ORNL-5337
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Quantitative Analysis of Soil Chromatography

I. Water and Radionuclide Transport

M. Reeves
C. W. Francis
J. O. Duguid

Environmental Sciences Division
Publication No. 1105

OAK RIDGE NATIONAL LABORATORY
OPERATED BY UNION CARBIDE CORPORATION · FOR THE DEPARTMENT OF ENERGY

Printed in the United States of America. Available from
National Technical Information Service
U.S. Department of Commerce
5285 Port Royal Road, Springfield, Virginia 22161
Price: Printed Copy $9.00; Microfiche $3.00

ORNL-5337
Dist. Category UC-70

Contract No. W-7405-eng-26

COMPUTER SCIENCES DIVISION

ENVIRONMENTAL SCIENCES DIVISION

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Computer Sciences Division

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FOREWORD

In February 1976 the Energy Research and Development Administration (ERDA) announced a greatly expanded waste management program for defense and commercial radioactive waste. In that announcement, ERDA indicated that the Oak Ridge Operations Office (ORO) of ERDA would have lead responsibility for overall coordination of the expanded commercial geologic disposal program and that an Office of Waste Isolation (OWI) would be created within Union Carbide Corporation-Nuclear Division (UCC-ND) with the responsibility for program management of that activity.

The commercial geologic disposal program was named the National Waste Terminal Storage (NWTS) program. The principal objective of the NWTS program is to provide facilities in various deep geologic formations at multiple locations in the United States which will safely dispose of commercial radioactive waste.

In addition to the geologic studies, the NWTS program includes a number of technical support activities which are required to identify a waste repository site, demonstrate its feasibility, confirm its suitability, and thoroughly analyze all aspects of the repository design proposed for the site. The material presented in this report is related to the category of activity identified as waste/rock interaction projects. These projects are concerned with chemical, physical-chemical, geochemical, and radiochemical reactions and processes between emplaced radioactive waste and the surrounding rock which might affect the design, safe operation, and long-term containment of a geologic repository. This document discusses soil chromatography and evaluates the potential for this analytical technique to provide useful cation exchange property data for soil and rock materials.

ACKNOWLEDGMENTS

The authors gratefully acknowledge the Office of Waste Isolation. Without the initial scientific interest of its representatives and the subsequent financial support, this research would not have been possible. Credit is also due Ms. Janice W. Arwood for both her promptness and her skill in computerized phototypesetting, and to Ms. Nancy C. Smith for the artistic manner in which she set up the many equations of this document. Finally, the authors express their appreciation to Ms. Linda B. Maddox, who was most helpful in editing and debugging the computer program.

QUANTITATIVE ANALYSIS OF SOIL CHROMATOGRAPHY
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ABSTRACT

Soil chromatography has been used successfully to evaluate relative mobilities of pesticides and nuclides in soils. Its major advantage over the commonly used suspension technique is that it more accurately simulates field conditions. Under such conditions the number of potential exchange sites is limited both by the structure of the soil matrix and by the manner in which the carrier fluid moves through this structure. The major limitation of the chromatographic method, however, has been its qualitative nature. This document represents an effort to counter this objection. A theoretical basis is specified for the transport both of the carrier eluting fluid and of the dissolved constituent. A computer program based on this theory is developed which optimizes the fit of theoretical data to experimental data by automatically adjusting the transport parameters, one of which is the distribution coefficient k_d. This analysis procedure thus constitutes an integral part of the soil chromatographic method, by means of which mobilities of nuclides and other dissolved constituents in soils may be quantified.

I. INTRODUCTION

In order to simulate the movement of a radionuclide through geologic formations, it is necessary to describe the adsorption of the radionuclide. A parameter which is frequently used for this purpose is the distribution coefficient k_d. This quantity is defined simply as the ratio of the solid-phase concentration to the liquid-phase concentration, and in the dilute-solution limit it assumes a constant value. Conventionally, values of k_d are obtained under equilibrium conditions using the suspension method. Determined in this manner, k_d values represent the maximum adsorption of a nuclide and may be greater than similar values obtained under "field conditions" [Prokhorov, 1962] by more than an order of magnitude. The large difference is, of course, attributable to insufficient exchange between solid and liquid phases in the moist soil relative to that which takes place in liquid suspension.

One method that appears to simulate environmental conditions better than suspension k_d measurements is soil chromatography [Helling and Turner, 1968, and Rhodes, Belasco, and Pease, 1970]. This method has been proposed by the AIBS-EPA environmental chemistry task group as the most suitable technique for evaluating the relative mobilities of pesticides in soils. It consists basically in the preparation of a thin layer of soil, the transport of the dissolved constituent through the soil by the carrier fluid, and the observation of migration profiles. We have modified this method experimentally for the study of radionuclide movement patterns and have developed a computer model capable of extracting values of k_d from these patterns.

Chapter II presents a brief overview of the experimental techniques. The purpose there, however, is not to present an exhaustive description of such techniques but to introduce the remaining part of the document, which contains the principal thrust of this report. These chapters and appendices form a complete description of our computer model. Moisture- and mass-transport are the subjects of Chapters III and IV, respectively. The optimization procedure used to adjust the transport parameters so as to theoretically "fit" the experimental data is briefly discussed in Chapter V. The next chapter, Chapter VI, describes the organization of the computer program, and Chapter VII demonstrates its application. A test case, a listing of the computer program, and a complete description of the input may be found in the appendices.

II. EXPERIMENTAL SOIL CHROMATOGRAPHY

Soil thin-layer chromatography (TLC) has been successfully used to evaluate the mobility of pesticides in soils [Helling, 1971]. The major advantage of this technique is the ease in which the mobility of a number of pesticides can be assessed under nearly identical conditions. The technique is rapid and allows for the comparison of the mobility of pesticides in a large number of soils with a minimum of expense and equipment. Ascending chromatography, using water as a solvent, is the conventionally accepted eluting procedure. Operating in this manner, the water flux is determined by the soil properties. Unlike soil-column studies, excessive plugging and hydraulic short circuiting do not occur and are thus eliminated as potential sources of error. Because of these characteristics, the technique is also appropriate for evaluating the movement of radionuclides in soils and porous media.

CHROMATOGRAPHIC SOIL COLUMNS

Instead of the conventional TLC plates, we use column-layered chromatographic (CLC) plates. These plates are 20 by 20 cm with nine channels or columns measuring 10 mm in width and 2 mm in depth. Soils are slurried with water until moderately fluid and then applied to the plates (Photo. 1) by using a spreader. Strips of blotter paper, approximately 0.7 mm wide and 5 cm long, are used as wicks for transporting the eluting solution to the soil layered in the channels. The wicks are held in place by clamping a 20 by 20 cm conventional TLC plate on top of the CLC plate (Photo. 2). By using these wicks, the soils in the CLC plates may be eluted again after drying. If wicks are not used, soil will usually slough off during immersion in the eluting, or feed, solution since the CLC plates are positioned at 68 degrees relative to the surface of the eluting solution.

GENERATION OF DISTRIBUTION PATTERNS

The radionuclide to be considered may be introduced into the soil column either through the feed solution or by spotting the radionuclide directly onto the soil. In the latter case a spot containing 10^4–10^5 dpm is placed at 4 cm from the base of the chromatographic soil column. The wicks are then submerged in the feed solution. We have used H_2O, 0.01 N $NaHCO_3$, and solutions of $Ca(CO_3)_2$ having varying ionic strengths. Such an eluting solution is allowed to disperse the radionuclide for a measured period of time. The entire CLC plate is then removed from the eluting solution, and radionuclide patterns are determined.

MEASUREMENT OF DISTRIBUTION PATTERNS

In some of our earlier work autoradiography and a dissection method were used to determine distribution patterns. Medical X-ray film was used for the autoradiography. The film was enclosed in thin sheets of plastic to prevent its contamination. It was then clamped securely between the TLC plate and the CLC plate and exposed for periods ranging from 48 to 72 hours. Measuring the movement of radionuclides in this manner sufficed only in that it gave the general characteristics of the mobility of one radionuclide relative to another. For instance, Photo. 3 shows that ^{106}Ru, ^{131}I, ^{60}Co, and ^{99}Tc were quite mobile compared to ^{85}Sr, ^{109}Cd, ^{95}Nb, and ^{137}Cs. There appeared to be a mobile and non-mobile specie of ^{106}Ru and ^{131}I. Autoradiography, however, is not satisfactory for quantitatively measuring the movement of the radionuclides. Another method for obtaining distribution patterns consisted of dissecting each column into 1.5 cm increments of soil. The radioactivity of each increment was then counted separately with a NaI detector. Although this technique was capable of quantitative measurement, it was extremely laborious and its resolution was limited to the lengths of the soil increments.

