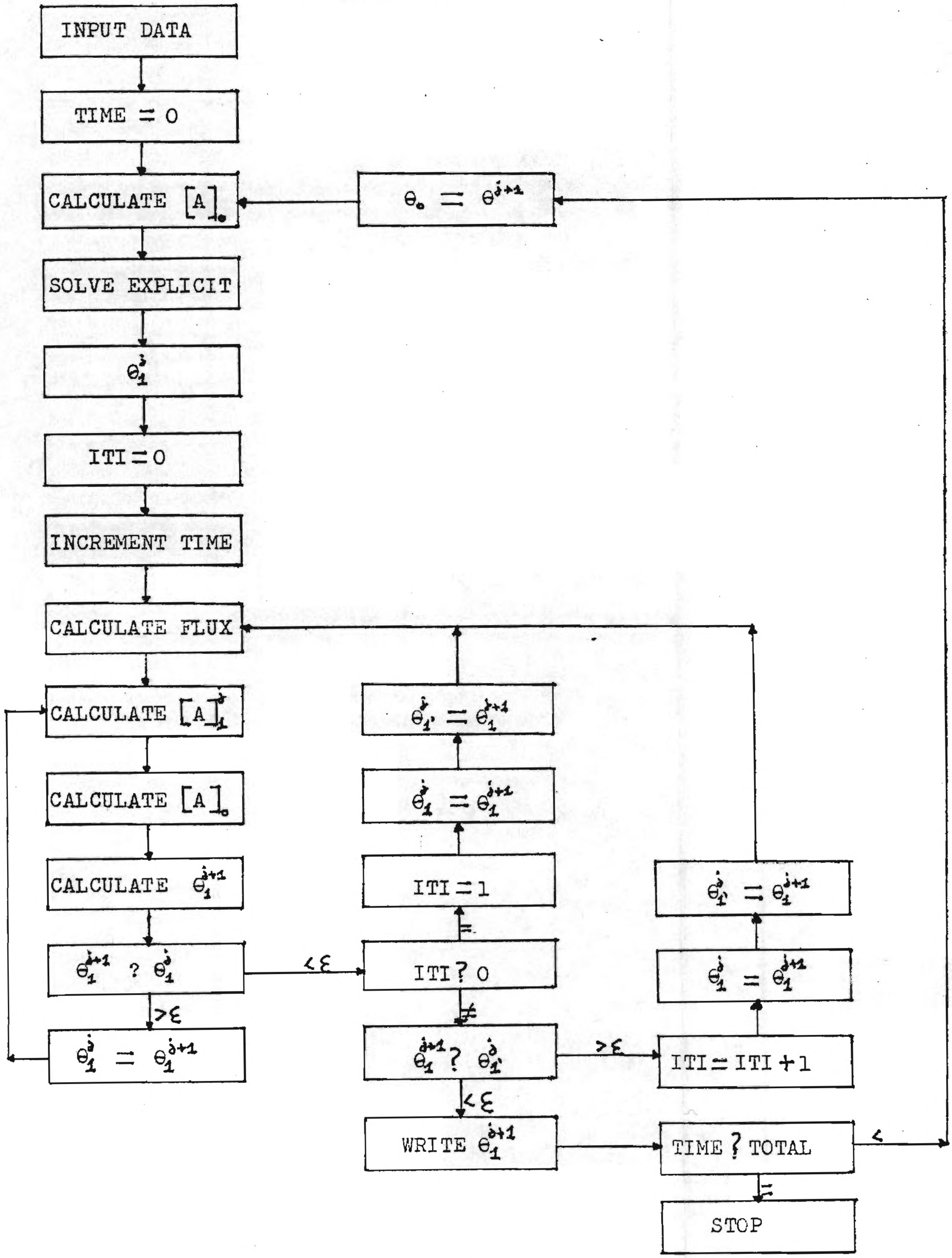
The relations used in the model between water content and pressure head and water content and hydraulic conductivity are:

$$\left(\frac{\theta - \theta_r}{m - \theta_r}\right) = \left(\frac{\psi_e}{\psi}\right)^{\lambda} \qquad \text{(Ref.25)}$$

$$K(\theta) = K_s\, S^{m} \qquad \text{(Ref.25)} \qquad (27)$$

where $\lambda$ is the pore size distribution index, $K_s$ is the saturated hydraulic conductivity, S is the moisture saturation ($S=\theta/m$), n is the porosity, $\theta_r$ is the residual water content, and $\psi_e$ is the air-entry value. As has already been mentioned, the derivation of the 2-dimensional model is similar to that presented for the 1-dimensional model.

Fig. 5 Flow diagram for the water Flow Model



Although the model was a simple one, with many assumptions, it was useful in checking the basic structure of the finite element formulation, since the finite element structure of a model is always the same (only the matrix coefficients change when the differential equation is changed).

## 3. Model Development

The water flow model is now being developed for the equation using the pressure head as the dependent variable. This model is being developed in a more general way than the previous one was and the simplifications adopted in the water content model are being eliminated. When the model is ready, then it will be possible to compare it with some analytical solutions for both saturated and unsaturated conditions. Once the flow model is running properly, the transport model will be implemented. Table 1 presented the capabilities of the model being developed; it also compares the unsaturated model with the saturated model that was used before by the Savannah River Plant. Some of the possible options that can be included in the future are also shown in the table.

# IV - MODEL IMPLEMENTATION

## 1 - INTRODUCTION

The general description of the water flow model using the water content as the dependent variable was presented in the last section. This section presents the numerical implementation of the equations derived previously. Both 1-dimensional and 2-dimensional models are described, and a brief explanation of each subroutine is shown. Also, the results obtained for a simple situation are presented.

## 2 - MODEL DESCRIPTION

In order to develop a finite element model, there are some standard steps that are usually taken. First of all the region under study is divided into elements and nodes. For the 1-D model, the region was divided in 10 nodes, 19 elements equally spaced, although different element length was also possible. For the 2-D model, the region was divided in 24 triangular elements, 21 nodes. After the region is characterized, the base functions are defined for each mode. For the 1-D model, a linear base function was used

$$\bar{\theta} = \sum_{i=1}^{2} N_i \, \theta_i$$

$$N_i = a_i + b_i \, Z \qquad (28)$$

For the 2-D model, the base functions used are

$$\bar{\theta} = \sum_{i=1}^{3} N_i \, \theta_i \qquad (29)$$

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

After the base functions are chosen, the weighting functions are selected. The method used was the Galerkin method, and in this case the weighting functions are chosen to be equal to the base functions.

The next step is then to approximate the functions in terms of basis functions and node values. This was shown in section III.2 for the 1-D model; the same procedure is applied to the 2-D model.

Once the approximating functions are prepared, the residual is defined as the difference between the correct solution and the approximate solution; the weighted residual is then set equal to zero and the matrix equation is then derived. The boundary condition is then incorporated and the resultant differential matrix equation is then solved using a finite difference scheme. All these steps are also shown in section III.2 for the 1-D model.

After the matrix equations and the finite difference schemes were prepared, the numerical model was developed.

## 3. 1-D MODEL

The 1-D model consists of one main program and 10 subroutines.

The main program is responsible for the organization of the model. Basically, it performs the scheme shown in Figure 5.

Subroutine ERROR is responsible for the convergence of the results; it uses the following equation to determine if there is convergence or not of the dependent variable.

$$\left[ \frac{\sum \left[ \theta_2 - \theta_1 \right]^2}{\sum \theta_1^2} \right]^{1/2} < \varepsilon$$

where $\varepsilon$ is the desired precision.

Subroutine INPU is used to introduce the values of all variables needed; these variables are: length of the column, total time of analysis, time increment, number of elements, coordinates of the nodes, initial water content, boundary condition time during which the boundary conditions applied, residual water content, air entry value, pore size distribution index, saturation, hydraulic conductivity, and porosity.

Subroutine SET performs the coordinate transformation; it changes the global coordinates of each element to local coordinates.

Subroutine ELEM generates the local element matrices by calculating each coefficient of the matrices necessary to solve the matrix equation.

Subroutine ASSEM is used to assemble the local matrices in a global matrix.

Subroutine BOUN introduces the value of the boundary condition (infiltration rate)

Subroutine CALC1 solves eq. (24)

Subroutine CMULT multiplies a non-synmetric band matrix by a vector

Subroutine CALC2 solves eq. (25)

Subroutine OUT prints the value of the water content of each node at each time interval.

Subroutine LEQT2B calculates the inverse of a matrix.

The resultant 1-D model is shown in Appendix A.

## 4. 2-MODEL

The 2-D model is basically composed of six subroutines. The MAIN subroutine represents the structure of the program; it performs the scheme shown in Figure 5. It also introduces all the values needed by the program (such as INPU of the 1-D model) and is also responsible for the output; it presents the water content values of each node at each time interval. It also solves Eq. 26

The ABC Subroutine evaluates the coefficients of the matrices necessary to formulate the base functions.

The ITGL Subroutine performs the integration of the terms which form the residual, over each element.

The SETUP Subroutine is called by the ITGL subroutine in order to perform the necessary integrations.

The UNSAT Subroutine calculates the diffusivity and the derivative of the hydraulic conductivity in relation to the water content, at each iteration.

The MKMTX Subroutine assembles the local element matrices in a global matrix.

The 2-D model is shown in Appendix B.

# 5 - RESULTS OF THE MODEL DEVELOPMENT WORK

A very simple situation is being used to check the output of the models. A 20 cm long sand column is simulated. The initial water content of the sand column is uniform and equal to 0.2. A constant infiltration rate is assumed at the top of the column; no flow is allowed at the bottom. The following parameters were used.

Saturated hydraulic conductivity = 4.5 m/day
Porosity = 0.4
Total time = 2.0 min.
Time internal = 0.01 min
Flux at boundary = 0.05 cm/min
Error = 0.002
Residual water content = 0.1.
Air-entry value = 30.0 cm
Pore size distribution index = 5.0
m = 3.0

The output of the 1-D model is shown in Table 3. It is seen that the results were consistent and that there are no longer fluctuations in the water content values. These results show that the structure of the program is working well, and so the hydraulic head flow equation is now being developed. When it is working, it will be possible to compare the output with some analytical situations for saturated cases. The 2-D model still presented some output fluctuations, but these have since been eliminated. This work is being continued in the coming months.

# 1 - D MODEL RESULTS

| NODE | COORDINATE | WATER CONTENT |
| --- | --- | --- |
| 1 | 0.000 | .202 |
| 2 | 1.000 | .199 |
| 3 | 2.000 | .200 |
| 4 | WAIT | |
| .000 | .200 | |
| 5 | 4.000 | .200 |
| 6 | 5.000 | .200 |
| 7 | 6.000 | .200 |
| 8 | 7.000 | .200 |

1STO

TIME = .020

| NODE | COORDINATE | WATER CONTENT |
| --- | --- | --- |
| 1 | 0.000 | .203 |
| 2 | 1.000 | .199 |
| 3 | 2.000 | .200 |
| 4 | 3.000 | .200 |
| 5 | 4.000 | .200 |
| [illegible] | 5.000 | .200 |
| [illegible] | [illegible] | .200 |
| [illegible] | 7.000 | .200 |

TIME = .030

| NODE | COORDINATE | WATER CONTENT |
| --- | --- | --- |
| [illegible] | 0.000 | .204 |
| 2 | 1.000 | .200 |
| [illegible] | 2.000 | .200 |
| 4 | 3.000 | .200 |
| [illegible] | 4.000 | .200 |
| [illegible] | 5.000 | .200 |
| [illegible] | 6.000 | .200 |
| [illegible] | 7.000 | .200 |

TIME = .040

| NODE | COORDINATE | WATER CONTENT |
| --- | --- | --- |
| [illegible] | [illegible] | .205 |
| [illegible] | [illegible] | .200 |
| [illegible] | [illegible] | .200 |
| [illegible] | [illegible] | .200 |
| [illegible] | 4.000 | .200 |
| [illegible] | [illegible] | .200 |
| [illegible] | [illegible] | .200 |
| 8 | 7.000 | .200 |

| NODE | COORDINATE | WATER CONTENT |
| --- | --- | --- |
| 1 | 0.000 | .203 |
| 2 | 1.000 | .200 |
| 3 | 2.000 | .200 |
| 4 | 3.000 | .200 |
| 5 | 4.000 | .200 |
| 6 | 5.000 | .200 |
| 7 | 6.000 | .200 |
| 8 | 7.000 | .200 |

1STO

TIME = .060

| NODE | COORDINATE | WATER CONTENT |
| --- | --- | --- |
| 1 | 0.000 | .207 |
| 2 | 1.000 | .201 |
| 3 | 2.000 | .200 |
| 4 | 3.000 | .200 |
| 5 | 4.000 | .200 |
| 6 | 5.000 | .200 |
| 7 | 6.000 | .200 |
| 8 | 7.000 | .200 |

1STO

TIME = .070

| NODE | COORDINATE | WATER CONTENT |
| --- | --- | --- |
| 1 | 0.000 | .207 |
| 2 | 1.000 | .201 |
| 3 | 2.000 | .200 |
| 4 | 3.000 | .200 |
| 5 | 4.000 | .200 |
| 6 | 5.000 | .200 |
| 7 | 6.000 | .200 |
| 8 | 7.000 | .200 |

1STO

TIME = .080

| NODE | COORDINATE | WATER CONTENT |
| --- | --- | --- |
| 1 | 0.000 | .208 |
| 2 | 1.000 | .201 |
| [illegible] | 2.000 | .200 |
| 4 | 3.000 | .200 |
| 5 | 4.000 | .200 |
| [illegible] | 5.000 | .200 |
| 7 | 6.000 | .200 |
| 8 | 7.000 | .200 |

1STO

```
1970

TIME =      .190

NODE     COORDINATE     WATER CONTENT
  1        0.000            .212
  2        1.000            .205
  3        2.000            .201
  4        3.000            .200
  5        4.000            .200
  6        5.000            .200
  7        6.000            .200
  8        7.000            .200
1970

TIME =      .200

NODE     COORDINATE     WATER CONTENT
  [illegible]  0.000        .212
  2        1.000            .206
  3        2.000            .202
  [illegible]  3.000        .200
  5        4.000            .200
  [illegible]  5.000        .200
  [illegible]  6.000        .200
  8        7.000            .200
1970

TIME =      .210
[illegible]
[illegible]
[illegible]
[illegible] .320

WAIT
TIME =      .[illegible]
[illegible]

WAIT
TIME =      .2[illegible]

NODE     COORDINATE     WATER CONTENT
  [illegible]  0.000        .215
  [illegible]  1.000        .208
  [illegible]  2.000        .204
  [illegible]  3.000        .201
  5        4.000            .200
  [illegible]  5.000        [illegible]
  [illegible]  6.000        [illegible]
  8        7.000            [illegible]
[illegible]

                                   TIME =      .410
55277 #13

WAIT

TIME =      .430

NODE     COORDINATE     WATER CONTENT
  1        0.000            .218
  2        1.000            .211
  3        2.000            .206
  4        3.000            .202
  5        4.000            .201
  6        5.000            .200
  7        6.000            .200
  8        7.000            .200
1970

55477 17,500

EXECUTE
DELIMITER
END OF FILE
[illegible]
      TIME LIMIT EXCEEDED    IN LEGT19  NEAR LINE 131
[illegible]

[illegible]
      [illegible]     [illegible]     .200
[illegible]

WAIT
      8         7.000         .2[illegible]
55077 [illegible]
1970

TIME =      .430

NODE     COORDINATE     WATER CONTENT
  [illegible]  0.000        .218
  2        1.000            .212
  3        2.000            .206
  4        3.000            .203
  5        4.000            .201
  6        5.000            .200
  7        6.000            .200
  8        7.000            .200
      TIME LIMIT EXCEEDED    IN LEGT19  NEAR LINE 131
END OF FILE
[illegible]
MEDIA [illegible]
[illegible] LINE*
[illegible]
FILE FUNCTION ILLEGAL
[illegible]

FILE FUNCTION ILLEGAL
[illegible]
```

## EXPERIMENTAL FLOW TESTS

One of the basic uncertainties in the lysimeter tests concerns the nature of the source term and the type of flow that exists in the waste material region itself. For instance, it is not intuitively obvious, whether the waste material on compaction by the overlying soil will form a barrier to throughflow or will leave cavities that may invite perched water. Depending on these flow conditions, it then becomes important to determine if water from the overlying area is diverted around the waste, in effect greatly reducing the leach rate, or diverted into it from neighboring flow cells, thus relatively increasing flow through the waste volume and, potentially, raising the leach rate.