Currently, a radiochromatographic scanner (Berthold Model LB 2760) equipped with a gas-flow detector is being used for measuring the movement of the various radionuclides (see Photo. 4). Because of the large selections of scanning speeds available (6000, 3000, 1500, 1200, 600, 300, 120,

PHOTO 5629-76

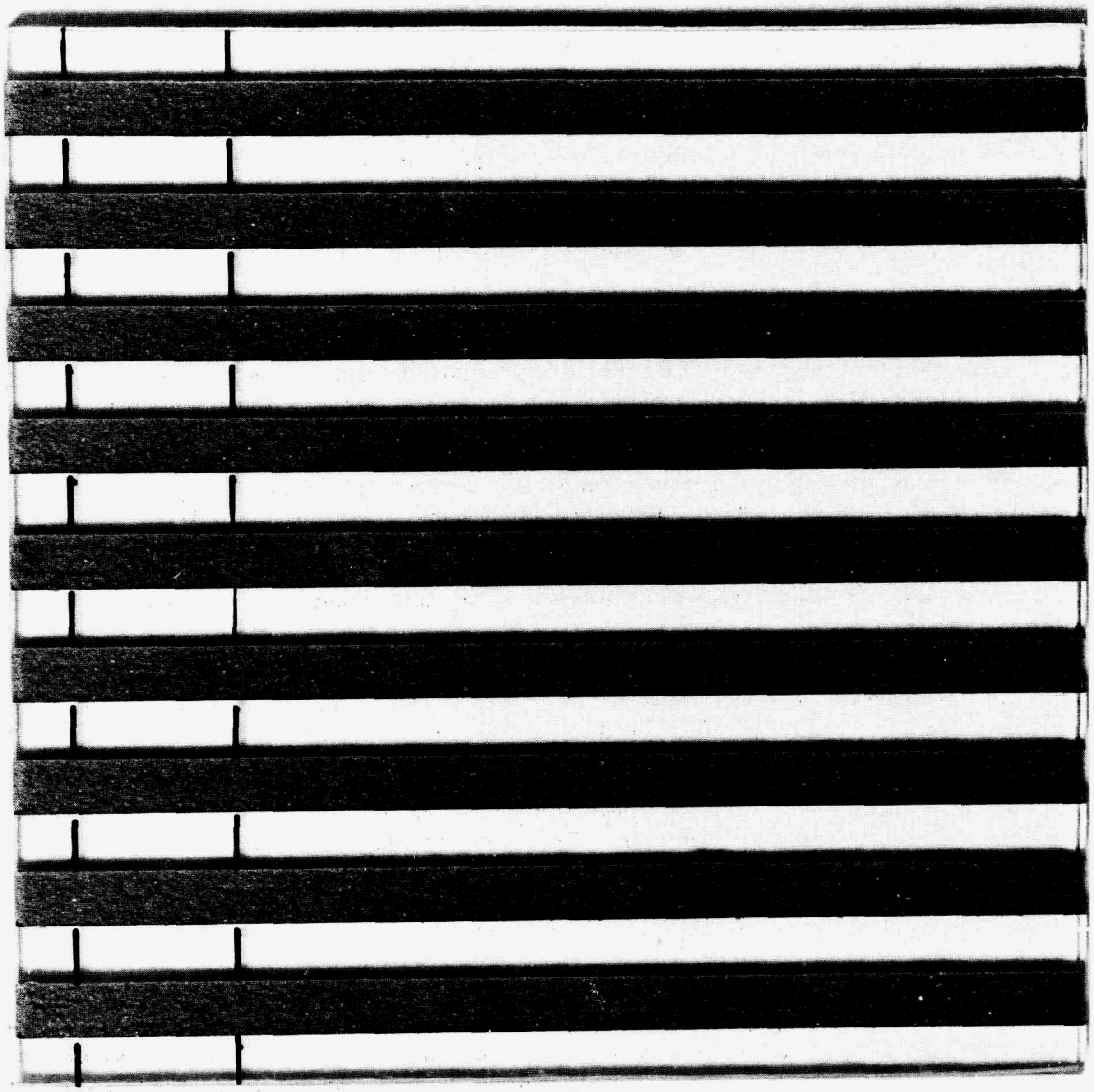


Photo. 1. The column-layered chromatographic (CLC) plate after loading with soil

PHOTO 5627-76

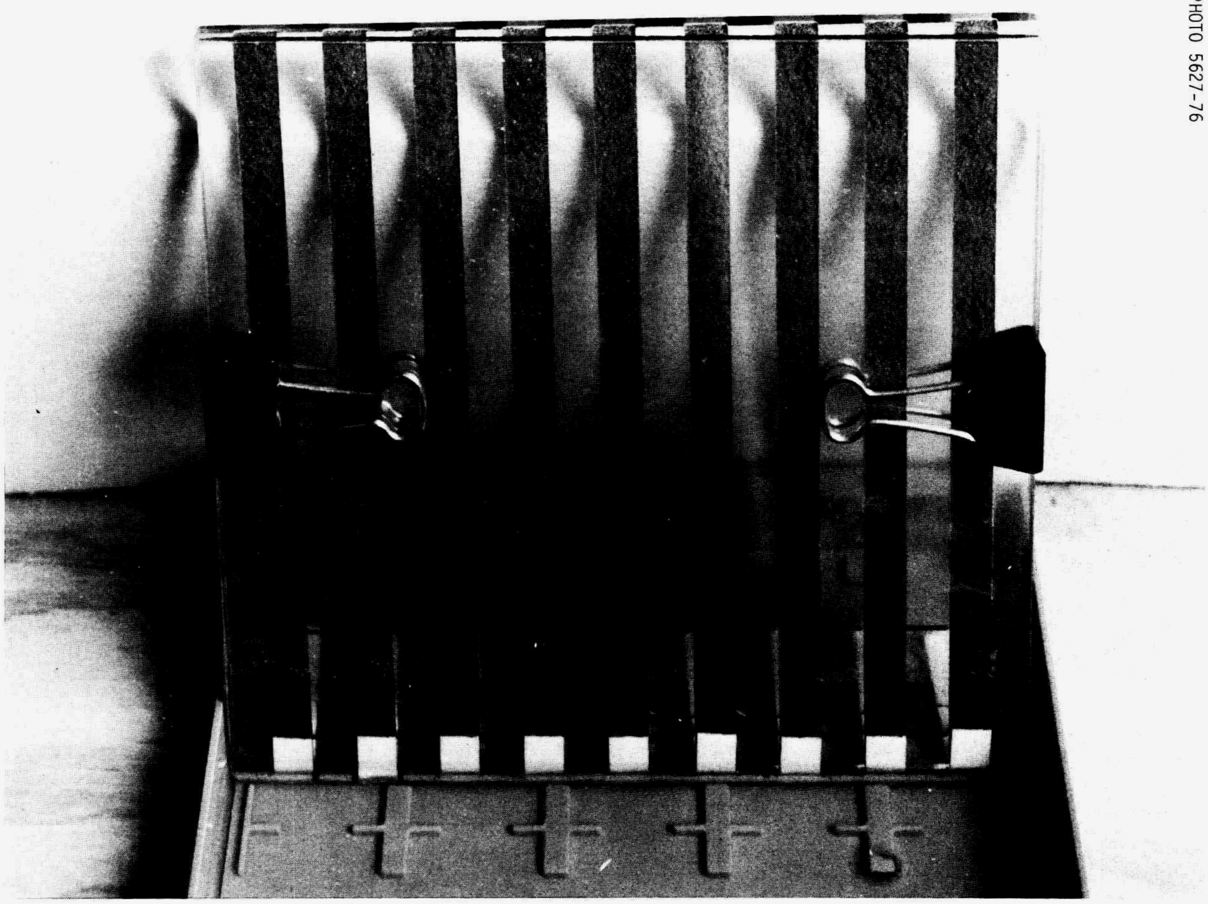


Photo. 2. A picture of the soil columns, the TLC plate clamped to the CLC plate, and the wicks submerged in an eluting solution

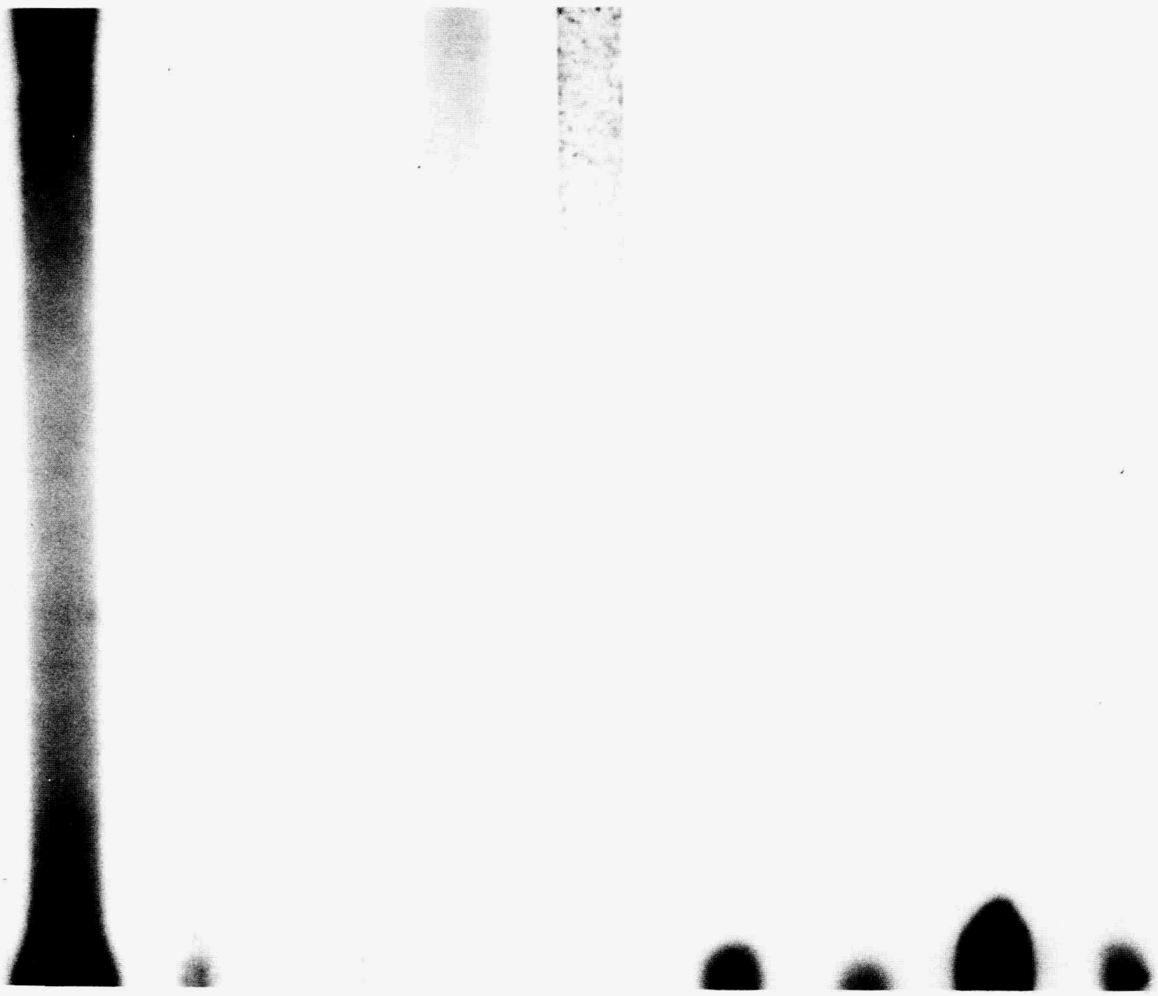


Photo. 3. Radionuclide mobilities as determined by medical x-ray film .