To answer these questions several tests were devised that, on a smaller scale, attempted to reproduce conditions in the lysimeters.

### A. Condition of Waste Material

Reference 9 contains several pictures of the type of laboratory trash loaded into the lysimeters. A listing of the composition was obtained from SRL and is presented in Table 4. Comparable waste material was collected from the Nuclear Research Center at Georgia Tech for compression tests. At SRP the waste was loaded into the lysimeters in plastic bags that were then punctured to admit water flow. That the waste degrades and perishes to a variable extent was evident when some SRP trenches were exhumed after 14 years of burial (DP-1456); Figs 6 and 7 are examples of what was found.

The simulation waste was placed into 3-gallon ice cream cartons for ease of handling. Two aspects of the behavior of the waste material were of interest: a)the degree of collapse or compression the waste would suffer after backfilling of the trenches or lysimeters; and b)the change in permeability to water flow the collapsed waste would present.

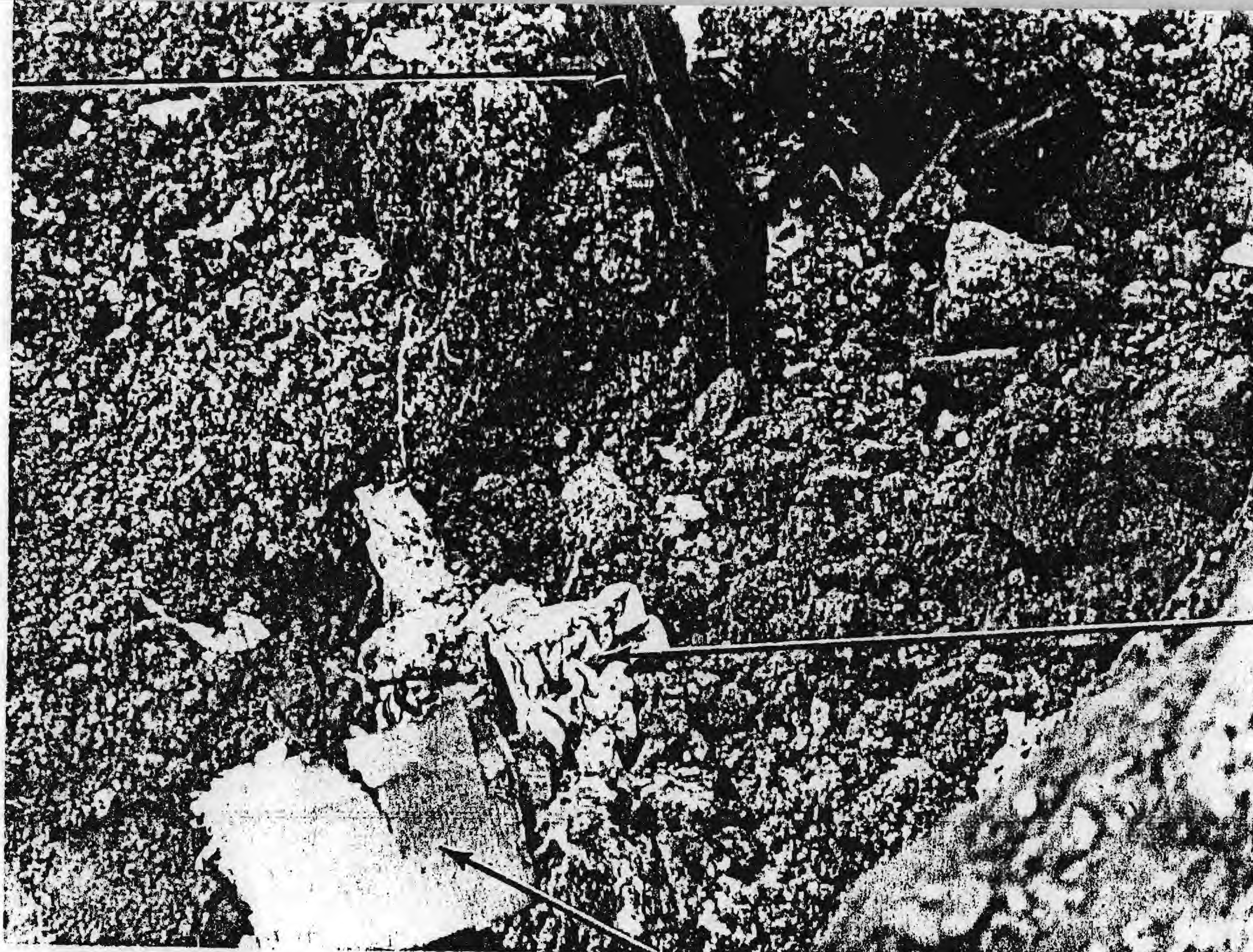


Fig. 6 Example of exhumed waste

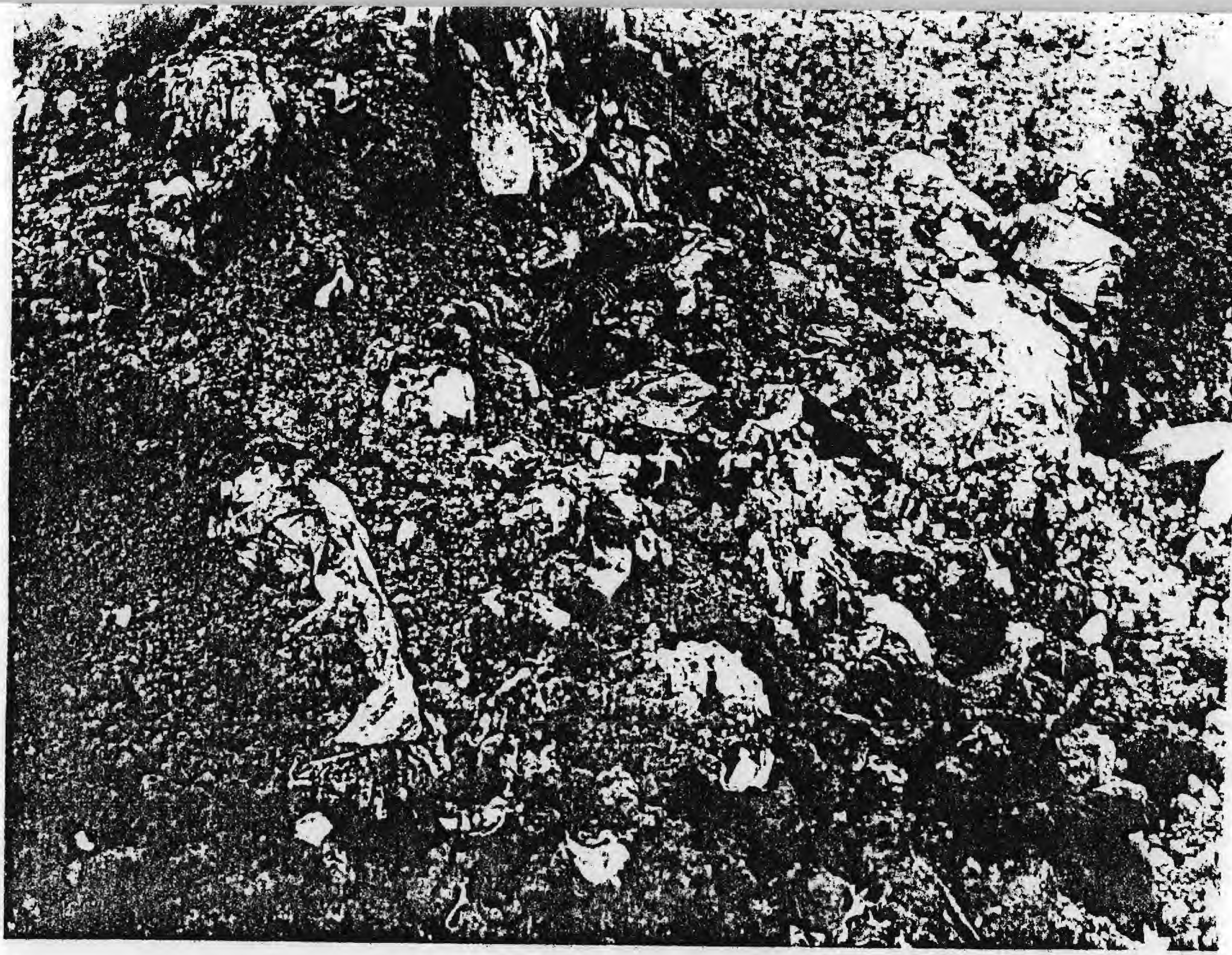


Fig. 7 Example of exhumed SRP waste

TABLE 4

FORMULA FOR SYNTHETIC SOLID WASTE
(VOLUME BASIS)

| | |
|---|---|
| 25% | Kimwipes, handiwipes, paper towels, and atomic wipes (sanitary pads) |
| 20% | Plastic bags |
| 20% | Assorted glassware and glass sample vials |
| 15% | Polyethylene bottles and caps (500 cc and smaller) |
| 10% | Disposable pipette tips |
| 10% | Metallic waste (small tools, bolts, clamps, forceps, etc.) |

The pressure of the moist overlying soil under 6 feet of backfill was estimated to be about 11 $lb/in.^2$ To measure changes in permeability, without changing the consistency of the waste, it was decided to measure changes in permeability to air flow only. Fig. 8 illustrates the set up.

To perform the compression tests, a tight-fitting ram had to be constructed to fit the inside of the cartons. The material was then compressed several times in succession and the flow rate measured under constant conditions. Table 5 summarizes the results for two different waste batches. It is evident, that even after applying a pressure of over 13 psi, well above the estimated soil load, there are still appreciable gaps in the waste package, allowing ample air flow, and therefore water flow, easily in excess of that passing through the surrounding soil. Fig. 9 shows a picture of the compacted waste in its container.

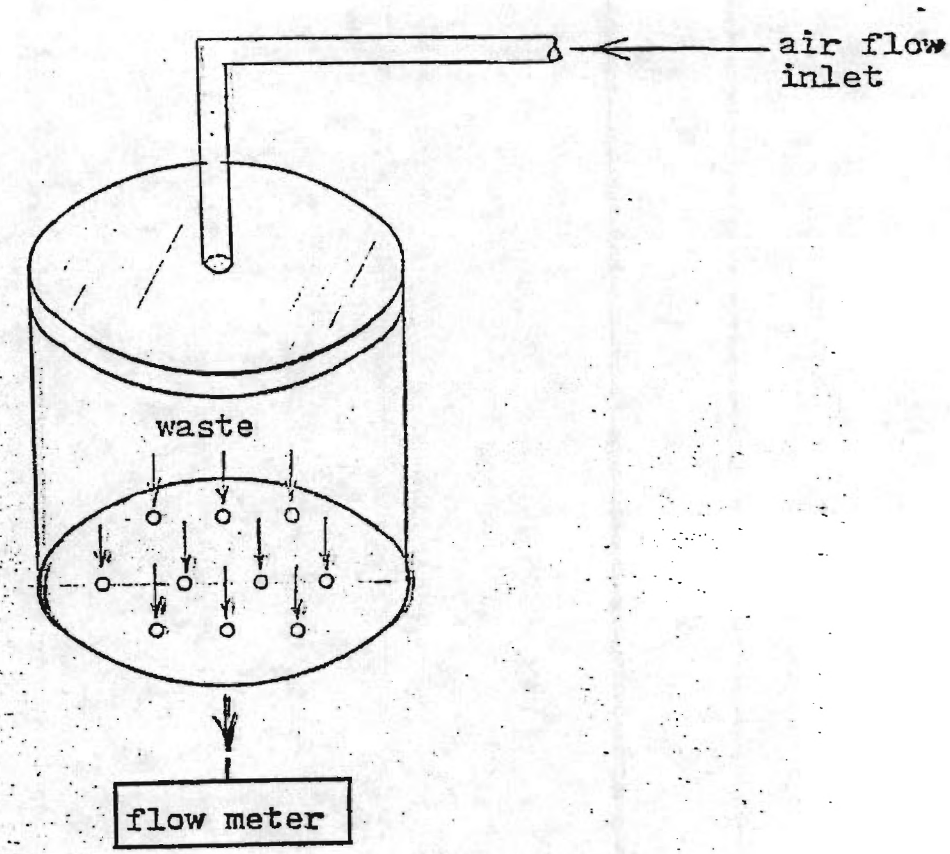
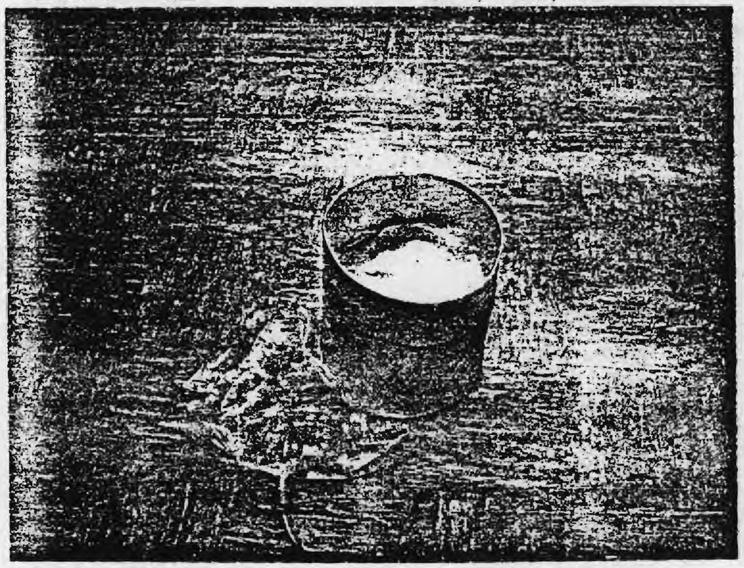



Fig. 8 Flow Test Arrangement

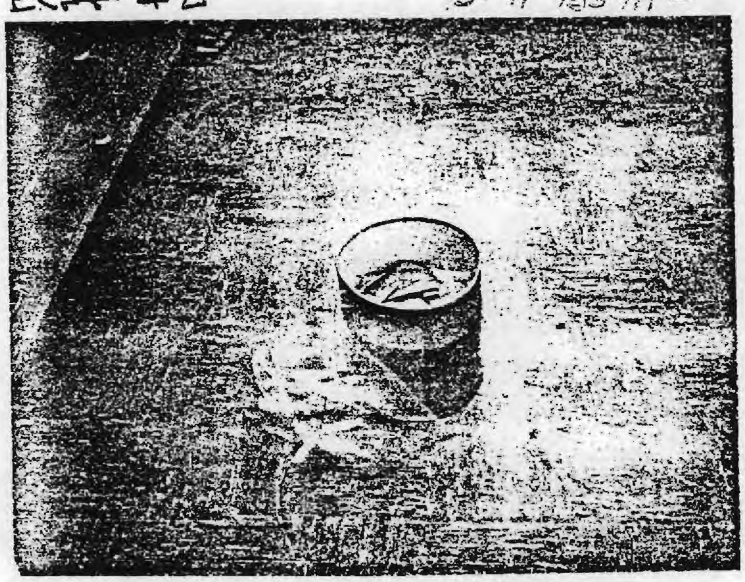
EXPT #2 9.17 lb/in²



650 lbs 10 → 4.75 inches

Experiment #2: 2nd Compaction; 9.17 lbs/in$^2$
Airflow: 5.11 ft$^3$/min
Volume: 336.69 inches$^3$
Height Reduction: to 4.75 inches

EXPT #2 13.41 lbs/in²



450 lbs 10 → 3 5/8 inches

Experiment #2: 3rd Compaction; 13.41 lbs/in$^2$
Airflow: 4.47 ft$^3$/min
Volume: 257.3 inches$^3$
Height Reduction: 5.62inches