PHOTO 5631-76

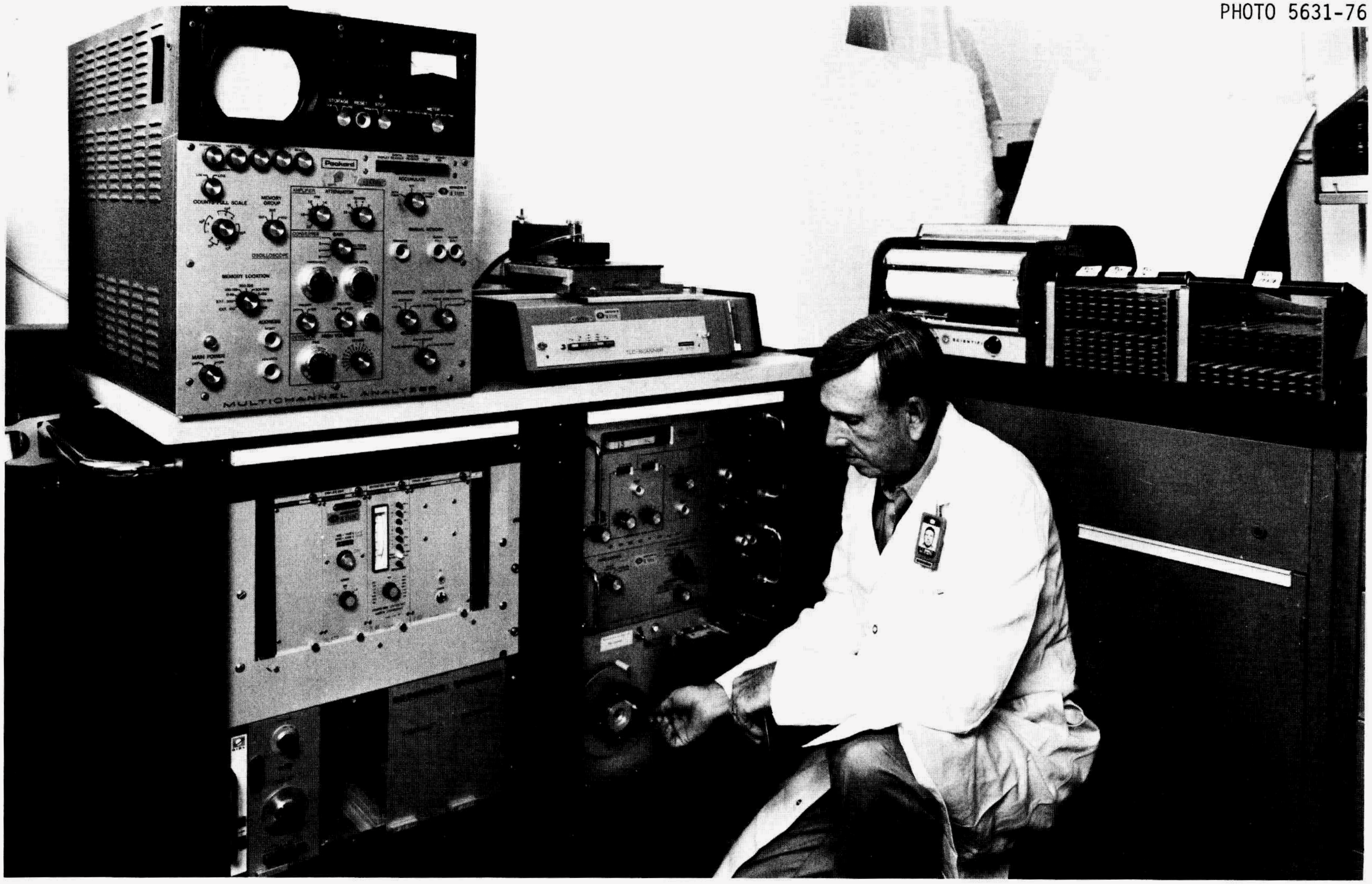
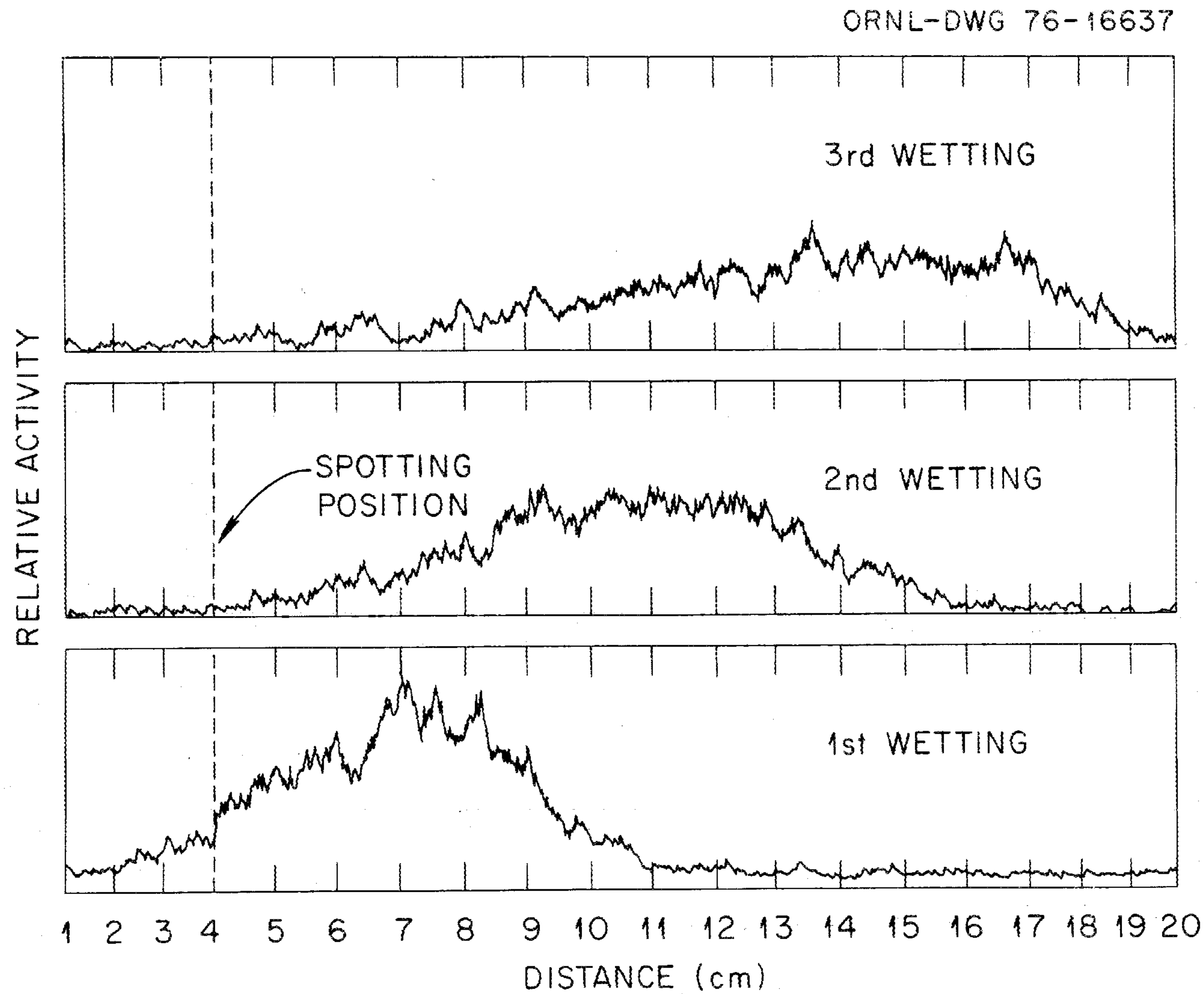


Photo. 4. The radiochromatographic scanner (top center) together with its associated recording apparatus: a multichannel analyzer (left) with its paper-tape punch attended by a technician and a strip-chart recorder (right).

60, 30 and 15 mm/hr) and the time selections available for integrating the counts per channel in the multichannel analyzer (12.5, 25, 50, 100, 200, 400 and 4800 sec), the resolution and sensitivity is much greater than any comparable type of recording apparatus. The multichannel analyzer, with its paper-tape punch, produces output suitable for computer analysis. For quick visual inspection, however, the scanner may be coupled to a strip-chart recorder. The charts exhibited as Figs. 1 and 2 are examples. They show a much more rapid movement of ^{85}Sr in Fuquay sand than in Captina silt loam for the same eluting solution.