Fig. 9

Table 5

Waste Compression Tests

Initial height of waste in container: 10 inches

SUMMARY OF AIR FLOW EXPERIMENTS

| Experiment | Pressure ($lb/in^2$) | Height (inches) | Air Flow (cf/m) |
|---|---|---|---|
| 1 | 0 | 10 | 9.90 |
| | | 6.62 | 12.78 |
| | | 4.5 | 9.27 |
| | | 3.0 | 9.27 |
| 2 | 0 | 10 | 10.68 |
| | 4.6 | 6.25 | 6.39 |
| | 9.17 | 4.75 | 5.11 |
| | 13.41 | 3.25 | 4.47 |
| 3 | 0 | 10 | 15.01 |
| | 4.7 | 5.5 | 12.14 |
| | 9.17 | 4.25 | 6.39 |
| | 13.41 | 3.25 | 6.39 |
| 4 | 0 | 10 | 15.33 |
| | 4.7 | 5.25 | 12.41 |
| | 9.17 | 4.25 | 9.59 |
| | 13.41 | 3.25 | 6.39 |

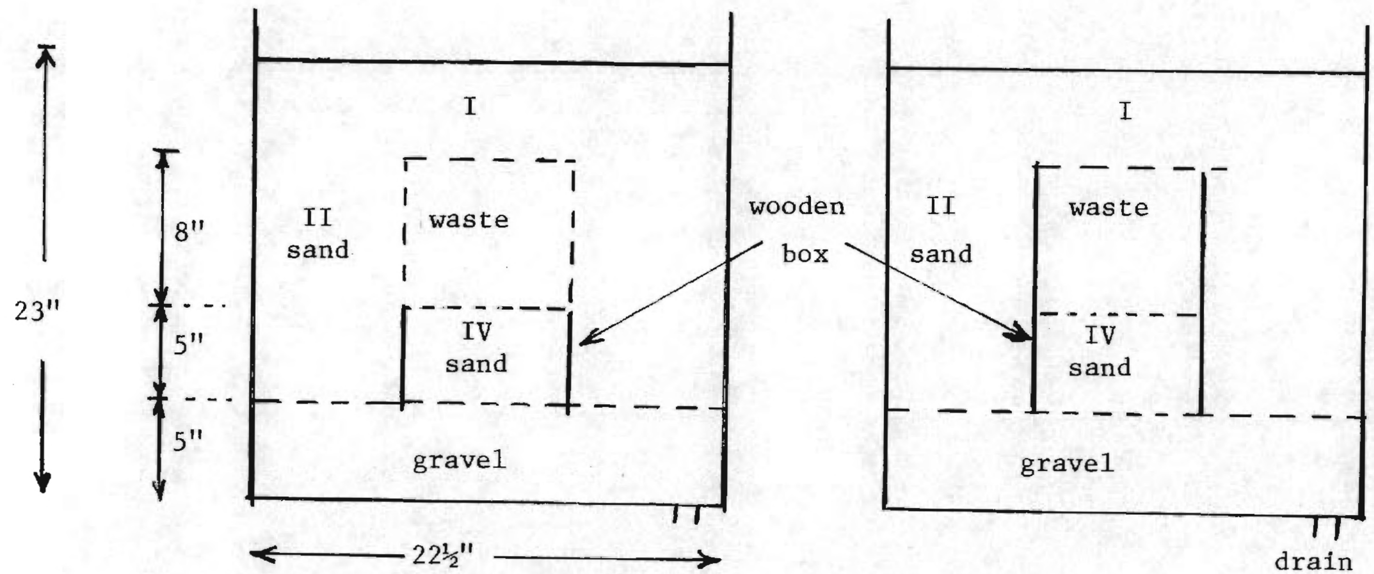
These tests show that for the type of waste material employed the waste volume, under compression, would not present a barrier to vertical flow nor encourage flow diversion around the waste volume. Instead, it is possible that water is diverted into the waste region from surrounding soil, at least until the waste material has degraded further, to the condition shown in Figures 6 and 7. Since the waste material in the SRP lysimeters is relatively fresh, any modeling of the flow process must envisage the possibility of lateral infiltration into the waste cavities and, even, for relatively impermeable backfill soil, the occurrence of perched water within the waste region. The next section discusses test work under way to study those processes.

B. Flow diversion through the Waste Volume

To provide some input data to the two-zone computer model of Fig. 4, experimental tests have been undertaken to measure the change in flow rate resulting from the presence of the permeable waste. These tests are still in progress. The tests consists of two phases which are illustrated in Fig 10. Sand initially, later SRP soil, is loaded into a drum designed to provide a two-zone flow regime. The compacted waste is loaded on top of an isolated sand bed, separated from the outer zone by a wooden barrier. By embedding electrical conductivity electrodes at various levels in the inner and outer zones moisture conditions can be monitored to indicate any flow diversion through the waste volume or into it as the test bed is wetted at intervals with known amounts of water. At this writing the first test, with the waste volume open to lateral flow, has been operating for three weeks and no significant diversion has been observed while the bed is running at low total moisture content. Moisture content will be stepped up gradually and it hoped to maintain a material balance to account for all water present. Fig. 11 shows the location of the electrodes and their general design. The electrodes were calibrated in a separate bed against moisture measurements by conventional means.

Conductivity Measurements

In order to avoid the problems due to hysteresis, the electrodes used were in direct contact with the soil, without the porous block. As is reported by Gardner (25), the major drawbacks of this method are uncertain electrical contact between electrodes and the soil, and soil heterogeneity, which prevents uniform flow of current in the soil. Since the soils used were artificially packed, and since the soils are well characterized, it seems that the soil heterogeneity does not represent a major problem in the present case. Consequently, if good electrical contact is obtained when the electrodes are placed in the soil, the method should give satisfactory results.




Experiment #1

Experiment # 2

Fig. 10 Diagram of Flow Diversion Experiments.

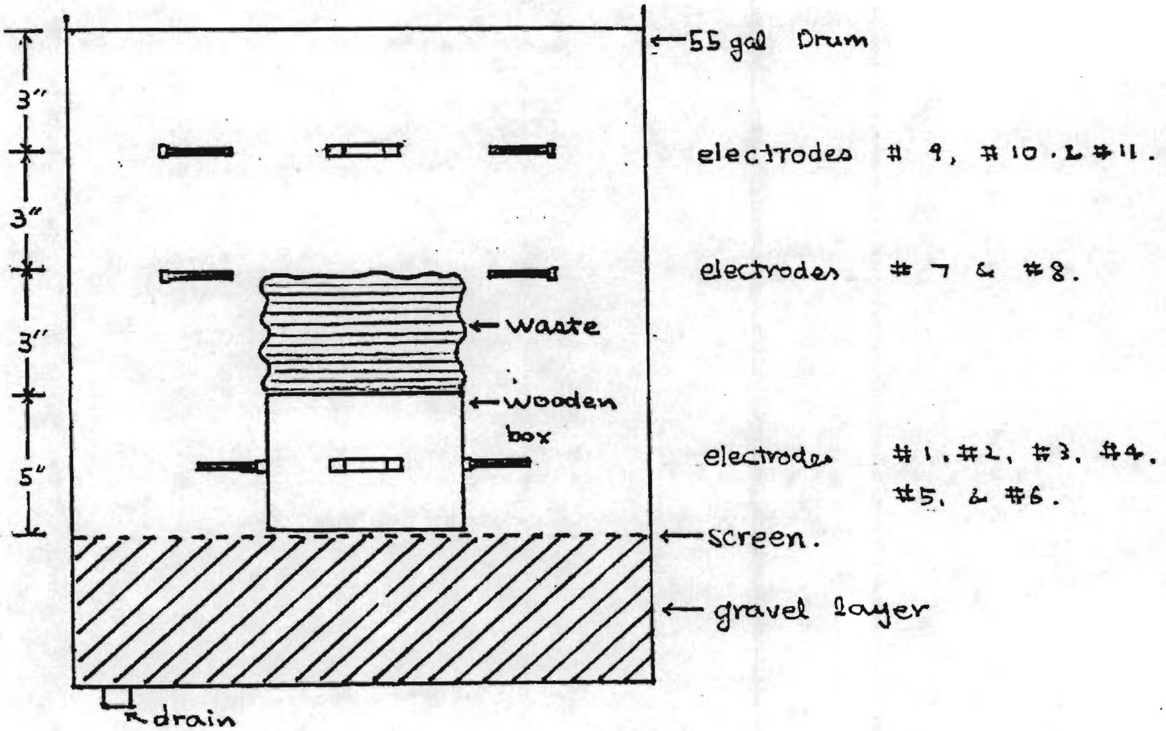



Fig. 11a. Drum Design and Electrodes.

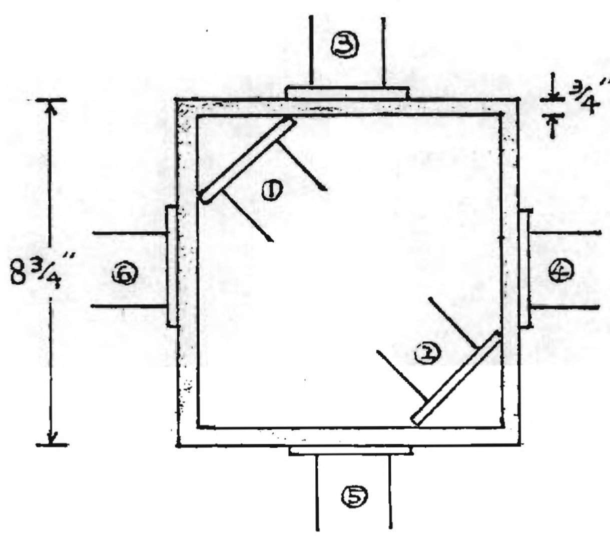



Fig. 11b. Wooden Box with Electrodes.

For each of the four soils used, the indirect method should be calibrated against a direct method; the direct method was chosen to be the gravimetric one with oven drying which is explained in a later section.

The electrodes that were used in this study are shown in Figure 11. Two copper electrodes are held together by a rigid plastic bar; the plastic bar has 2 small holes, 5 cm apart, through which two solderless terminals are inserted. One end of the terminal is connected to the copper electrode, while the other end is connected to an electrical cable, which connects the electrode to the measuring device. In order to avoid corrosion of the copper electrodes, they were nickel-plated. The plating procedure was adapted from Rodgers (1960), and Gray (1953). Basically, the copper electrodes were first degreased with detergent (Alconox); they were then rinsed with water and acid-dipped (20 parts of water to 1 part of $H_2SO_4$); after being rinsed with hot and cold water, the electrodes were plated for 15 minutes in a nickel sulfate-nickel chloride bath.

The electrodes were checked for reproducibility with excellent results.

The conductivity measurement system was calibrated for each type of soil by preparing progressively wetter samples and determining the moisture content for each. The volumetric water content is obtained as

$$\theta = w \frac{\rho_b}{\rho_w}$$

where $\rho_b$ and $\rho_w$ are the bulk density and water density respectively. The percent saturation is given by

$$S = \frac{\theta}{m} \times 100$$

and this quantity is related to the current measured when a standard voltage is applied to the electrode system. To avoid electrochemical changes it was found to be important to use pre-equilibrated water in making up the wet soil samples. Figs. 12 to 15 show the calibration curves obtained. For most measurements the error in the resistance measurement was of the order of 1.5 percent.

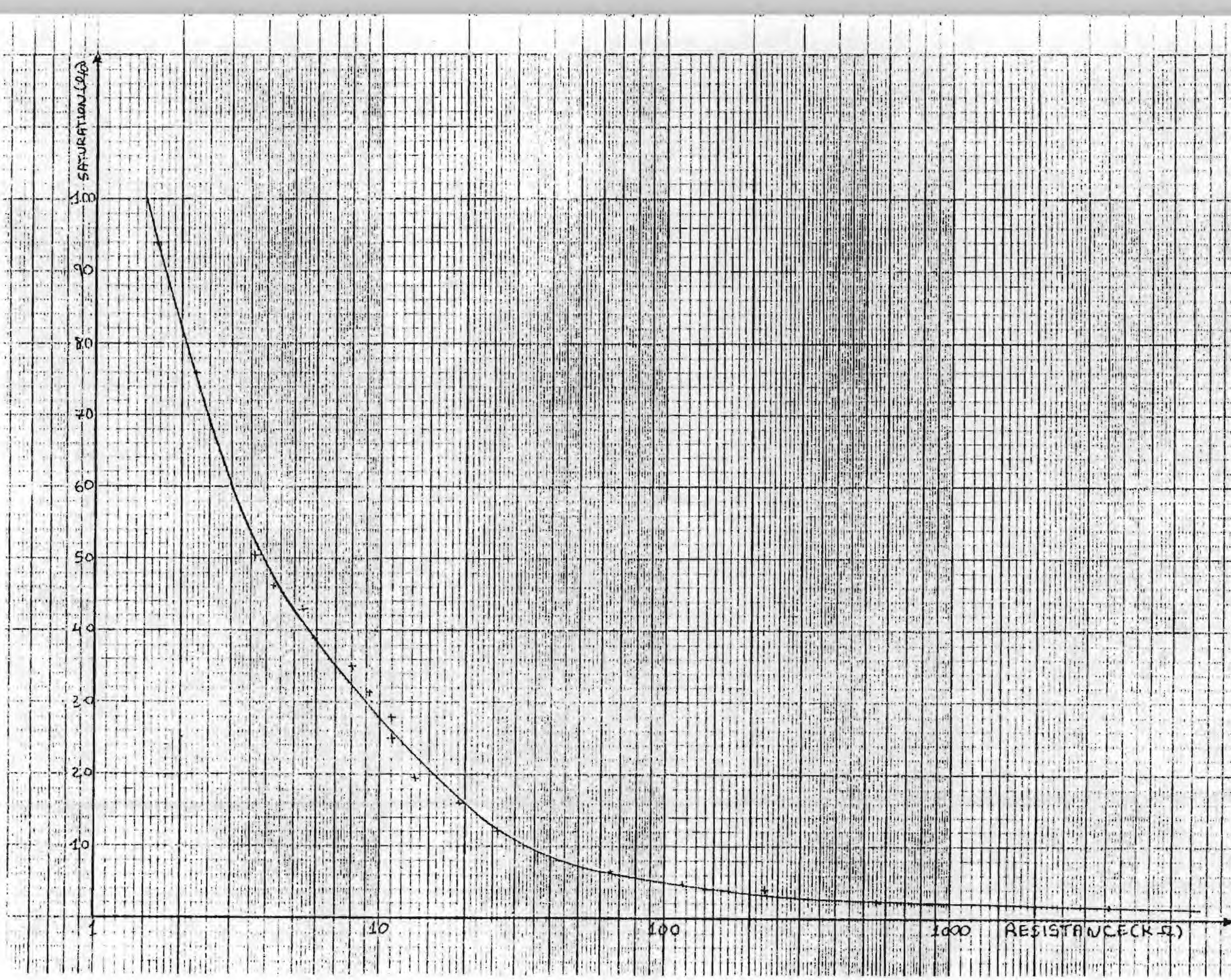



Fig. 12 Electrode Calibration: G.T. Sand

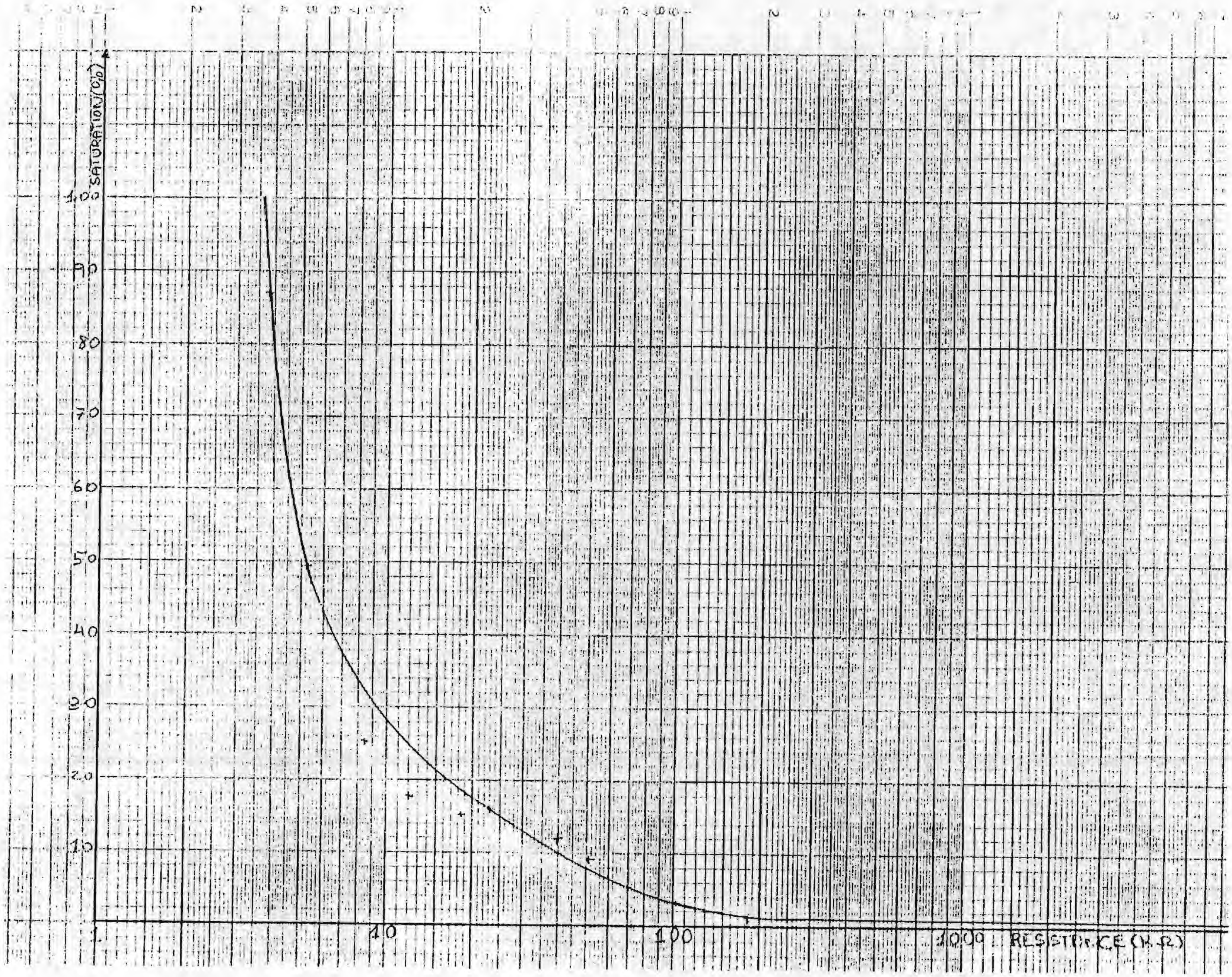



Fig. 13. Electrode Calibration; Rollo Sand.

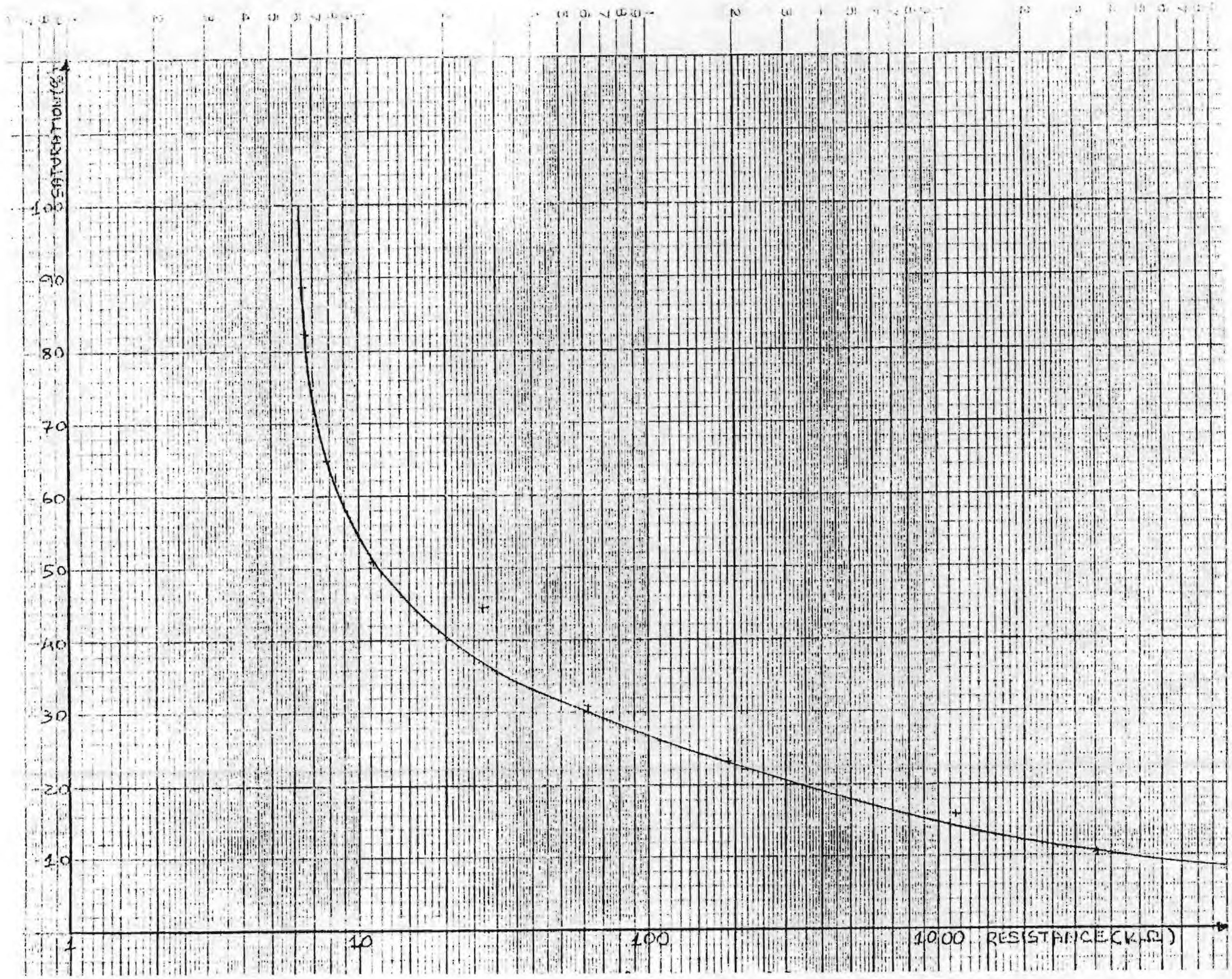



Fig.14. Electrode Calibration: SRP #1 Soil.

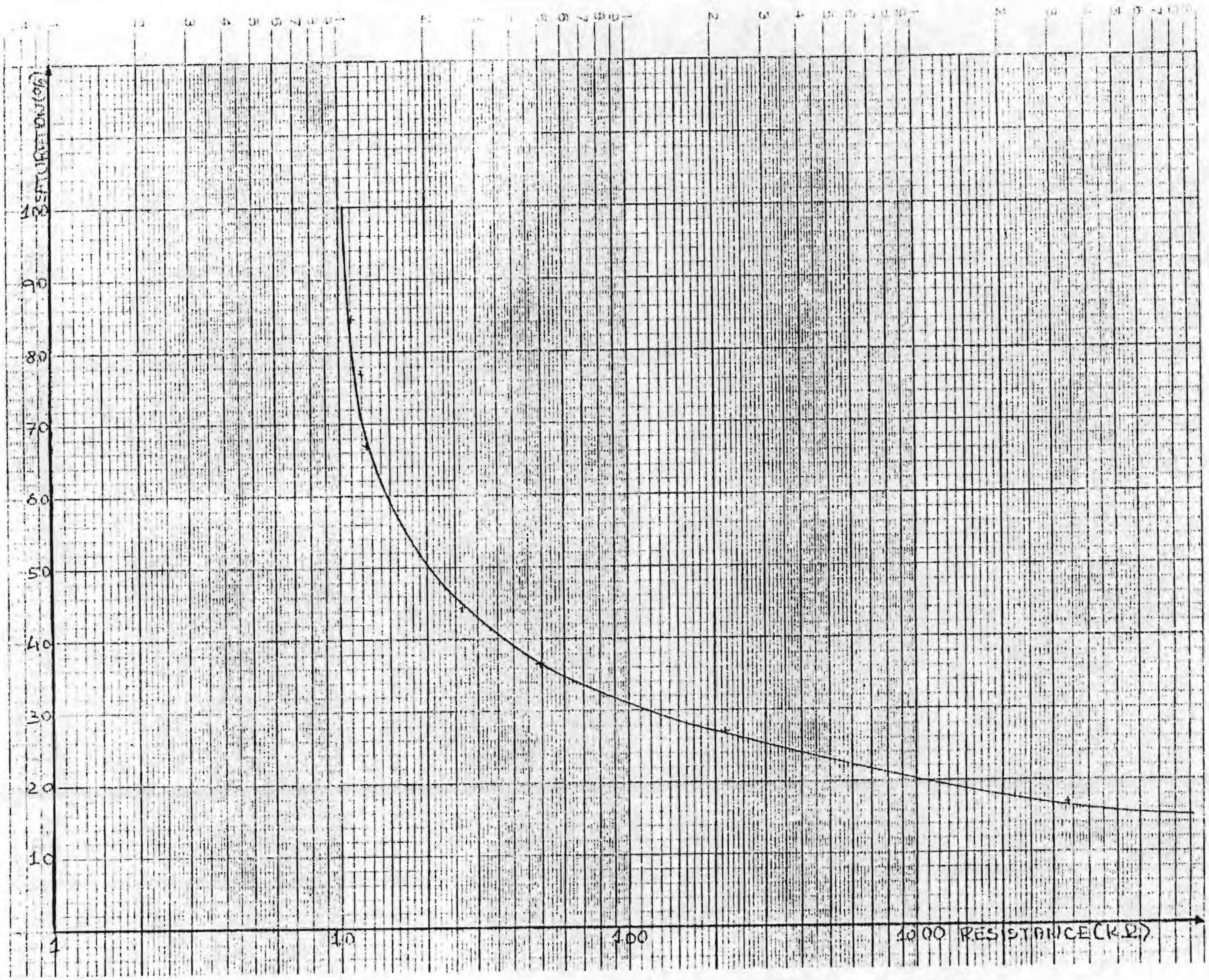



Fig. 15. Electrode Calibration: SRP #2 Soil.

Flow Diversion Test

As mentioned before, these tests are under way at the time of writing. The following procedure is being used:

1. The sand being used for the first run was analyzed with the results presented in the following section.
2. After calibrating the conductivity probes the drum was filled with the material listed in Table 6 which had been compressed from 10 in. to 3 in. in height.
3. Eleven sets of probes were inserted in the sand bed as it was filled and compacted in the locations indicated in Fig 16. Figure 17 shows the appearance of the drum after filling.
4. Baseline measurements were obtained with the dry bed.
5. Subsequent runs, involving vertical moisture profiles and comparison of the inner and outer zone were obtained after injecting 2 gallons of distilled water with a watering can on successive occasions.

TABLE 6

Material Used in Flow Diversion Tests

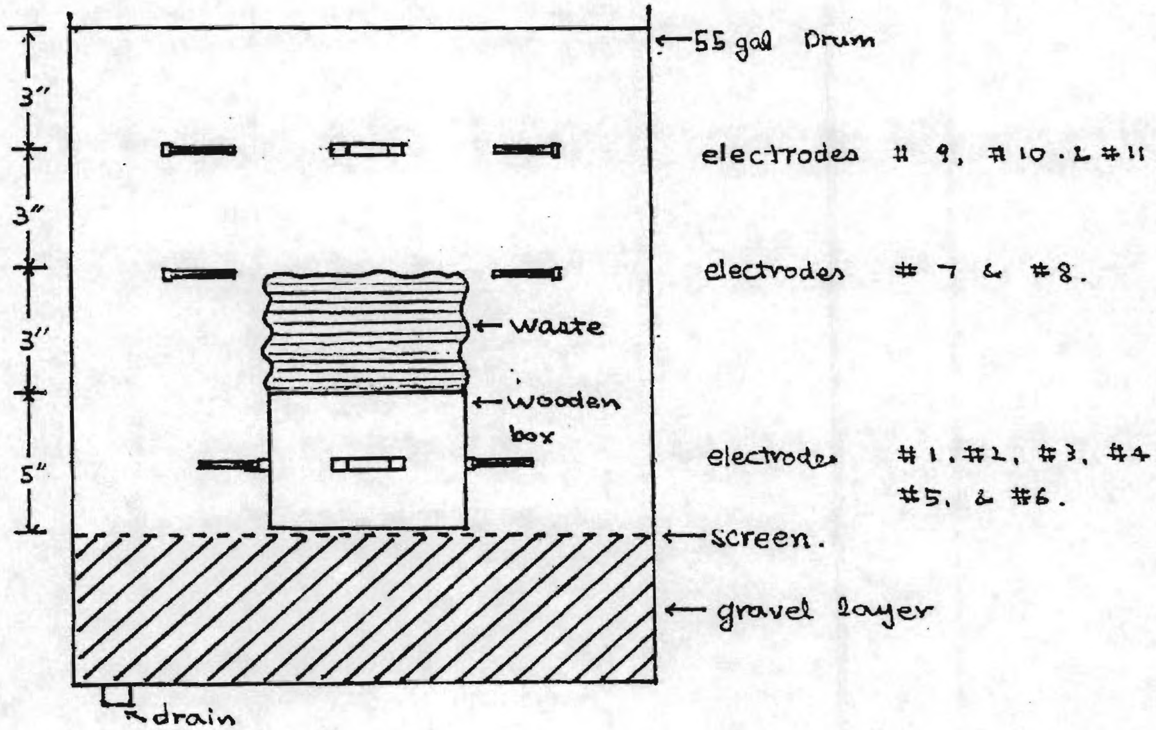
1. Uncontaminated clinical waste materials.

| | | Volume |
|---|---|---|
| Kim wipes, paper towels, and etc | 130.5g | 25% |
| plastic bags | 73.5g | 20% |
| assorted glass ware | 336.6g | 20% |
| polyethylene bottles and cups | 210.0g | 15% |
| disposable pipet tips | 119.6g | 10% |
| metals | 253.6g | 10% |
| total weight | 1223.6g | |

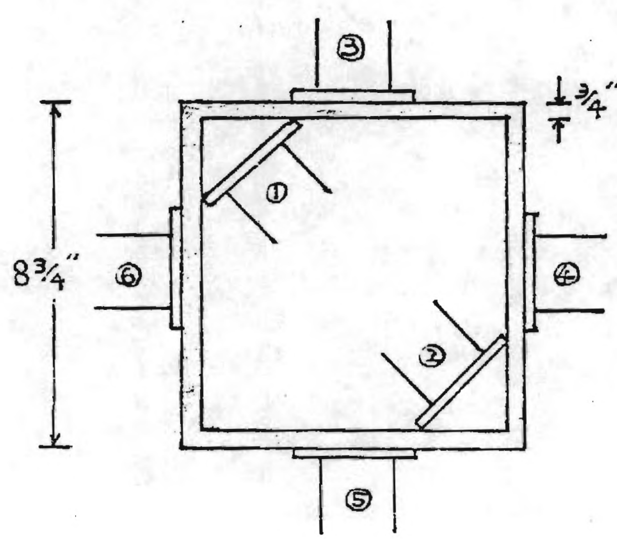
2. 3 gallon ice cream carton.

9.5" diameter, 10" height.

The waste, at first, had 10" of height in the carton and then was compacted to 3" height by pressing it from the top with 13.5 lb/in of weight on it.