MOVEMENT OF THE ELUTING SOLUTION

Profiles such as those shown in Figs. 1 and 2 are amenable to quantitative interpretation providing the movement of the eluting solution can be understood. Observed movements of water fronts in two types of soils are shown in Fig. 3. As would be expected, a $t^{1/2}$ dependence is observed initially due to the dominance of capillary pressures over gravitational pressures. An important deficiency in Fig. 3 is that it yields the Darcy velocity V only at the water front, where the reduced moisture content $\alpha \approx 0.5$. However, this velocity can vary substantially as a function of α, ranging from a value which is sometimes in excess of the saturated conductivity K_s at $\alpha = 1$ to a value of zero at $\alpha = 0$. To obtain this additional information, we introduce a tracer, tritium, into the feed solution, and then generate and measure distribution patterns as described above. These patterns are then analyzed theoretically to obtain complete velocity profiles. The formalism used for this purpose is examined in the next chapter, Chapter III, and it is applied to the Fuquay soil in Chapter VII.



^{85}Sr Movement in Fuquay Sand 200 ppm Ca in Eluting Solution.

Fig. 1. Mobility of ^{85}Sr in Fuquay sand for an eluting solution containing 200 ppm Ca.

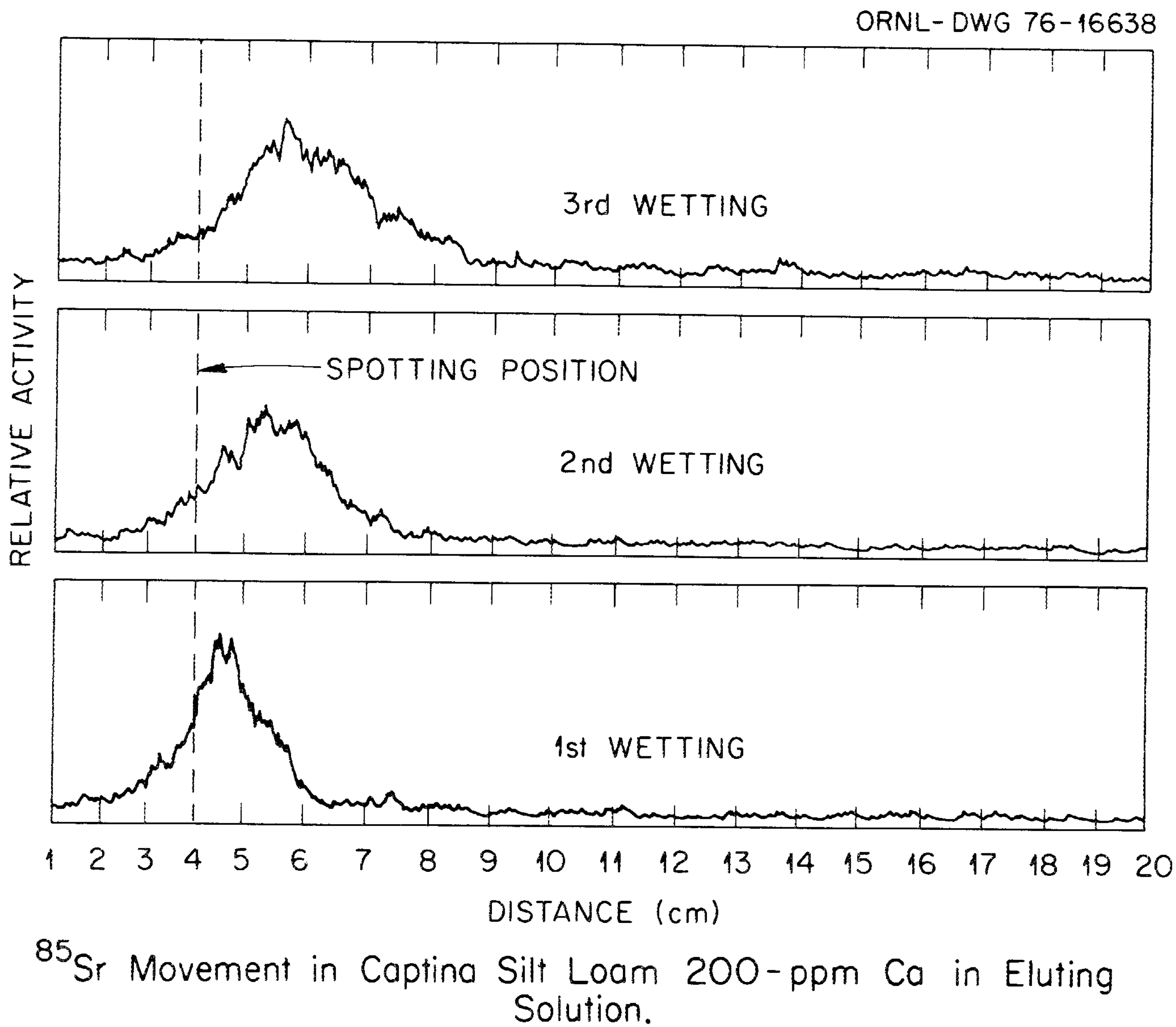


Fig. 2. Mobility of ^{85}Sr in Captina silt loam for an eluting solution containing 200 ppm Ca.

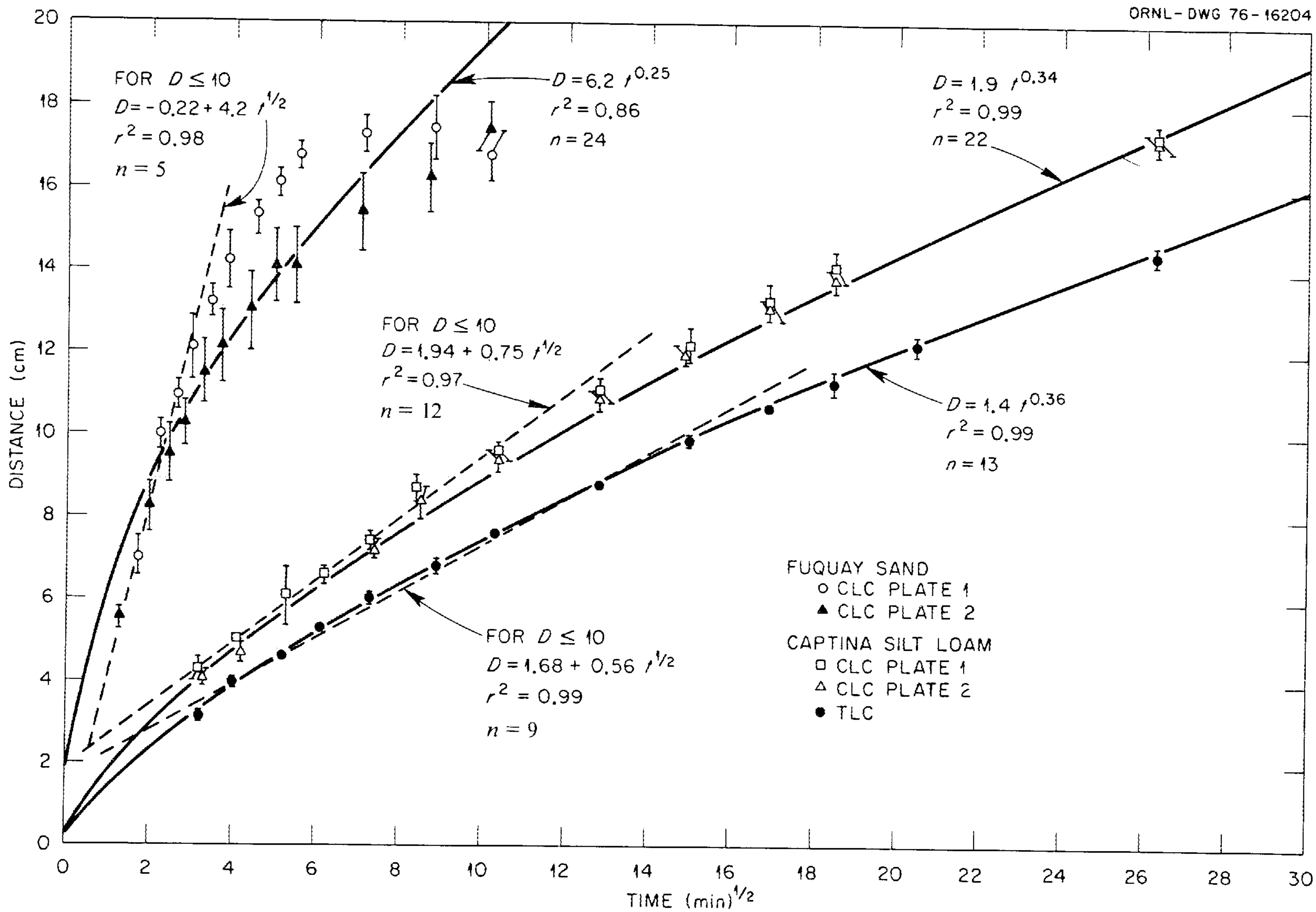


Fig. 3. Water-front movement with respect to time. Here only does D represent the distance, r^2 the correlation coefficient, and n the number of points.

III. WATER TRANSPORT

THEORY

1. **Transport equations.** Fortunately the water-movement is sufficiently restricted that it may be treated analytically. The boundary-initial conditions may be prescribed simply as

$$\theta(x = 0, t) = \theta_1 \qquad \text{and} \qquad \theta(x > 0, t = 0) = \theta_0 \tag{1}$$

where θ is the moisture content. Also, the transport equation

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial x}\left(Q \frac{\partial \theta}{\partial x}\right) + \frac{\partial K}{\partial x} \sin \epsilon \tag{2}$$

for a chromatographic column inclined at an angle ϵ (see Fig. 4) is one dimensional. (Symbols which are not defined in the discussion to follow may be found in the notation, Chapter IX.)