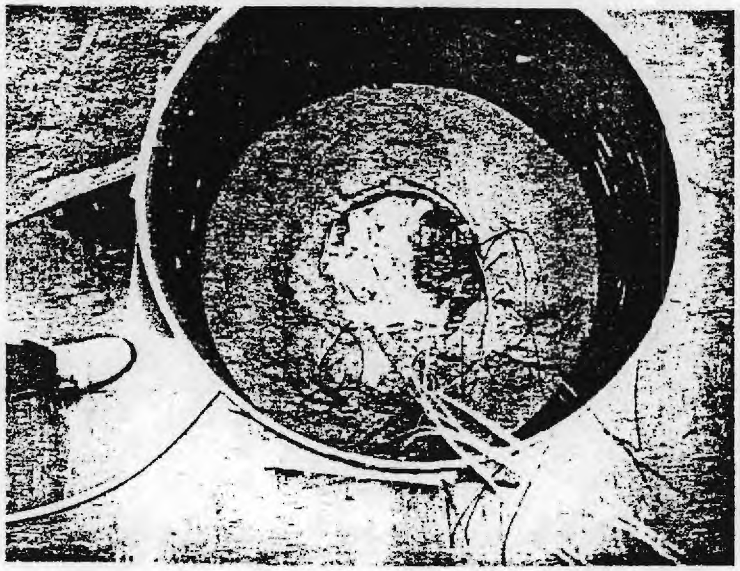



Drum Design and Electrodes.

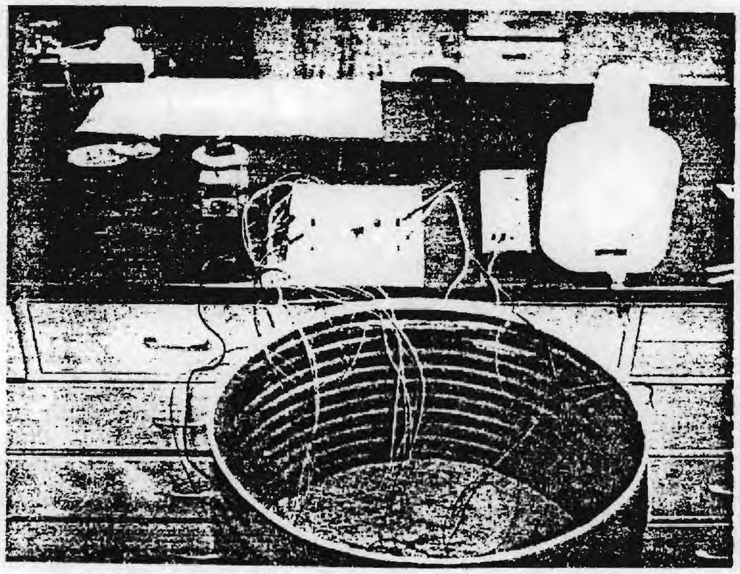



Wooden Box with Electrodes.

Fig. 16 Details on Flow Test



Drum (half-filled with Sand and Waste).



Drum with Measuring Equipments.

Fig. 17 Flow Test Installation

Results and Discussion

It was found that, in the initial state, water was not distributed homogeneously in the sand which filled the drum. In filling the drum, the sand contained a small amount of water and due to the time interval of filling the drum layer by layer, evaporation of moisture from the sand happened. This resulted in inhomogeneous distribution of water in the sand.

Although water content at each position of electrode had changed after watering, this uneven distribution of the initial water content in the sand maintained the same profile as the initial state of this experiment, even 15 days after watering with 2 gallons of distilled water. For example, the water content at electrode positions #1 to #6 increased to about 300% of that at the initial state identically.

In the initial experiment, results were not expected to be obtained quantitatively. However several facts could be observed qualitatively:

One fact observed is that, with very low initial water content, water infiltration rate through the sand was very low; comparing runs #2 and #3 with run #1, this can be seen easily. After 2 gallons of watering, it took 50 min for water to infiltrate through 13 inches of height of the sand; this might be caused by low hydraulic conductivity of the sand when it is relatively low in water content.

Another important fact observed is that, although the initial distribution of water in the sand was not homogeneous, the existence of waste seemed to retard infiltration of water. Looking at saturation values at positions of electrodes #1 to #6, which were located at identical depth, the sand right below the waste seemed to have less water content than the sand outside the wood box. This effect can be explained by the fact that while the free volume in the waste is being filled by water, all gradients are inward and after pressure is applied, equilibrium pressure in the free volume with that of the surrounding soil is established, fluid within the volume of waste will flow with its regional ground water flow. (30).

Another reasonable consideration can be that there was water-absorbing material, like kimwipes and papertowels, which might absorb a considerable amount of water to retard the flow of water.

Experiment 2 started with the initial state of water content which was the last state of run #1. This means that, as the initial water content, the sand contained about 300% higher water content than that of the initial state in experiment 1.

The first results of run #2 showed fast changes of saturation values which were measured right after watering: The deepest electrodes (#1 to #6) read about 200% increase in water content. However, at $t = o$, water content values began to increase or decrease slowly, but faster than in experiment #1. For rapid and big changes in saturation values at $t = o$ one may assume that water might have filled and been kept in the big voids of the waste volume from the experiment 1, and then the water in the voids was flushed out rapidly by the change of pressure caused by the new water source.

Following this, the same retardation of water flow through the waste occurred as was observed in experiment 1.

In run #3, fast and large changes of water content at the deepest positions were not observed. This was thought to be because of the long drainage time in experiment #2 (15 days). Because of that, the water which might have filled the voids in the waste volume is thought to have been drained down.

## C. Soil Material Characterization

To compare the behavior of SRP soil with other soil materials and to enable one to extrapolate measured values to a more general case that can be projected by the calculational model, it is important to characterize the soil materials used. The principal parameters of interest are hydraulic conductivity or permeability, ion exchange capacity, residual moisture content and draining rate. These must be experimentally determined and related to the inherent properties of the soil materials, i.e. bulk density, porosity, particle size and composition.

1 - Bulk Density

One of the important parameters for any soil study is the bulk density. The bulk density is defined as the ratio between the dry weight of the soil and the total volume in undisturbed conditions.

Samples of the four soils under study (Georgia Tech Sand, Rollo Sand, Savannah River Plant Soil #1 and #2) were oven dried for 24 hours at 105+5 $^{o}C$ as is recommended by the ASTM (34). A plastic vial with known volume ($21.3 cm^3$) was then used to obtain 3 samples of each soil; these samples were then weighed and the obtained result are shown in Table 7 .

TABLE 7 - BULK DENSITIES ($g/cm^3$)

| SAMPLE # | G.T.SAND | ROLLO SAND | SRP #1 | SRP #2 |
|---|---|---|---|---|
| 1 | 1.38 | 1.40 | 1.25 | 1.19 |
| 2 | 1.39 | 1.39 | 1.24 | 1.20 |
| 3 | 1.37 | 1.41 | 1.24 | 1.21 |
| AVERAGE | 1.38 | 1.40 | 1.24 | 1.20 |

The bulk density was obtained with two different measurements: the weight and the volume of the dry soil. The volume of the sample vial was determined by weighing the vial, filling it with distilled water and weighing again; the difference between these weighings is then divided by the density of the water at the temperature the measurements were done.

$$V = \frac{W_{v+w} - W_v}{\rho_w}$$

Where V is volume, $W_{v+w}$ and $W_v$ are the weights of the vial with water and the empty vial, respectively, and $\rho_w$ is the density of the water.

Three measurements were performed and all three presented the same result, 21.30 $cm^3$. Since there was no variability in the results, the error associated with this measurement is the error due to the instrument readings, which can then be assumed as half the value of the smallest instrumental division, in this case, 0.05g. Assuming the error associated with the water density is negligible, and using the water density at 25° as 0.997g/$cm^3$ the error associated with the volume determination is 0.07 $cm^3$ and V = 21.30 ± 0.07 $cm^3$. Table 8 presents the results of these measurements.

TABLE 8 - BULK DENSITY

| | WEIGHT (g) | VOLUME ($cm^3$) | BULK DENSITY (g/$cm^3$) |
|---|---|---|---|
| ROLLO SAND | 29.879±0.159 | 21.30±0.07 | 1.40±0.01 |
| G.T.SAND | 29.394±0.095 | 21.30±0.07 | 1.38±0.01 |
| SRP #1 | 29.484±0.113 | 21.30±0.07 | 1.24±0.01 |
| SRP #2 | 25.503±0.179 | 21.30±0.07 | 1.20±0.01 |

2 - Porosity

Porosity is another soil parameter that has to be determined in order to well characterize the soils. The porosity of a soil is defined as the fraction of the total volume of the material which is occupied by pores or interstices; these pores may be filled with water if the soil is saturated, or with air and water if the soil is unsaturated. The porosity may be written a function of the bulk density.

$$n = 1 - \frac{\rho_b}{\rho_d}$$

where n is the porosity, $\rho_b$ is the bulk density, and $\rho_d$ is the particle density.

For soils and gravels, the predominant mineral is quartz, and a density of 2.65 g/$cm^3$ is generally used as the density of the solid fraction of the soil (Bauer et al., 1972). Consequently, using a particle density value of

$2.65 \pm 0.01 g/cm^3$ will cover the whole range of interest. With the values given in Table 8 for the bulk density, the porosity of the four soils was calculated and the results are shown in Table 9. The errors were calculated by applying the error propagation formula; these errors are also shown in Table 9.

TABLE 9 - POROSITY

| | BULK DENSITY ($g/cm^3$) | PARTICLE DENSITY($g/cm^3$) | POROSITY |
|---|---|---|---|
| ROLLO SAND | 1.40±0.01 | 2.65±0.01 | 0.472±0.004 |
| G.T.SAND | 1.38±0.01 | 2.65±0.01 | 0.479±0.004 |
| SRP #1 | 1.24±0.01 | 2.65±0.01 | 0.532±0.005 |
| SRP #2 | 1.20±0.01 | 2.65±0.01 | 0.547±0.005 |

## 3 - Particle Size Analysis

The porosity and the bulk density are not the only parameters used to characterize a soil; among some others, the size range of particle in the soil is important. The determination of the particle-size distribution of a soil sample is called mechanical analysis; the results of the mechanical analysis are generally presented in graphical form, known as the distribution curve.

The method used in this study to determine the distribution curve is that recommended by the American Society for Testing and Materials (35, 36). Basically, the soil sample is allowed to contact a dispersive agent (sodium hexameta phosphate) for about 16 hours; the sample is then placed overnight in a shaker in order to disperse all particles. At the end of the dispersion stage, the sample is introduced in a sedimentation cylinder, and hydrometer readings are taken at fixed time intervals. The hydrometer used was the 151H, which is recommended by the ASTM (36). After the readings are taken, a sieve analysis is performed in order to determine the size distribution of the sand fraction. The calculation are then done as shown in Ref. 36.

The distribution curve of the four soils under study was determined, and the results are shown in Table 10-13; Figures 18-21 show the distribution curve of the four soils, and Table 14 shows the resultant sand, silt, and clay fractions of the four soils.

TABLE 10 - PARTICLE SIZE DISTRIBUTION - G. T. SAND

| DIAMETER ($\mu$m) | % PASSING (%) | DIAMETER ($\mu$m) | % PASSING (%) |
|---|---|---|---|
| 1410.0 | 90.7 | 23.0 | 1.5 |
| 1000.0 | 80.7 | 13.0 | 1.5 |
| 707.0 | 65.8 | 9.3 | 0.7 |
| 500.0 | 46.6 | 6.6 | 0.7 |
| 250.0 | 10.4 | 5.0 | 0.7 |
| 105.0 | 2.9 | 3.5 | 0.0 |
| 75.0 | 2.6 | 2.7 | 0.0 |
| 36.0 | 1.5 | 1.3 | 0.0 |

TABLE 11 - PARTICLE SIZE DISTRIBUTION - ROLLLO SAND

| DIAMETER ($\mu$m) | % PASSING (%) | DIAMETER ($\mu$m) | % PASSING (%) |
|---|---|---|---|
| 1410.0 | 86.0 | 36.4 | 1.2 |
| 1000.0 | 51.3 | 23.0 | 1.2 |
| 707.0 | 12.8 | 13.3 | 1.2 |
| 500.0 | 4.5 | 9.4 | 1.2 |
| 250.0 | 1.3 | 6.7 | 0.6 |
| 105.0 | 1.1 | 4.7 | 0.6 |
| 75.0 | 1.1 | 3.4 | 0.0 |

TABLE 12 - PARTICLE SIZE DISTRIBUTION - SRP #1

| DIAMETER ($\mu$m) | %PASSING (%) | DIAMETER ($\mu$m) | % PASSING (%) |
|---|---|---|---|
| 1410.0 | 97.1 | 7.6 | 30.4 |
| 1000.0 | 94.5 | 5.4 | 29.7 |
| 500.0 | 80.4 | 3.8 | 29.7 |
| 250.0 | 61.0 | 2.7 | 29.0 |
| 75.0 | 34.8 | 2.0 | 28.3 |
| 63.0 | 34.2 | 1.1 | 27.7 |
| 29.0 | 33.1 | 1.0 | 27.0 |
| 18.4 | 32.4 | 0.8 | 26.3 |
| 10.7 | 31.7 | 0.7 | 25.6 |

TABLE 13 - PARTICLE SIZE DISTRIBUTION -SRP #2

| DIAMETER ($\mu$m) | % PASSING (%) | DIAMETER ($\mu$m) | % PASSING (%) |
|---|---|---|---|
| 1410.0 | 97.1 | 16.5 | 42.3 |
| 1000.0 | 94.6 | 9.6 | 41.6 |
| 500.0 | 84.2 | 6.9 | 40.9 |
| 250.0 | 62.1 | 4.9 | 40.3 |
| 75.0 | 43.3 | 2.4 | 39.6 |
| 63.0 | 43.1 | 1.0 | 38.9 |
| 25.8 | 43.0 | | |

TABLE 14 - SOIL PROPERTIES

| SOIL TYPE | BULK DENSITY ($g/cm^3$) | POROSITY | SAND FRACTION (%) | SILT FRACTION (%) | CLAY FRACTION (%) | RESIDUAL* WATER CONTENT (%) |
|---|---|---|---|---|---|---|
| ROLLOSAND | 1.40 | 0.472 | 98.9 | 1.1 | 0.0 | 0.8 |
| G.T. SAND | 1.38 | 0.479 | 97.4 | 2.6 | 0.0 | 0.7 |
| SRP #1 | 1.24 | 0.32 | 62.0 | 9.0 | 29.0 | 10.0 |
| SRP #2 | 1.20 | 0.547 | 56.0 | 4.0 | 40.0 | 16.0 |

*Approximate values from Figs. 12 - 15

D. Residual Water Content

The residual water content is defined as the amount of water retained by a material when water is removed by the force of gravity; although it has a very simple definition, the residual water content is very difficult to determine in practical situations. The importance of this soil parameter is that it reflects the maximum degree of unsaturation that a soil can reach and, consequently, the minimum rate that a solute in the soil will be transported by the water.

In order to determine the residual water content, a large column filled with a soil would have to be left draining for a long time and, when no more water flows from the column, the water content is then determined; this is not a very practical procedure, and so the electrical resistance of the soil was used to estimate the residual water content.

In a previous experiment, Whang (1984) used the electrical resistance method to estimate the residual water content of several sands. Basically, several short columns (8.2 cm long, electrodes 5 cm apart) were filled with saturated sand and were allowed to drain, while the electrical resistance was measured from time to time. When the current reached zero (infinite resistance), the residual water content was determined. When the resistance reaches zero, it means that the water in the soil is no longer interconnected, and although it may not be the point at which the water stops flowing due to gravity, as it is defined, it is at least a good indication of the residual water content. When Whang applied the same method for soils containing an appreciable amount of clay (SRP#1 and SRP#2), the current did not reach zero; consequently, the point used for the residual water content was chosen when the current reading remained constant for some time. This result is expected, since as the soil particle decrease in size, the force attracting the water to the soil particles increase and, although the water in the soil is still interconnected, the gravity force is not enough to separate the water from the soil particles, and there is no water flow in the soil. Whang's results are shown in Table 15.

TABLE 15 - RESIDUAL WATER CONTENT

| SOIL TYPE MESH SIZE | RESIDUAL WATER CONTENT (%) |
|---|---|
| 14-16 | 0.50 |
| 16-20 | 0.16 |
| 25-30 | 0.18 |
| 30-55 | 0.25 |
| 40-50 | 0.33 |
| 50-60 | 0.61 |
| SRP#1 | 12.50 |
| SRP#2 | 16.70 |

In the experiments described in this report, the calibration of the soils was done starting from dry soils; consequently, it is almost impossible to use the results in order to estimate the residual water content. However, if the point at which the current changes from zero to any value is used as an indication of the residual water content, it is possible to compare the results obtained with the results obtained by Whang; the values shown in

Table 16 were obtained from Figs 12-15.