In published work **by Parlange [1971a, 1971b, 1972] a singular perturbation theory** is used to obtain a second-order solution to the above problem subject to only one additional condition, namely that the column be semi-infinite, i.e.

$$0 \leqslant x \leqslant \infty \ . \tag{3}$$

Invoking such a condition will restrict applications to situations in which the wetting front is sufficiently well removed from the top end of the chromatographic columns. However, this is a very mild restriction and is indeed a small price to pay for the computational efficiency of an analytic or, more precisely, a partially analytic solution. Equation (2) is notoriously difficult to solve for unsaturated moisture conditions due to the highly nonlinear nature of the conductivity $K(\theta)$ and the diffusivity $Q(\theta)$, and, in general, one must resort to a strictly numerical and computer-time-consuming treatment such as that of Reeves and Duguid [1975].

Using the theory of implicit functions [Margenau and Murphy, 1956], as is frequently done in thermodynamic analyses, the water-content variable θ may be employed as the independent variable in Eq. (2), i.e.

$$\frac{\partial x}{\partial t} = \frac{\partial V}{\partial \theta} \ . \tag{4}$$

Here the Darcy velocity

$$V = -\frac{Q}{\partial x / \partial \theta} - K \sin \epsilon \tag{5}$$

has been separately identified since it is the coupling variable between moisture transport and mass transport.

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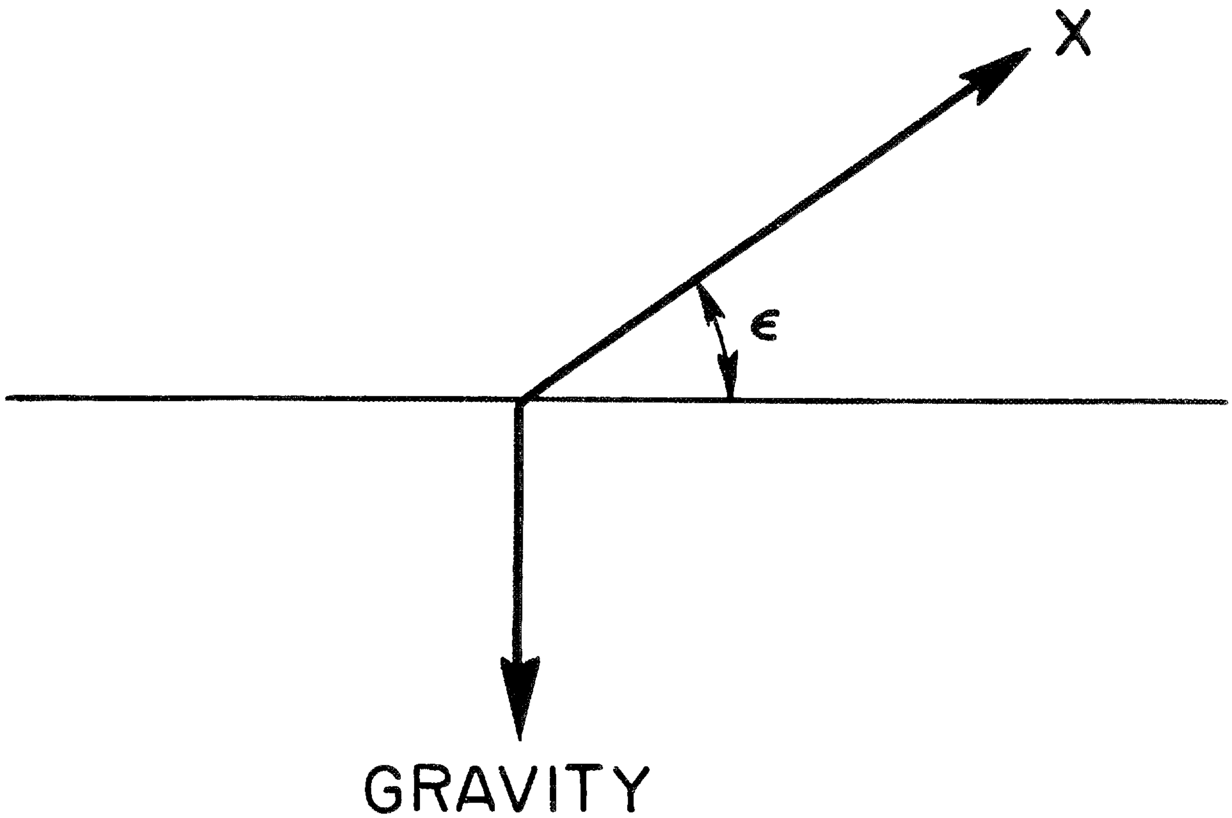

Fig. 4. Definition of the angle ϵ.

In terms of the reduced variables

$$\alpha = \frac{\theta - \theta_0}{\theta_1 - \theta_0} \qquad \text{and} \qquad \kappa = \frac{K(\theta) - K(\theta_0)}{\theta_1 - \theta_0} \quad . \tag{6}$$

Eqs. (4) and (5) become

$$\frac{\partial x}{\partial t} = \frac{\partial W}{\partial \alpha} \tag{7}$$

and

$$W = -\frac{Q}{\partial x/\partial \alpha} - \kappa \sin \epsilon \quad . \tag{8}$$

The reduced velocity W is related to the Darcy velocity by the equation

$$V = (\theta_1 - \theta_0)\, W - K_0 \sin \epsilon \tag{9}$$

where $K_o = K(\theta_o)$. Expressed in terms of variable α, the boundary and initial conditions become

$$x\,(\alpha = 1, t) = 0 \qquad \text{and} \qquad x\,(\alpha = 0, t = 0) > 0 \ . \tag{10}$$

since position x is a single-valued function of water content.

2. **General application of the Parlange method.** To apply the perturbation method, Parlange [1971b] first integrates Eq. (7) as follows:

$$\int_{\alpha}^{1} d\alpha \; \frac{\partial x}{\partial t} = W_1 - W \tag{11}$$

where $W_1(t) = W(\alpha = 1,t)$. He then reasons that since

$$\left.\frac{\partial x}{\partial t}\right|_{\alpha = 1} = 0 \tag{12}$$

[see Eq. (10a)] the time-derivative term will be small compared to other terms in Eq. (11) provided α is sufficiently close to unity. Thus this quantity may be represented by a lower ordered approximation. Expressing the reduced velocity in expanded form of Eq. (11), Eq. (8) yields, for the n-th approximation to $\partial x/\partial\alpha$, the quantity

$$\frac{\partial x^{(n)}}{\partial \alpha} = -\frac{Q}{\kappa \sin \epsilon + W_1 - \int_{\alpha}^{1} d\beta \, \frac{\partial x^{(n-1)}}{\partial t}} \tag{13}$$

as a first integral, which defines the velocity [Eq. (8)]:

$$W^{(n)} = W_1 - \int_\alpha^1 d\beta \, \frac{\partial x^{(n-1)}}{\partial t} \quad . \tag{14}$$

The second integral

$$x^{(n)} = \int_\alpha^1 \frac{Q d\gamma}{\kappa \sin \epsilon + W_1 - \int_\alpha^1 d\beta \, \frac{\partial x^{(n-1)}}{\partial t}} \tag{15}$$

is easily obtained by applying the boundary condition, Eq. (10a). Evaluation of the time derivative in these two equations is considered in Sections 3 and 5, below.

3. **First-order solution.** Although Eqs. (14) and (15) are appropriate for general n-th order approximations, Parlange [1971a, 1971b, 1972] found that second order was quite adequate for practical applications. To start the iterative scheme, it is assumed that Eq. (12) is also valid for $\alpha \neq 1$, i.e.

$$\frac{\partial x^{(0)}}{\partial t} = 0 \quad . \tag{16}$$

The first-order solutions of Eqs. (14) and (15) then become

$$W^{(1)} = W_1 \tag{17}$$

and

$$x^{(1)} = \int_\alpha^1 d\gamma \, \frac{Q}{\kappa \sin \epsilon + W_1} \quad . \tag{18}$$

Equation (17) simply says that for each water-content value $\alpha > 0$, the velocity of advance of the wetting front is independent of α and is a function of time only [$W^{(1)} = W^{(1)}(t)$].

4. **Temporal behavior of the end-point Darcy velocity.** At this point a problem associated with W_1 is identified in Parlange's [1971b] analysis. This quantity, the velocity at $\alpha = 1$ or $x = 0$, is at this point an unknown function of time $W_1(t)$. However, a relation may be found for this quantity by extending the range of integration in Eq. (11) to $\alpha = 0$:

$$\int_0^1 d\alpha \, \frac{\partial x}{\partial t} = W_1 - W_0 \tag{19}$$

where, from Eq. (8),

$$W_0 = - \frac{Q}{\partial x / \partial \alpha} \bigg|_{\alpha = 0} - \kappa \sin \epsilon \bigg|_{\alpha = 0} \quad . \tag{20}$$

Now, by definition [Eq. (6b)], $\kappa(0) = 0$ since $\alpha = 0$ implies $\theta = \theta_0$ [Eq. (6a)]. In addition, it may be inferred from the initial condition [Eq. (10b)] that $\partial x/\partial\alpha$ becomes indeterminantly large as α approaches zero. Hence Eq. (20) gives $W_0 = 0$, and Eq. (19) becomes

$$W_1 = \int_0^1 d\alpha \frac{\partial x}{\partial t} \quad . \tag{21}$$

From the first-order result, Eq. (18), one obtains

$$\frac{\partial x^{(1)}}{\partial t} = -\frac{\partial W_1}{\partial t} \int_\alpha^1 d\gamma \frac{Q}{(\kappa \sin\epsilon + W_1)^2} \quad . \tag{22}$$

Inserting this relation into Eq. (21) and integrating the resulting equation from 0 to t yields

$$t = \int_0^1 d\alpha \int_\alpha^1 d\gamma \, Q(\gamma) \, I(\gamma) \tag{23}$$

where

$$\begin{aligned} I &= -\int_{W_1(0)}^{W_1} \frac{dW_1}{W_1 (\kappa \sin\epsilon + W_1)^2} \\ &= \frac{1}{\kappa^2 \sin^2\epsilon} \left(\ln\left(\frac{\kappa \sin\epsilon + W_1}{W_1}\right) - \frac{\kappa \sin\epsilon}{\kappa \sin\epsilon + W_1} \right) \quad . \end{aligned} \tag{24}$$

The last line of the above equation uses the fact that $W_1(0)$ is infinite.