TABLE 16 - RESIDUAL WATER CONTENT

| SOIL TYPE | RESIDUAL WATER CONTENT |
|---|---|
| ROLLO SAND | 0.89 % |
| G.T. SAND | 1.59 |
| SRP #1 | 10.51 |
| SRP #2 | 17.37 |

Comparing the results presented in Tables 15 and 16, it is seen that they are in good agreement. In order to check if these results could be assumed as a valid estimation of the residual water content, a long sand column (26 cm long, 2 cm diameter) was filled with sand (15-20 mesh size) and saturated. It was then left draining for more than 3 months. After that time, the current readings (electrodes at each 2cm) were equal to zero in the top portion of the column (top 10cm), and then the readings increased reaching a maximum at the bottom of the column. The water content corresponding to the top 10cm was found to be $w = 3.4 \times 10^{-4}$, which is close to the value reported by Whang for the same sand size ($w = 4.5 \times 10^{-4}$). However, the bottom of the column presented an average water content of $w = 1.5 \times 10^{-3}$, which is an order of magnitude higher. One possible explanation for this high water content at the bottom is that a paper filter was used to support the sand, and it is suspected that this filter was not very permeable, and so it did not allow the water to drain freely. These tests are being repeated and expanded.

# CONCLUSION

This report constitutes a progress report on work done at the Georgia Institute of Technology in support of the Savannah River Laboratory lysimeter studies. These investigations centered on the development of a suitable computer model and on experimental tests to establish realistic flow paths within the lysimeters and to study the unsaturated flow conditions existing there. Considerable progress has been made on all these tasks and is reported here. A two-dimensional model has been described and is at present in process of being debugged and tested. The program presented in Appendix B is indicative of the nature of the model, but should be considered as preliminary only at this stage.

The experimental tests have shown that the Savannah River soils tested will retain a residual moisture level of 10-16%. Ordinarily, unsaturated flow conditions prevail and both waste leach rates and migration rates would be expected to be well below those indicated for saturated flow. Waste compression tests have been performed and show that material of the type placed in the lysimeters will not be flattened entirely by the overlying soil and may well present a preferred pathway for the infiltrated water. The possibility of water perching in the waste volume then depends on the drainage rate in the lower half of the lysimeter.

These and related aspects will be the subject of continuing investigations.

## REFERENCES


1. G. E. Siple, Geology and Ground Water of the Savannah River Plant and Vicinity, South Carolina. U.S. Geological Survey Water Supply Paper 1841, U.S. Govt. Printing Office, Washington D.C., 1967

2. I.W. Marine, Geochemistry of Ground Water of the Savannah River Plant. Rept DP-1356, Savannah River Lab. 1976.

3. W.E. Prout. Adsorption of Radioactive Wastes by Savannah River Plant Soil. Soil Science 86, 13-17 (1958).

4. J.H. Horton and J.C. Corey. Storing Solid Radioactive Wastes at the Savannah River Plant. Rept. DP-1366, Savannah River Lab. 1976.

5. National Academy of Sciences. An Evaluation of the Concept of Storing Radioactive Wastes in Bedrock below the Savannah River Plant Site. National Academy of Sciences, Washington, D.C. 1972.

6. Final Environmental Impact Statement. Defense Waste Processing Facility, Savannah River Plant, Aiken, S.C. Rept. DOE/EIS-0082, U.S. Dept of Energy, Washington, D.C. 1982.

7. D.L. Shaeffer and E.L. Etnier. AQUAMAN - A Computer Code for Calculating Dose Commitments to Man from Aqueous Releases of Radionuclides. Rept. ORNL/TM-6618, Oak Ridge National Laboratory, 1979.

8. G.G. Killough and L.R. McKay. A Methodology for Calculating Radiation Doses from Radioactivity Released to the Environment. Rept. ORNL-4992. Oak Ridge National Lab., 1976.

9. R. L. Hooker and R.W. Root. Lysimeter Tests of SRP Waste Forms. Rept. DP-1591, Savannah River Lab., 1981.

10. S.B. Oblath, J.A. Stone and J.R. Wiley. Special Wasteform Lysimeter Program at the Savannah River Laboratory. Proc. 5th Annual Participants Information Meeting, DOE Low-level Waste Management Program, Denver, 1983, p. 441. CONF-8308106.

11. J.A. Stone, S.B. Oblath, R.H. Hawkins, R.H. Emslie, J.P. Ryan and C.M. King. Migration Studies at the Savannah River Plant Shallow Land Burial Site. Proc. 5th Annual Participants Information Meeting, DOE Low-level Waste Management Program, Denver, 1983, p. 577. CONF-8308106.

12. C.S. Simmons and C.R. Cole. Ground Water Transport Model Selection and Evaluation Guidelines. Proc. 5th Annual Participants Information Meeting, DOE-LLWMP Denver, 1983, p 542, CONF-8308106.

13. M. Reeves and J.O. Duguid. Water Movement through Saturated-unsaturated Porous Media - A finite-element Galerkin Model. Repts ORNE 4927,4928, Oak Ridge National Lab. 1975.

14. S.S. Papadopoulos and L.T. Winograd. Storage of Low-level Radioactive Wastes in the Ground: Hydrogeologic and Hydrochamical Factors. Rept. EPA 74-344, U.S. Environmental Protection Agency, 1974.

15. A.H. Lu. Modeling of Radionuclide Migration from a Low-level Radioactive Burial Site. Health Physics, 34, 39-44 (1978).

16. O.I. Oztunali and A.E. Aikens. A Model to Assess Migration from Shallow Land Burial Facilities. Engineering Bull. 50, 21-30, Dames & Moore, Los Angeles, 1979.

17. D.T. Silvieira, M.A. Harwell, B.A. Napier, J.T. Zellner and G.L. Benson, A Short Description of the AEGIS Aproach. Rept. PNL-3398, Battelle Pacific Northwest Laboratory, 1980.

18. R. Cleary and M. Ungs. Analytical Models for Ground-Water Pollution and Hydrology. Rept. 78-WR-15, Water Resources Program, Princeton University, 1978.

19. H.C. Burkholder and E.L.T. Rosinger. A Model for the Transport of Radionuclides and their Decay Products through Geologic Media. Nuclear Technology 49, 150-158 (1980).

20. G.T. Yeh and R.T. Lumoore, Modeling moisture and thermal transport in unsaturated porous media. J. Hydrology 64, 299-309 (1983).

21. F.N.C. DE Sousa. Movement of Radionuclides through Unsaturated Soils. Georgia Institute of Technology, Program in Health Physics (unpublished), 1983.

22. J.H. Horton. Soil Moisture Flow as Related to the Burial of Solid Radioactive Wastes. Rept. DPST-75-218, Savannah River Lab., 1975.

23. G.L. Poorter, G.J. Langhorst and J.G. Steger. Field Studies and Modeling of Chemical Processes in the Unsaturated Zone. Proc. 5th Annual Participants Information Meeting, DOE-LLWMP., CONF 8308106, Denver, 198 p 548

24. R.H. Brooks, and A.T. Corey. "Hydraulic Properties of Porous Media" Hydrology Paper N 3, Colorado State University. Ft. Collins, Colorado, 1964

25. V.R. Gardner, "Soil Water Relations in Acid and Semi-Acid Conditions". UNESCO 15, 37-61., (1960)

26 R.W. Gilham, et al. "Hydraulic Properties of a Porous Medium: Measurement and Empirical Representation". Soil Sci. Soc. Am. J. 40(2): 203-207 (1976).

27. A.J. Raudkivi, and R. A. Callander, "Analysis of Ground-water Flow" Edward Arnold, London, 1976.

28. M. Th. Van Genuchten, "Numerical Solutions of the One-dimensional Saturated - Unsaturated Flow Equation". Water Resources Program, Princeton University. New Jersey, (1978).

29. G.T. Yeh, Training Course No2: The Implementation of FEMWASTE Computer Program. NUREG/CR-2706, ORNL/TM-8328. Oak Ridge National Laboratory, Oak Ridge, Tennessee, (1982).

30. C.E. Bailey and I.W. Marine, Parametric Study of Geohydrologic Performance Characteristics for Geologic Waste Repositories. Rept. DP-1555, Savannah River Laboratory, (1980).

31. Dames & Moore. "Detailed Seepage Investigation of Mill Waste Disposal Alternatives, West Gas Hills, Wyoming, Dames & Moore, Salt Lake City, Utah., 1980

32. Segol, Genevieve. "A Three-Dimensional Galerkin Finite Element Model for the Analysis of Contaminant Transport in Saturated-Unsaturated Porous Media", International Conference on Finite Element in Water Resources, Princeton University, Princeton, New Jersey, 1976.

33. Reisenauer, A. E., S. K. Gupta, R. W. Nelson, and C. A. Newbill. "Advective Radionuclide Transport with Soil Interaction Under Variably Saturated Flow Conditions". Rept. PNL-3994, Pacific Northwest Laboratory, Richland, Wash. 1981.

34. ASTM. "Standard Method of Laboratory Determination of Moisture Content of Soil". 1974 Annual Book of ASTM Standards, Part 19. Am. Soc. For Testing and Materials, Philadelphia, 1974.

35. ASTM. "Standard Method for Dry Preparation of Soil Samples For Particle Size Analysis and Determination fo Soil Constants". 1975 Annual Book of ASTM Standards, Part 19. Am. Soc. for Testing and Materials, Philadelphia, 1975.

36. ASTM. "Standard Method For Particle-Size Analysis of Soils", 1975 Annual Book of ASTM Standards, Part 19. Am. Soc. For Testing and Materials, Philadelphia, 1975