Interchanging the order of integration in Eq. (23) yields

$$t = \int_0^1 d\gamma \, \gamma \, Q(\gamma) \, I(\gamma) \tag{25}$$

which, when combined with Eq. (24), gives

$$t = \int_0^1 d\gamma \frac{\gamma Q}{\kappa^2 \sin^2\epsilon} \left(\ln\left(\frac{\kappa \sin\epsilon + W_1}{W_1}\right) - \frac{\kappa \sin\epsilon}{\kappa \sin\epsilon + W_1} \right), \quad \sin\epsilon \neq 0 \quad . \tag{26a}$$

If $\sin\,\epsilon = 0$, the indeterminate form may be evaluated to yield

$$t = \frac{1}{2 W_1^2} \int_0^1 d\gamma \, \gamma \; Q(\gamma) \, , \sin\epsilon = 0 \quad . \tag{26b}$$

Equations (26) may be inverted numerically to obtain the desired relation $W_1(t)$. Actually, this function should be denoted by $W_1^{(1)}(t)$ since it is based on the first-order quantity $x^{(1)}$. However, we follow Parlange in not updating this function with an approximation of higher order. Thus there is no need to make such a notational distinction. As a consequence, the familiar $t^{1/2}$ dependence is observed for both first and second order in the horizontal-flow case, i.e. $x^{(1)} \sim t^{1/2}$ and $x^{(2)} \sim t^{1/2}$.

5. Second-order solution. In proceeding to second order one should note that the time derivative of $x^{(1)}$ in Eqs. (14) and (15) will introduce the troublesome quantity $\partial W_1/\partial t$, just as it did in Eq. (22). This quantity, however, may be eliminated algebraically. Using Eq. (21) twice the following relation is obtained:

$$\begin{aligned} W_1 - \int_\alpha^1 d\beta \frac{\partial x^{(1)}}{\partial t} &= \int_0^\alpha d\beta \frac{\partial x^{(1)}}{\partial t} \\ &= W_1 \int_0^\alpha d\beta \frac{\partial x^{(1)}}{\partial t} \Big/ \int_0^1 d\beta \frac{\partial x^{(1)}}{\partial t} \quad . \end{aligned} \tag{27}$$

Differentiating Eq. (18) with respect to time yields

$$W_1 - \int_\alpha^1 d\beta \frac{\partial x^{(1)}}{\partial t} = W_1\, J(\alpha)/J(1) \tag{28}$$

where

$$J = \int_0^\alpha d\beta \int_\beta^1 d\gamma \frac{Q}{(\kappa \sin \epsilon + W_1)^2} \quad . \tag{29}$$

Parlange [1971b] used Eq. (29) directly, combining it with Eqs. (28) and then with Eq. (15) to achieve the second-order result [Eq. (14) in the (1971b) article]. Here Eq. (29) will be simplified before taking these final steps. By interchanging the order of integration, Eq. (29) becomes the sum of two single integrals:

$$J(\alpha) = \int_0^\alpha d\gamma \frac{\gamma Q}{(\kappa \sin \epsilon + W_1)^2} + \alpha \int_\alpha^1 d\gamma \frac{Q}{(\kappa \sin \epsilon + W_1)^2} \quad . \tag{30}$$

The second integral, of course, vanishes when $\alpha = 1$.

Combining Eq. (28) with Eqs. (14) and (15) yields the second-order approximations

$$W^{(2)} = W_1\, J(\alpha)/J(1) \tag{31}$$

and

$$x^{(2)} = \int_\alpha^1 d\gamma \frac{Q}{\kappa \sin \epsilon + W_1\, J(\alpha)/J(1)} \quad . \tag{32}$$

In contrast to $W^{(1)}(t)$ the second-order approximation to the reduced velocity is a function of both water content and time, i.e. $W^{(2)} = W^{(2)}(\alpha,t)$. The unreduced Darcy velocity

$$V^{(2)} = (\theta_1 - \theta_0)\, W^{(2)} - K_0 \sin \epsilon \tag{33}$$

obtained from Eq. (9), is the desired result.

RESULTS FOR YOLO CLAY

Parlange's applications to one-dimensional moisture flow are of interest here. They pertain to capillary rise [Parlange and Aylor, 1972], infiltration [Parlange, 1971b], and horizonatal flow [Parlange, 1971a]. Our purpose here is threefold: (1) to demonstrate the solution procedure, (2) to compare results of our computer program with those presented in the above-mentioned papers, and (3) to supplement the moisture profiles with their corresponding Darcy-velocity profiles.

1. **Soil properties.** In each case the soil used is Yolo clay. Values of the conductivity and diffusivity for this material are given in Phillip [1957] in tabular form. Here they are presented in graphical form as Fig. 5. The only other soil properties which are required are the residual moisture content $\theta_0 = 0.2376$ cm^3/cm^3 and the end-point moisture content $\theta_1 = 0.4950$ cm^3/cm^3, respectively.

2. **Capillary rise.** The case of capillary rise ($\epsilon = 90°$) is used to demonstrate the solution procedure. Generation of the time curve (Fig. 6) is the initial step. In general this must be done in order to invert the transcendental equation, Eq. (26a), between the time t and the end-point reduced Darcy velocity W_1. [Such a procedure is not required, however, for the special case of horizontal flow, where the appropriate relation, Eq. (26b), may be inverted analytically.] To produce the time curve, various values are chosen for W_1. [Actually, values of the more physical quantity V_1, in units of the saturated conductivity, are required for the computer program, which converts them to W_1 using Eq. (9).] Corresponding values of the elapsed time t are then obtained via numerical integration of Eq. (26).

Determination of positions $x(\alpha,t)$ and velocities $W(\alpha,t)$ [or equivalently $V(\alpha,t)$] is the second and final step in the solution procedure. For a specified time t the corresponding end-point velocity $W_1(t)$ is obtained from Fig. 6 by interpolation. Equations (30), (31), and (32), which depend on W_1, are then evaluated to obtain the second-order approximations $x^{(2)}(\alpha,t)$ and $W^{(2)}(\alpha,t)$. Figure 7 exhibits $x^{(2)}(\alpha,t)$ and $V^{(2)}(\alpha,t)$, which is related to $W^{(2)}(\alpha,t)$ by Eq. (9), at four different values of the elapsed time for the case of capillary rise; the agreement with Parlange and Aylor [1972] is quite satisfactory.

3. **Infiltration and horizontal flow.** Comparisons with Parlange's work for $\epsilon \neq 90°$, however, although acceptable, are not of the same quality. This may be seen in Fig. 8 for the case of infiltration ($\epsilon = -90°$) and in Fig. 9 for the case of horizontal flow ($\epsilon = 0°$). One possible source of this discrepancy is the diffusion in the region near $\alpha = 1$. Since there are no experimental data there, extrapolation must be employed. Logarithmic extrapolation yields the value $Q_1 = Q(\alpha = 1) = 1.85 \times 10^{-2}$ cm^2/sec, resulting in a position profile lying above Parlange's [1971a] results, as indicated in Fig. 9. If Q_1 is arbitrarily reduced by a factor of 10, then the position profile falls beneath Parlange's calculation for $\alpha > 0.5$. Thus different extrapolations would appear to account for the discrepancy between our results and that of Parlange for $\alpha > 0.5$.

As yet, however, we do not have a comparable explanation for the region $\alpha < 0.5$. As shown in Fig. 9, our first-order profiles for $x^{(1)}(\alpha,t)$ agree rather well with those of Parlange. Such a circumstance would appear to indicate that our logarithmic interpolation for $Q(\alpha)$ and $K(\alpha)$ [see Eqs. (6) and (18)] and our adaptive Gauss quadrature [see Eq. (18) only] are consistent with the