# Appendix A

## Program of the one-dimensional model.

```
      PROGRAM NUNO (DADOS,OUTPUT,SAIDA,TAPE5=DADOS,TAPE6=OUTPUT,
     1              TAPE7=SAIDA)
      DIMENSION Z(20),TETIN(20),ICON(20,2),NEWN(2),ZE(2),SE(2,2),
     1          BE(2,2),XM(2,2),AE(2,2),AG(20,3),XMG(20,3),PG(20),
     2          AGT(20,3),AGP(20),XMT(20,20),TETIX(20),AGZ(20,3),
     3          XA(20,3),TETIS(20),U(20,5),XY(200),TETEN(20)
      CALL INPU(XL,TIME,TIVAL,NELEM,Z,TETIN,BOUND,ICON,TIMEX,
     1 XERR,AI,BI,PM,HCOS,PORO,PL,ISP,ISS,NNODE)
      TI=0
1     DO 5 I=1,20
**********                                          MCH29
      PG(I)=0.
*******                                             MCH29
      DO 5 J=1,3
      AG(I,J)=0
5     XMG(I,J)=0
*     PG(1)=0      ********************************DELETED ON MCH29******
      DO 20 I=1,NELEM
      TETI1=TETIN(I)
      TETI2=TETIN(I+1)
      DO 10 J=1,2
10    NEWN(J)=ICON(I,J)
      CALL SET(NEWN,ZE,Z,NNODE,ISP,XL,NELEM)
      CALL ELEM(ZE,TETI1,SE,BE,XM,AE,AI,BI,PM,HCOS,PORO,PL,
     1 TETI2)
20    CALL ASSEM(NEWN,AE,AG,XM,XMG)
      CALL BOUN(BOUND,PG,TIMEX,TI,TETIN,HCOS,PORO,PM)
      CALL CALC1(TIVAL,PG,AG,TETIN,XMG,AGP)
      IJOB=0
      N=20
      NLC=1
      NUC=1
      IA=20
      DO 110 I=1,20
      DO 110 J=1,20
      XMT(I,J)=0.
      IF(I.EQ.J) XMT(I,J)=1.
110   CONTINUE
      CALL LEQT2B(XMG,N,NLC,NUC,IA,XMT,N,IA,IJOB,U,N,XY,IER)
      WRITE(6,*)'1ST',IER
      CALL CMULT(XMT,AGP,TETIX)
      ITI=0
      TI=TI+TIVAL
115   CALL BOUN(BOUND,PG,TIMEX,TI,TETIX,HCOS,PORO,PM)
120   DO 150 I=1,20
      DO 150 J=1,3
      AGZ(I,J)=AG(I,J)
150   CONTINUE
      PI=PG(1)
      DO 200 I=1,20
      DO 200 J=1,3
      AG(I,J)=0.
200   XMG(I,J)=0.
```

```
      DO 300 I=1,NELEM
      TETI1=TETIX(I)
      TETI2=TETIX(I+1)
      DO 250 J=1,2
250   NEWN(J)=ICON(I,J)
****************                                            MCH29
      CALL SET(NEWN,ZE,Z,NNODE,ISP,XL,NELEM)
****************                                            MCH29
      CALL ELEM(ZE,TETI1,SE,BE,XM,AE,AI,BI,PM,HCOS,PORO,PL,
     1 TETI2)
300   CALL ASSEM(NEWN,AE,AG,XM,XMG)
      CALL CALC2(TIVAL,PG,AG,TETIN,XMG,AGP,PI,AGZ,XA)
      DO 310 I=1,20
      DO 310 J=1,20
      XMT(I,J)=0
      IF(I.EQ.J) XMT(I,J)=1
310   CONTINUE
      CALL LEQT2B(XA,N,NLC,NUC,IA,XMT,N,IA,IJOB,U,N,XY,IER)
      CALL CMULT(XMT,AGP,TETIS)
C  FEB29
C
      CALL ERROR(TETIX,TETIS,IE,XERR)
      IF(IE.EQ.0)GO TO 350
      TETIX(I)=TETIS(I)
      GO TO 120
 350  IF(ITI.GE.1)GO TO 380
      ITI=1
 360  DO 370 I=1,20
      TETIX(I)=TETIS(I)
 370  TETIN(I)=TETIS(I)
      GO TO 115
 380  CALL ERROR(TETEN,TETIS,IE,XERR)
      IF(IE.EQ.0)GO TO 400
      ITI=ITI+1
      GO TO 360
 400  WRITE(7,*)ITI
 410  CALL OUT(TI,TETIS,Z)
      IF(TI.GE.TIME)GO TO 450
      DO 420 I=1,20
420   TETIN(I)=TETIX(I)
      GO TO 1
 450  CONTINUE
      STOP
      END
      SUBROUTINE ERROR(TETEN,TETIS,IE,XERR)
      DIMENSION TETEN(20),TETIS(20)
****                                TETIN>>TETEN         MCH29
      TTI=0
      TTII=0.
      DO 1 I=1,20
      TTT=TETEN(I)-TETIS(I)
      TT=(ABS(TTT))**2.
      TTI=TTI+TT
      TTII=TTII+(TETEN(I))**2.
```

```
 1    CONTINUE
      TTIII=SQRT(TTI/TTII)
      IF(TTIII.GT.XERR)GO TO 2
      IE=0
      GOTO 3
 2    IE=1
 3    RETURN
      END
C
C
C
C       FEB29
C
C
      SUBROUTINE INPU(XL,TIME,TIVAL,NELEM,Z,TETIN,BOUND,ICON,TIMEX,
     1  XERR,AI,BI,PM,HCOS,PORO,PL,ISP,ISS,NNODE)
      DIMENSION Z(20),TETIN(20),ICON(20,2)
      DO 1 I=1,20
      Z(I)=0.
 1    TETIN(I)=0.
      READ(5,*)XL,TIME,TIVAL,BOUND,NELEM,TIMEX,XERR
      WRITE(7,200)XL,TIME,TIVAL,BOUND,NELEM,TIMEX,XERR
      NNODE=NELEM+1
      READ(5,*)ISP,ISS
      IF(ISP.LT.1)GO TO 3
      DO 2 I=1,NNODE
      Z(I)=(I-1)*XL/NNODE
 2    WRITE(7,400)I,Z(I)
      GO TO 5
 3    DO 4 I=1,NNODE
      READ(5,*)Z(I)
 4    WRITE(7,400)I,Z(I)
 5    DO 6 I=1,NELEM
      DO 6 J=1,2
 6    ICON(I,J)=I+J-1
      IF(ISS.LT.1)GO TO 8
      READ(7,*)TETO
      WRITE(7,950)TETO
      DO 7 I=1,NNODE
 7    TETIN(I)=TETO
      GO TO 10
 8    DO 9 I=1,NNODE
      READ(7,*)TETIN(I)
      WRITE(7,400)I,TETIN(I)
 9    CONTINUE
 10   READ(5,*)AI,BI,PM,HCOS,PORO,PL
      WRITE(7,900)AI,BI,PM,HCOS,PORO,PL
 200  FORMAT(/,2X,3(4X,F8.3),4X,F8.5,4X,I4,2(2X,F8.3))
 400  FORMAT(4X,I4,6X,F8.3)
 900  FORMAT(/,4X,6(F8.3,4X))
 950  FORMAT(/,4X,F8.3)
      RETURN
      END
      SUBROUTINE SET(NEWN,ZE,Z,NNODE,ISP,XL,NELEM)
```

```
      DIMENSION Z(20),ZE(2),NEWN(2)
      IF(ISP.LT.1)GO TO 1
      ZE(1)=0.
      ZE(2)=(XL/NNODE)
      GO TO 5
1     J=NEWN(1)
      JJ=NEWN(2)
      ZE(1)=0.
      ZE(2)=Z(JJ)-Z(J)
5     RETURN
      END
      SUBROUTINE ELEM(ZE,TETI1,SE,BE,XM,AE,AI,BI,PM,HCOS,PORO,PL,
     1  TETI2)
      DIMENSION ZE(2),XM(2,2),SE(2,2),BE(2,2),AE(2,2)
      IF(PORO.GT.TETI1)GO TO 1
      TETI1=PORO
      GO TO 2
1     IF(TETI1.GE.AI)GO TO 2
      TETI1=AI+0.001
2     IF(PORO.GT.TETI2)GO TO 3
      TETI2=PORO
      GO TO 4
3     IF(TETI2.GE.AI)GO TO 4
      TETI2=AI+0.001
4     YN=(PORO-AI)
      YM=(TETI1-AI)
      YMM=(TETI2-AI)
      PPL=(1/PL)
      PPLL=(PL+1)/(PL)
      AL=ZE(2)-(ZE(1))
      XM(1,1)=AL/3
      XM(1,2)=AL/6
      XM(2,1)=AL/6
      XM(2,2)=AL/3
      PMM=PM-1
      BMM=-(PM*HCOS)*(TETI1**PMM)/(PORO**PM)
      AMM=((-1)*(HCOS*(TETI1**PM)/(PORO**PM))*(BI/PL)*(YN**PPL)/(YM**
     1PPLL))
      BMMM=-(PM*HCOS)*(TETI2**PMM)/(PORO**PM)
      AMMM=((-1)*(HCOS*(TETI2**PM)/(PORO**PM))*(BI/PL)*(YN**PPL)/(YMM
     1**PPLL))
      SE(1,1)=-1.*(AMM/AL)
      SE(1,2)=(AMMM/AL)
      SE(2,1)=(AMM/AL)
      SE(2,2)=(AMMM/AL)*(-1.)
      BE(1,1)=(BMM/2)
      BE(1,2)=(BMMM/2)*(-1.)
      BE(2,1)=(BMM/2)
      BE(2,2)=(BMMM/2)*(-1.)
      DO 10 I=1,2
      DO 10 J=1,2
10    AE(I,J)=SE(I,J)+BE(I,J)
      RETURN
      END
```

```
      SUBROUTINE ASSEM(NEWN,AE,AG,XM,XMG)
      DIMENSION NEWN(2),AE(2,2),AG(20,3),XM(2,2),XMG(20,3)
      IUBW=2
      DO 10 I=1,2
      DO 10 J=1,2
      II=NEWN(I)
      JJ=NEWN(J)
      KK=IUBW+JJ-II
      AG(II,KK)=AG(II,KK)+AE(I,J)
      XMG(II,KK)=XMG(II,KK)+XM(I,J)
10    CONTINUE
      RETURN
      END
      SUBROUTINE CALC1(TIVAL,PG,AG,TETIN,XMG,AGP)
      DIMENSION PG(20),AG(20,3),TETIN(20),XMG(20,3),AGT(20,3)
     1,AGP(20)
      DO 1 I=1,20
      AGP(I)=0.
1     CONTINUE
      DO 2 I=1,20
      DO 2 J=1,3
      AGT(I,J)=(XMG(I,J)-(TIVAL*AG(I,J)))
2     CONTINUE
      DO 3 J=2,3
      L=J-1
      AGP(1)=AGP(1)+((AGT(1,J))*(TETIN(L)))
3     CONTINUE
      AGP(1)=AGP(1)+TIVAL*PG(1)
      DO 4 I=2,19
      DO 4 J=1,3
      K=I+J-2
      AGP(I)=AGP(I)+((AGT(I,J))*(TETIN(K)))
4     CONTINUE
      DO 5 J=1,2
      L=18+J
5     AGP(20)=AGP(20)+((AGT(20,J))*(TETIN(L)))
      RETURN
      END
      SUBROUTINE BOUN(BOUND,PG,TIMEX,TI,TETIN,HCOS,PORO,PM)
      DIMENSION PG(20),TETIN(20)
      IF(TI.LE.TIMEX)GO TO 1
      PG(1)=0
      GO TO 2
1     PG(1)=BOUND-HCOS*(TETIN(1)/PORO)**PM
2     CONTINUE
      RETURN
      END
      SUBROUTINE CMULT(XMT,AGP,TETIX)
      DIMENSION XMT(20,20),AGP(20),TETIX(20)
      DO 1 I=1,20
1     TETIX(I)=0
      DO 2 I=1,20
      DO 2 J=1,20
2     TETIX(I)=TETIX(I)+XMT(I,J)*AGP(J)
```

```
      RETURN
      END
      SUBROUTINE CALC2(TIVAL,PG,AG,TETIN,XMG,AGP,PI,AGZ,XA)
      DIMENSION PG(20),AG(20,3),TETIN(20),XMG(20,3),AGP(20),
     1AGZ(20,3),TETIX(20),XA(20,3),AGT(20,3)
      DO 1 I=1,20
      AGP(I)=0
    1 CONTINUE
      DO 2 I=1,20
      DO 2 J=1,3
      XA(I,J)=0.
      AGT(I,J)=(((2/TIVAL)*(XMG(I,J)))-AGZ(I,J))
    2 XA(I,J)=(((2/TIVAL)*XMG(I,J))+AG(I,J))
      DO 3 J=2,3
      L=J-1
    3 AGP(1)=AGP(1)+(AGT(1,J)*TETIN(L))
      AGP(1)=AGP(1)+PG(1)+PI
      DO 4 I=2,19
      DO 4 J=1,3
      K=I+J-2
    4 AGP(I)=AGP(I)+AGT(I,J)*TETIN(K)
      DO 5 J=1,2
      L=18+J
    5 AGP(20)=AGP(20)+AGT(20,J)*TETIN(L)
      RETURN
      END
      SUBROUTINE OUT(TI,TETIX,Z)
      DIMENSION TETIX(20),Z(20)
      WRITE(6,20)TI
      WRITE(6,150)
      WRITE(6,200)(I,Z(I),TETIX(I),I=1,8)
   20 FORMAT(//,15X,"TIME =",1X,F8.3)
  150 FORMAT(/,4X,"NODE",8X,"COORDINATE",8X,"WATER CONTENT")
  200 FORMAT(4X,I4,9X,F8.3,10X,F8.3)
      RETURN
      END
D OF FILE
```