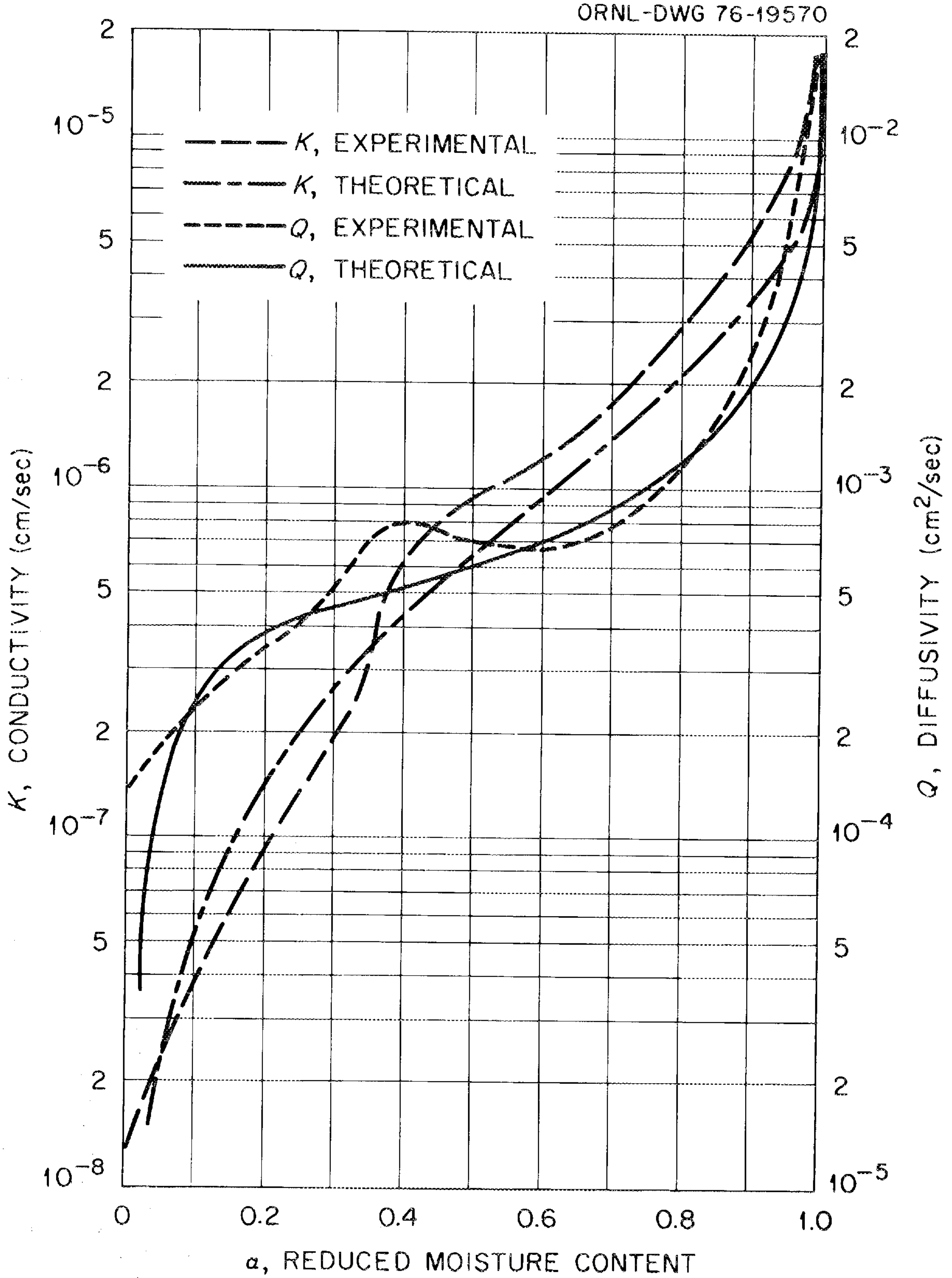

Fig. 5. Soil properties of Yolo clay.

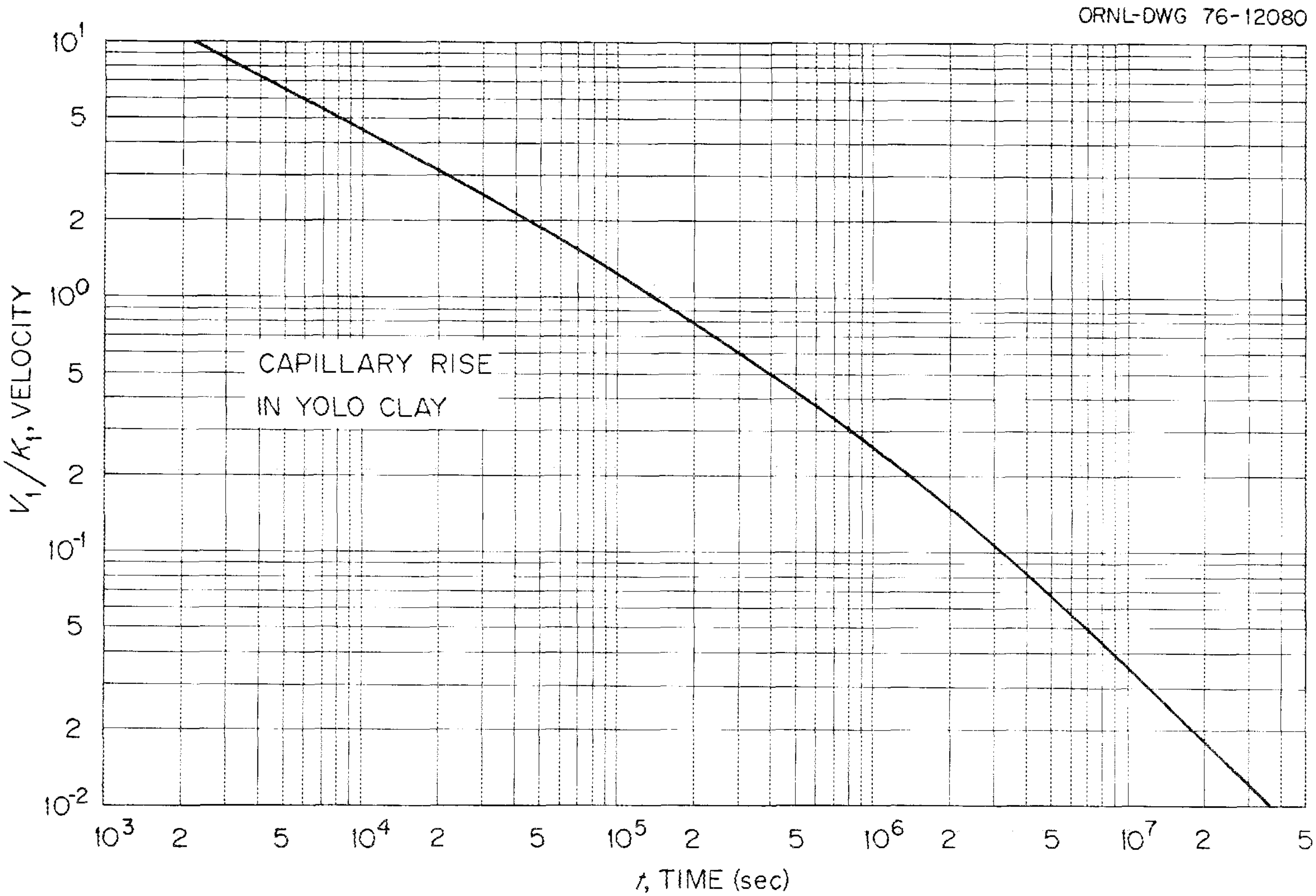

Fig. 6. End-point Darcy velocity as a function of time for capillary rise in Yolo clay.

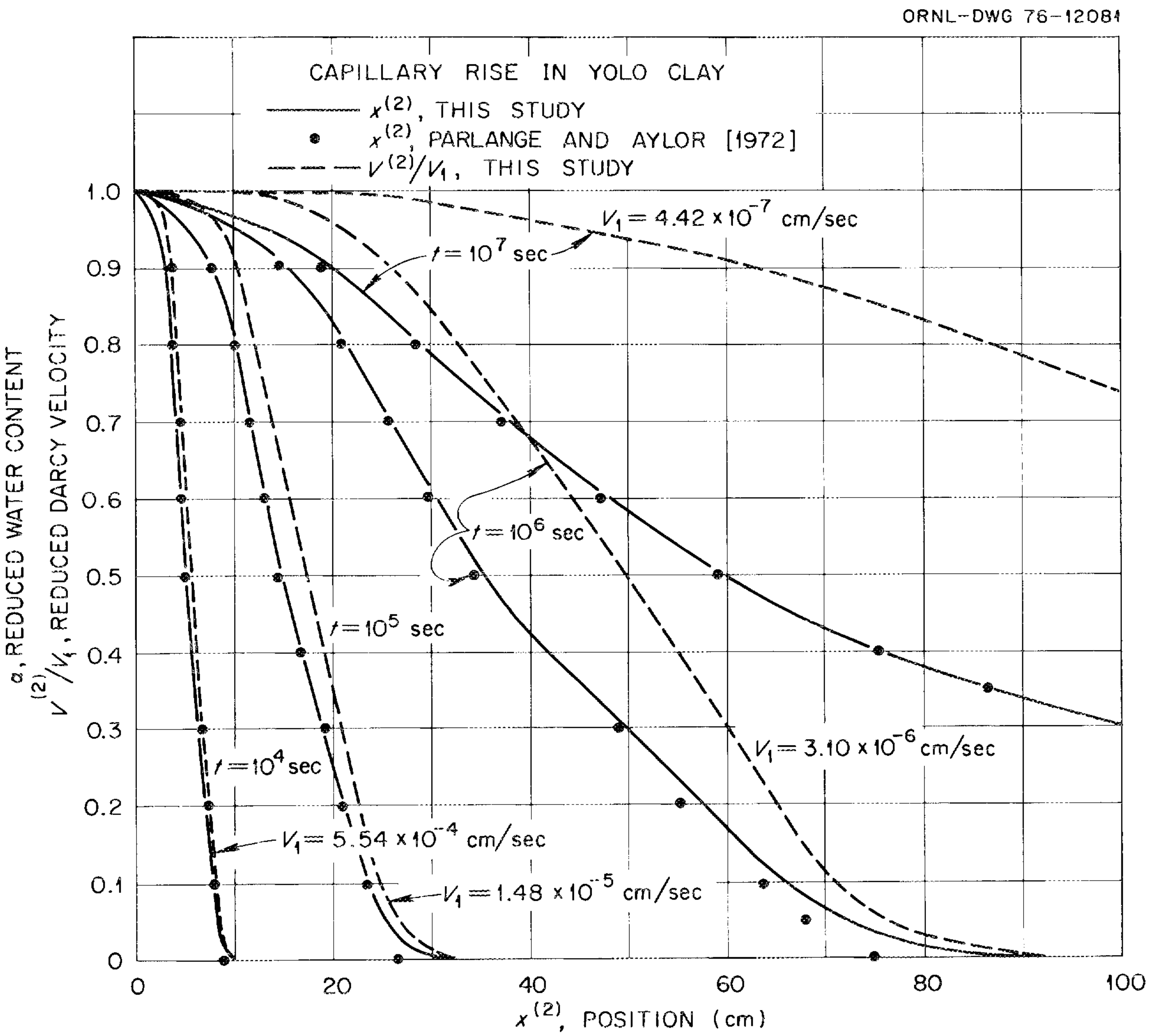

Fig. 7. Water content and Darcy velocity as functions of time for capillary rise in Yolo clay.