Appendix B

Program of the two-dimensional model.

```
*****************************************
*      Q=+K(PHI)*GRAD.H                 *
*  BASIC FN.=  A + B*Z + C*R            *
*****************************************
*  APRIL 29  1984
************************************
*   PREPARED BY DEOG YOUNG SUH      *
*   MARCH 25 02:18,1984             *
************************************
**************************************************************************
*                                                                        *
*    PROGRAM CAPABILITY :  TO SOLVE 2 DIMENSIONAL UNSTEADY               *
*                      UNSATURATED WATER FLOW OR RADIOACTIVE MATERIAL    *
*                      TRANSPORTATION                                    *
*                                                                        *
*    GENERAL VARIABLES                                                   *
*                                                                        *
*     ND               NUMBER OF NODES                                   *
*     NE               NUMBER OF ELEMENTS                                *
*     NOD(NE,3)        NODES OF AN ELEMENT                               *
*     R(ND)            RADIUS OF A NODE                                  *
*     Z(ND)            ELEVATION OF A NODE                               *
*                                                                        *
*                                                                        *
*    PARAMETERS IN EACH ELEMENT FOR EACH MODEL                           *
*                                                                        *
*     NSAT             UNSAT. = 1      SAT. = 0
*     BTH(NE)          D(K(TH))/D(TH)                                    *
*     DTH(NE)          HYDTAULIC DIFFUSIVITY                             *
*     KS               SATURATED CONDUCTIVITY                            *
*     RAMM(NE)         CCCCCCCCCCPARAMETERS USED TO UNSATURATED MODEL    *
*     EM(NE)           M          PARAMETERS USED TO UNSATURATED MODEL   *
*                      DTH(NE) FOR SAT. CONDITION
*     EN(NE)           N          PARAMETERS USED TO UNSATURATED MODEL   *
*                      BTH(NE) FOR SAT. CONDITION
*     PHL(NE)          PHI-L      PARAMETERS USED TO UNSATURATED MODEL   *
*     THR(NE)          THETA-R    PARAMETERS USED TO UNSATURATED MODEL   *
*                                                                        *
*                                                                        *
*     BOUNDARY CONDITIONS-NODES AND RELATED VALUES                       *
*                                                                        *
*                                                                        *
*                                                                        *
*                                                                        *
*                                                                        *
*    PARAMETERS TO CONTROL THE PROGRAM                                   *
*                                                                        *
*                                                                        *
*     AL(PHA)          OPTION FOR TIME INTEGRATION                       *
*                      AL=0       EXPLICIT                               *
*                      AL=1/2     CRANK-NICOLSON                         *
*                      AL=1       IMPLICIT                               *
*     TIN              TIME INTERVAL                                     *
*     TMAX             TIME LIMIT                                        *
*     ITMAX            ITERATION LIMIT                                   *
*     ERR              TOLERANCE OF CONVERGENCY                          *
```

```
*                                                                        *
**************************************************************************
      PROGRAM TWOD(IN,OUT,TAPE5=IN,TAPE6=OUT)
      PARAMETER(NE=18,ND=16)
      REAL LPI,LHS,KS
      COMMON/COEFF/R(ND),Z(ND),A(NE,3),B(NE,3),C(NE,3),VOL(NE)
      COMMON/ITGR/DTI(NE,3,3),DZI(NE,3,3),LPI(NE,3,3),BC(ND)
      COMMON/GAUS/LHS(ND,ND),RCLMN(ND)
      COMMON NOD(NE,3)
      COMMON RHS(ND,ND)
      COMMON/THS/TH(ND),THL(ND)
      COMMON/SAT/DTH(NE),BTH(NE)
      COMMON/ELM/RAMM(NE),EM(NE),EN(NE),PHL(NE),THR(NE),KS(NE)
*---------------------------------------------------------------
*    READ # OF NODES AND ELEMENTS
*---------------------------------------------------------------
      CALL MAIN
      STOP
      END
***************************************************************
***  MAIN ROUTINE OF THIS PROGRAM  ****************
***************************************************************
      SUBROUTINE MAIN
      PARAMETER(NE=18,ND=16)
      REAL LPI,LHS,KS
      CHARACTER FEM(3)*15
      COMMON/ELM/RAMM(NE),EM(NE),EN(NE),PHL(NE),THR(NE),KS(NE)
      COMMON/COEFF/R(ND),Z(ND),A(NE,3),B(NE,3),C(NE,3),VOL(NE)
      COMMON/ITGR/DTI(NE,3,3),DZI(NE,3,3),LPI(NE,3,3),BC(ND)
      COMMON/GAUS/LHS(ND,ND),RCLMN(ND)
      COMMON NOD(NE,3)
      COMMON RHS(ND,ND)
      COMMON/THS/TH(ND),THL(ND)
      COMMON/SAT/DTH(NE),BTH(NE)
       DATA FEM/'EXPLICIT','CRANK-NICHOLSON','IMPLICIT'/
*---------------------------------------------------------------
*   READ  THE CONSTANTS FOR EACH ELEMENT
*---------------------------------------------------------------
      WRITE(6,121)
 121  FORMAT(////5X,'CONSTANTS FOR EACH ELEMENT'/5X,26('*')//3X,
     1'ELEMENT',T14,'NODE1 NODE2 NODE3',T33,'RAMMDA',T43,'M'
     1,T51,'N',T55,'PHI-L  THETA-R   K-S'/)
      DO 10 I=1,NE
      READ(5,*)(NOD(I,J),J=1,3),RAMM(I),EM(I),EN(I),PHL(I),THR(I),KS(I)
      WRITE(6,112)I,(NOD(I,J),J=1,3),RAMM(I),EM(I),EN(I),PHL(I)
     1,THR(I),KS(I)
 10   CONTINUE
 112  FORMAT(3X,I4,T12,3I6,2X,6F7.2)
*---------------------------------------------------------------
*   READ COORDINATES OF NODES
*---------------------------------------------------------------
      READ(5,*)(R(I),Z(I),I=1,ND)
*---------------------------------------------------------------
*    READ BOUNDARY CONDITIONS AND OPTIONS
*---------------------------------------------------------------
      READ(5,*)AL,TMAX,ITMAX,ERR,TIN,NSAT,G,IHC
```

```
      READ(5,*)TB,TS
      KM=INT(AL*2.+1.)
      WRITE(6,113)FEM(KM),TIN,TMAX,ITMAX,ERR,Q
      WRITE(6,116)TB,TS
      IF(NSAT.NE.0)THEN
      WRITE(6,114)
      ELSE
      WRITE(6,115)
      ENDIF
 113  FORMAT(//'     FEM TYPE                 :',A20
     1        //' TIME INTERVAL               :',F5.2,' MIN'
     2        //' MAXIMUM TIME                :',F5.2,' MIN'
     2        //' MAX. # OF ITERATION         :',I5
     2        //' CONVERGENCE                 :',F8.5
     2        //' WATER FLOW RATE             :',1PE10.3,' GM/MIN/CM**2')
 114  FORMAT(///' UNSATURATED CONDITION'//)
 115  FORMAT(///' SATURATED   CONDITION'//)
 116  FORMAT(/' FLOW-IN BEGINS AT      :',F5.2,' MIN'/
     1        ' FLOW-IN ENDS   AT     :',F5.2,' MIN'//)
*------------------------------------------------------------
*   INTIALIZE TH AND THL  AND PRINT TH
*------------------------------------------------------------
      DO 20 I=1,ND
      READ(5,*)TH(I)
      THL(I)=TH(I)
 20   CONTINUE
      WRITE(6,400)R(1)
      WRITE(6,500)(R(I),I=1,IHO)
      LL=ND/IHO
      DO 212 I=1,LL
      KK=I*IHO
      II=KK-IHO+1
 212  WRITE(6,502)Z(KK),(TH(LM),LM=II,KK)
*----------------------------------------------------------------------*
*   DETERMINE CONSTNATS OF BASIS FUNCTION FOR EACH ELEMENT             *
*                                                                      *
*    BASIS FUNCTION=A(I)+B(I)*Z(I)+C(I)*R(I)                           *
*----------------------------------------------------------------------*
      CALL ABC
*----------------------------------------------------------------------*
*   INTEGRATE OVER AN ELEMENT W.R.T. 1/DT    --- DTI                   *
*                                    LAPLACE-- LPI                     *
*                                    D/DZ    --- DZI                   *
*----------------------------------------------------------------------*
      CALL ITCL(TIN,Q)
*---------------------------------------------------------------------*-
*   ASSIGN ITERATION PARAMETER,BEGINNING TIME                         *
*                                                                     *
*   HERE IS BEGINNING OF TIME LOOP                                    *
*---------------------------------------------------------------------*
      TIME=0.
 111  TIME=TIME+TIN
      DO 30 I=1,ND
      THL(I)=TH(I)
 30   CONTINUE
      IT=0
```

```
      SUM=0.
*-----------------------------------------------------------------*
*   HERE IS BEGINNING OF ITERATION                                *
*   FOR UNSATURATED SPATIAL INTEGRATION                           *
*-----------------------------------------------------------------*
 222  IT=IT+1
      IF(TIME.GE.TB.AND.TIME.LT.TS)THEN
      DO 31 I=1,ND
 31   RCLMN(I)=BC(I)
      ELSE
      DO 32 I=1,ND
 32   RCLMN(I)=0.
      ENDIF
*-----------------------------------------------------------------*
*   DETERMINE CONDUCTIVITY AND DIFFUSIVITY FOR EACH ELEMENT       *
*                                                                 *
*   SUBROUTINE SHOULD BE SUPPLIED BY USER ACCORDING TO            *
*   THE MODELS TO BE USED.                                        *
*-----------------------------------------------------------------*
      IF(NSAT.EQ.0)THEN
      DO 33 I=1,NE
         DTH(I)=EM(I)
         BTH(I)=EN(I)
 33   CONTINUE
      ELSE
      CALL UNSAT
      ENDIF
*-----------------------------------------------------------------*
*   MAKE RIGHT HAND SIDE MATRIX                                   *
*   MAKE LEFT HAND SIDE MATRIX:                                   *
*-----------------------------------------------------------------*
      CALL MKMTX(AL)
*-----------------------------------------------------------------*
*    SOLVE THE MATRIX EQ. TO GET THE VALUE OF TH(ND)              *
*-----------------------------------------------------------------*
      CALL GAUSSE(IFLAG)
*-----------------------------------------------------*
*   CHECK THE CONVERGENCE                             *
*-----------------------------------------------------*
      SUML=SUM
      SUM=0.
      DO 40 I=1,ND
      TH(I)=RCLMN(I)
      SUM=SUM+ABS(TH(I))
 40   CONTINUE
      IF(IT.GE.ITMAX)THEN
      WRITE(6,300)IT
 300  FORMAT(////5X,'# OF ITERATIONS EXCEEDED ',I5,' TIMES'/////)
      GO TO 445
      ENDIF
      IF(SUML.EQ.0.)GO TO 222
      IF(ABS((SUM-SUML)/SUM).GE.ERR)GO TO 222
*-----------------------------------------------------------------*
*     INCREMENT IN TIME AND PRINT THE TH(ND)                      *
*-----------------------------------------------------------------*
 445  WRITE(6,400)TIME
```

```
400   FORMAT(////'       TH AT THE TIME OF',1PE15.3//)
      WRITE(6,500)(R(I),I=1,IHO)
500   FORMAT(//10X,'ELEVATION \ RADIUS',T30,':',1P6E15.3/9X,110('-')/)
      LL=ND/IHO
      DO 122 I=1,LL
      KK=I*IHO
      II=KK-IHO+1
122   WRITE(6,502)Z(KK),(TH(LM),LM=II,KK)
502   FORMAT(1PE22.3,T30,':',1P6E15.3/)
      WRITE(6,401)IT
401   FORMAT(/5X,I4,' TIMES ITERATED'///)
      IF(IT.EQ.ITMAX)RETURN
      IF(TIME.LE.TMAX)GO TO 111
      RETURN
      END
**************************************************************
**** SUBROUTINE TO GENERATE COEFFICIENTS OF BASIS FUNCTIONS ***
**************************************************************
      SUBROUTINE ABC
      PARAMETER(NE=18,ND=16)
      COMMON/COEFF/R(ND),Z(ND),A(NE,3),B(NE,3),C(NE,3),VOL(NE)
      COMMON 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)=ZE(2)*R2(3)-ZE(3)*R2(2)
      A(I,2)=ZE(3)*R2(1)-ZE(1)*R2(3)
      A(I,3)=ZE(1)*R2(2)-ZE(2)*R2(1)
      B(I,1)=R2(2)-R2(3)
      B(I,2)=R2(3)-R2(1)
      B(I,3)=R2(1)-R2(2)
      C(I,1)=ZE(3)-ZE(2)
      C(I,2)=ZE(1)-ZE(3)
      C(I,3)=ZE(2)-ZE(1)
      VOL(I)=(A(I,1)+A(I,2)+A(I,3))/2.
10    CONTINUE
      RETURN
      END
**************************************************************
***** INTEGRATE OVER AN ELEMENT ******************************
**************************************************************
      SUBROUTINE ITGL(TIN,Q)
      PARAMETER(NE=18,ND=16)
      REAL LPI
      COMMON/COEFF/R(ND),Z(ND),A(NE,3),B(NE,3),C(NE,3),VOL(NE)
      COMMON/ITGR/DTI(NE,3,3),DZI(NE,3,3),LPI(NE,3,3),BC(ND)
      COMMON NOD(NE,3)
      DIMENSION S(9),ZE(3),RE(3)
      PHI=3.141592
      SIGN=-1.
      DO 11 I=1,ND
11    BC(I)=0.
```

```
      DO 10 I=1,NE
      DO 20 J=1,3
      K=NOD(I,J)
      ZE(J)=Z(K)
      RE(J)=R(K)
 20   CONTINUE
*-------------------------------------------------------*
*  INTEGRAL OF BASIC VARIABLE IS S(K)                   *
*                                                       *
*    K=1   IS INTEGRAL OF        R                      *
*    K=2   IS INTEGRAL OF        ZR                     *
*    K=3   IS INTEGRAL OF        Z**2*R                 *
*    K=4   IS INTEGRAL OF        R**2                   *
*    K=5   IS INTEGRAL OF        Z*R**2                 *
*    K=6   IS INTEGRAL OF        R**3                   *
*    K=7   IS INTEGRAL OF        Z*R**3                 *
*    K=8   IS INTEGRAL OF        R**4                   *
*    K=9   IS INTEGRAL OF        R**5                   *
*-------------------------------------------------------*
**************** MAY 13 **********************************
      CALL SETUP(0,0,RE(1),RE(2),RE(3),ZE(1),ZE(2),ZE(3),S(1))
      CALL SETUP(0,1,RE(1),RE(2),RE(3),ZE(1),ZE(2),ZE(3),S(2))
      CALL SETUP(0,2,RE(1),RE(2),RE(3),ZE(1),ZE(2),ZE(3),S(3))
      CALL SETUP(1,0,RE(1),RE(2),RE(3),ZE(1),ZE(2),ZE(3),S(4))
      CALL SETUP(1,1,RE(1),RE(2),RE(3),ZE(1),ZE(2),ZE(3),S(5))
      CALL SETUP(2,0,RE(1),RE(2),RE(3),ZE(1),ZE(2),ZE(3),S(6))
      CALL SETUP(2,1,RE(1),RE(2),RE(3),ZE(1),ZE(2),ZE(3),S(7))
      CALL SETUP(3,0,RE(1),RE(2),RE(3),ZE(1),ZE(2),ZE(3),S(8))
      CALL SETUP(4,0,RE(1),RE(2),RE(3),ZE(1),ZE(2),ZE(3),S(9))
********************** MAY 13 **************************END
      VV=4.*VOL(I)**2
      DO 50 L=1,3
      DO 50 M=1,3
      DTI(I,L,M)=2.*PHI*((A(I,L)*B(I,M)+A(I,M)*B(I,L))*S(2)+
     5          A(I,L)*A(I,M)*S(1)+
     1                  (A(I,L)*C(I,M)+A(I,M)*C(I,L))*S(4)+
     2                   B(I,L)*B(I,M)*S(3)+
     3                  (B(I,L)*C(I,M)+B(I,M)*C(I,L))*S(5)+
     4                  C(I,L)*C(I,M)*S(6))/(TIN*VV)
      LPI(I,L,M)=2.*PHI*(C(I,L)*C(I,M)*S(1)+B(I,L)*B(I,M)*S(1))
     1          /VV*SIGN
      DZI(I,L,M)=2.*PHI*(A(I,L)*B(I,M)*S(1)+B(I,L)*B(I,M)*S(2)
     1                 +C(I,L)*B(I,M)*S(4))/VV*SIGN
*-------------------------------------------*
*   BOUNDARY CONDITION                      *
*      AT Z=0,Q=SOME VALUE                  *
*     (COUNT-CLOCKWISE INTEGRATION ONLY)    *
*-------------------------------------------*
      IF((ZE(L)+ZE(M)).NE.0.)GO TO 50
      NN=NOD(I,L)
      R1=RE(L)
      R2=RE(M)
      S2=R1**2-R2**2
      S3=R1**3-R2**3
      IF(S2.GE.0.)S2=-S2
      IF(S3.GE.0.)S3=-S3
```

```
******    AS(N,N) * X(N) = RCLMN(N)                            **************
******    RESULTS:      AS(N,N) >>> I(N,N) UNIT MATRIX ************
******                  RCLMN(N)    >>> X(N)    ROOTS          **************
******                  IFLAG=100  SINGULAR MATRIX    *************
****************************************************************************
      SUBROUTINE GAUSSE(IFLAG)
      PARAMETER(NE=18,ND=16)
      COMMON/GAUS/AS(ND,ND),RCLMN(ND)
      N=ND
      IFLAG=0
      DO 100 I=1,N
      J=I+1
 10   IF(AS(I,I).EQ.0.)THEN
      IFLAG=IFLAG+1
      IF(J.LT.N)THEN
      B=RCLMN(J)
      RCLMN(J)=RCLMN(I)
      RCLMN(I)=B
      DO 200 K=1,N
      A=AS(J,K)
      AS(J,K)=AS(I,K)
      AS(I,K)=A
 200  CONTINUE
      ELSE
      IFLAG=100
      RETURN
      ENDIF
      J=J+1
      GO TO 10
      ENDIF
      AI=AS(I,I)
      DO 50 II=1,N
 50   AS(I,II)=AS(I,II)/AI
      RCLMN(I)=RCLMN(I)/AI
      DO 300 K=1,N
      IF(K.EQ.I)GO TO 300
      AK=AS(K,I)
      RCLMN(K)=RCLMN(K)-RCLMN(I)*AK
      DO 400 L=1,N
      AS(K,L)=AS(K,L)-AS(I,L)*AK
 400  CONTINUE
 300  CONTINUE
 100  CONTINUE
      RETURN
      END
ND OF FILE
```

```
      QIN=2.*PHI*(A(I,L)*S2/2.+C(I,L)*S3/3.)/2./VOL(I)*Q*TIN
      BC(NN)=BC(NN)+QIN*SIGN
 50   CONTINUE
 10   CONTINUE
      RETURN
      END
**************** MAY 13 ***********************BEGIN
      SUBROUTINE SETUP(I,J,R1,R2,R3,Z1,Z2,Z3,S)
      C=(Z3-Z1)/(R3-R1)
      A=(Z2-Z1)/(R2-R1)
      D=(R3*Z1-R1*Z3)/(R3-R1)
      B=(R2*Z1-R1*Z2)/(R2-R1)
         S=0.
          R=R1
 10       RP2=R**(I+2)/(I+2)
         RP3= R**(I+3)/(I+3)
         RP4= R**(I+4)/(I+4)
         RP5= R**(I+5)/(I+5)
        IF(J.EQ.0)THEN
        S=S+RP3*(A-C)+RP2*(B-D)
        ELSE IF (J.EQ.1)THEN
        S=S+(RP4*(A*A-C*C)+RP3*(A*B-C*D)*2.+RP2*(B*B-D*D))/2.
        ELSE IF (J.EQ.2)THEN
         S=S+(RP5*(A**3-C**3)+(RP4*(A*A*B-C*C*D)+RP3*(A*B*B
     1          -C*D*D))*3.+RP2*(B**3-D**3))/3.
       ENDIF
        S=S*(-1.)
        IF(R.EQ.R1)THEN
        R=R2
        GO TO 10
       ENDIF
        RETURN
        END
*********************************** JUNE20
************************* MAY 13 ******************************END
**************************************************************
****** CALCULATE CONDUCTIVITY (BTH) AND DIFFUSIVITY (DTH) *****
**************************************************************
      SUBROUTINE UNSAT
      PARAMETER (NE=18,ND=16)
      REAL KS
      COMMON NOD(NE,3)
      COMMON/THS/TH(ND),THL(ND)
      COMMON/SAT/DTH(NE),BTH(NE)
      COMMON/ELM/RAMM(NE),EM(NE),EN(NE),PHL(NE),THR(NE),KS(NE)
*--------------------------------------------------------*
*     MODEL SHOULD BE SUPPLIED BY USER                   *
*--------------------------------------------------------*
      DO 10 I=1,NE
*--------------------------------------------------------*
*     GET AVERAGED TH VALUE OVER AN ELEMENT              *
*--------------------------------------------------------*
      THAV=(TH(NOD(I,1))+TH(NOD(I,2))+TH(NOD(I,3)))/3.
      DTH(I)=KS(I)*(THAV/EN(I))**EM(I)/(-RAMM(I)*PHL(I)/(EN(I)-THR(I)
     1       )/((THAV-THR(I))/(EN(I)-THR(I)))**(1.+1./RAMM(I))
      BTH(I)=KS(I)/EN(I)*EM(I)*(THAV/EN(I))**(EM(I)-1.)
```

```
 10    CONTINUE
       RETURN
       END
***********************************************************************
*** MAKE THE LEFT HAND SIDE MATRIX LHS(ND,ND) *****************
***********************************************************************
*** MAKE THE RIGHT HAND SIDE MATRIX RHS(ND,ND) THEN ***********
*** MAKE THE RIGHT HAND COLUMN MATRIX RCLMN(ND)=RHS(ND,ND)*THL(ND)
***********************************************************************
*-----------------------------------------------------------------------*
*       LHS(ND,ND=SYSTEM MATRIX OF (DTI-AL*(DTH*LPI+BTH*DZI))           *
*       RHS(ND,ND)=SYSTEM MATRIX OF ((1-AL)*(DTH*LPI+BTH*DZI)+DT)       *
*-----------------------------------------------------------------------*
       SUBROUTINE MKMTX(AL)
       PARAMETER(NE=18,ND=16)
       REAL LPI,LHS
       COMMON NOD(NE,3)
       COMMON/ITGR/DTI(NE,3,3),DZI(NE,3,3),LPI(NE,3,3),BC(ND)
       COMMON/GAUS/LHS(ND,ND),RCLMN(ND)
       COMMON RHS(ND,ND)
       COMMON/THS/TH(ND),THL(ND)
       COMMON/SAT/DTH(NE),BTH(NE)
*-------------------------------------------------------------     *
*     CLEAR MATRIX FOR NEW VALUE                                   *
*------------------------------------------------------------------*
       DO 10 I=1,ND
       DO 10 J=1,ND
       RHS(I,J)=0.
       LHS(I,J)=0.
 10    CONTINUE
*------------------------------------------------------------------------- *
*    GENERATE SYSTEM MATRIX                                                *
*--------------------------------------------------------------------------*
       DO 20 NNE=1,NE
       DO 20 I=1,3
       II=NOD(NNE,I)
       DO 20 J=1,3
       JJ=NOD(NNE,J)
       LHS(II,JJ)=LHS(II,JJ)+DTI(NNE,I,J)-AL*(DTH(NNE)*LPI(NNE,I,J)
      1            +BTH(NNE)*DZI(NNE,I,J))
       RHS(II,JJ)=RHS(II,JJ)+DTI(NNE,I,J)+(1.-AL)*
      1            (DTH(NNE)*LPI(NNE,I,J)+BTH(NNE)*DZI(NNE,I,J))
 20    CONTINUE
*------------------------------------------------------------------*
*    GENERATE RIGHT HAND SIDE COLUMN MATRIX                        *
*------------------------------------------------------------------*
       DO 30 I=1,ND
       DO 30 J=1,ND
       RCLMN(I)=RCLMN(I)+RHS(I,J)*THL(I)
 30    CONTINUE
       RETURN
       END
***********************************************************************
***********************************************************************
*** SOLVE MATRIX EQUATION BY GAUSSE ELIMINATION ****************
***********************************************************************
```