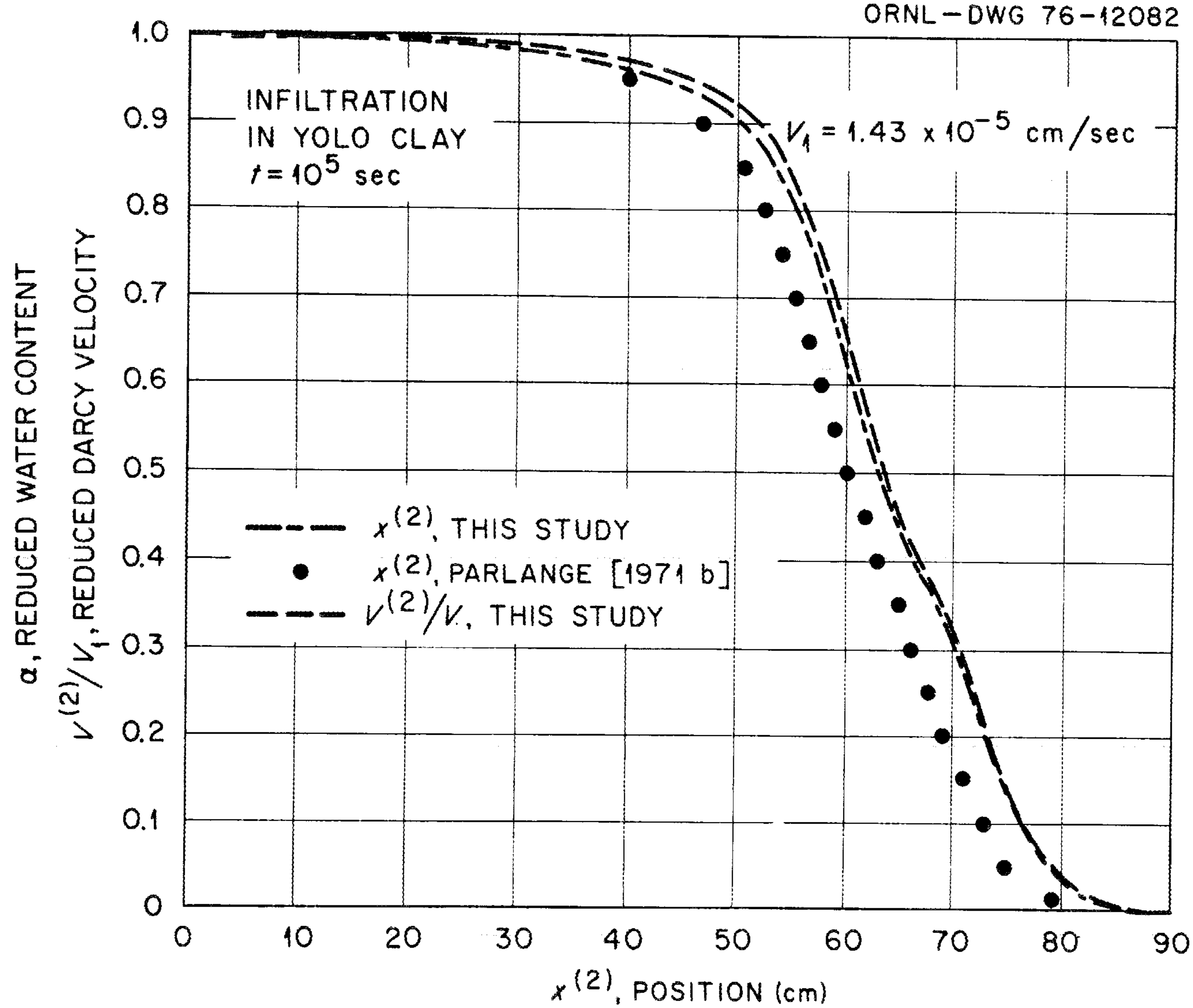

Fig. 8. Water content and Darcy velocity as functions of time for infiltration in Yolo clay.

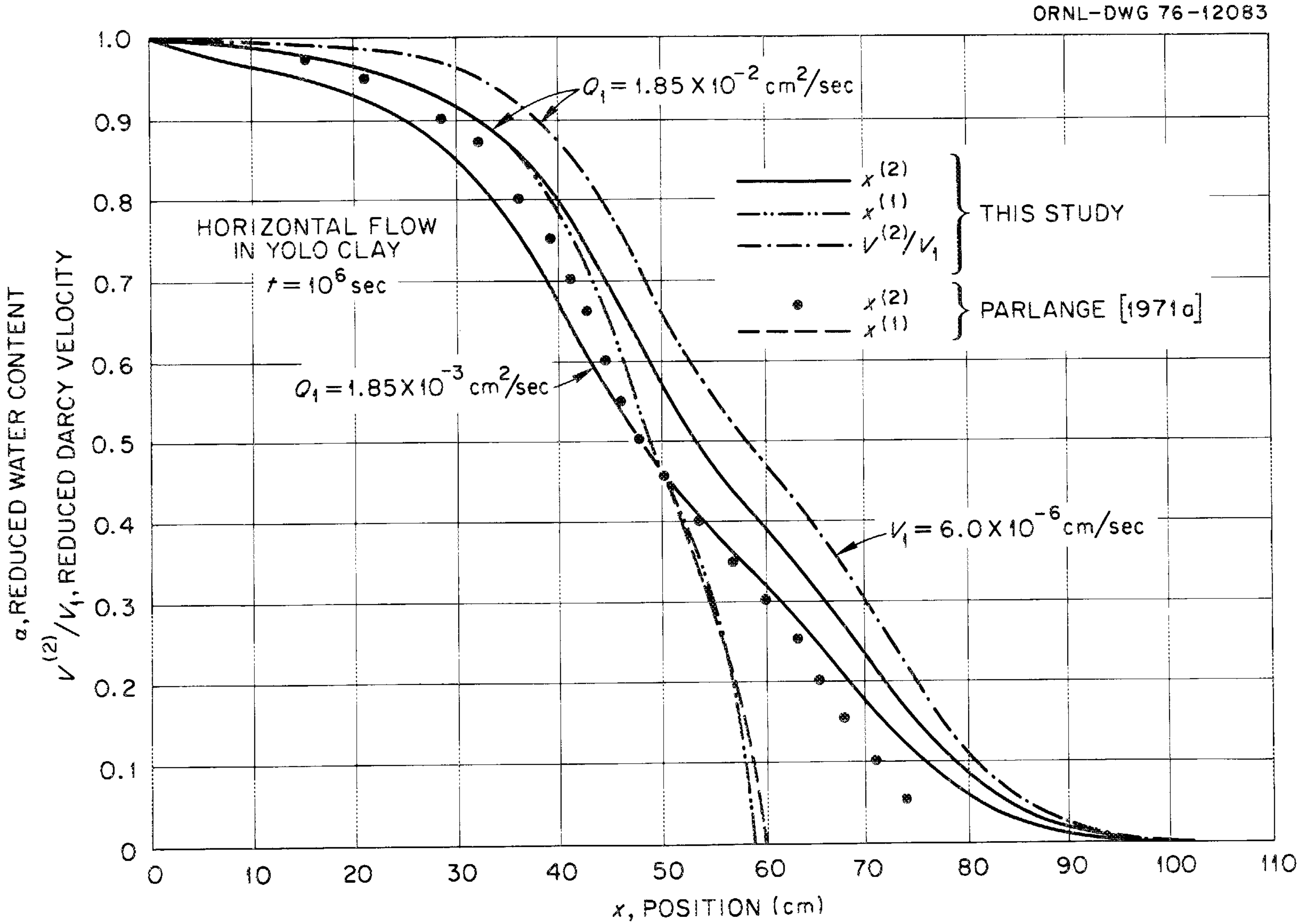

Fig. 9. Water content and Darcy velocity as functions of time for horizontal flow in Yolo clay.

numerical techniques used by Parlange. Since Eq. (32) for $x^{(2)}$ differs from Eq. (18) for $x^{(1)}$ only in the appearance of $J(\alpha)/J(1)$, the discrepancy would appear to lie in this quantity. However, increases in the order of the Gauss quadrature procedure used to evaluate $J(\alpha)$ at nodal points α_i [Eq. (30)] and in the order of the Lagrangian interpolation used to evaluate this quantity between nodal points have failed to produce significant changes in our results for $x^{(2)}$.

To place this discrepancy in perspective, one must consider the function of the water-transport formalism in the analysis of chromatographic results. Basically this is to provide a physics-based interpolation technique to realistically construct the moisture-content and Darcy-velocity profiles at arbitrary times using a minimal number of physical observations. The techniques of this chapter, we feel, are quite satisfactory for this purpose. By using the automatic-search methods described in a later chapter, measured moisture-content profiles may be synthesized to approximately six parameters. These parameters may then be used to obtain both moisture contents and Darcy velocities at the times and positions required by the mass-transport description. The water-transport parameters themselves are the subject of the following section.

PARAMETERIZATION OF SOIL PROPERTIES

For some specialized applications of the chromatographic technique, soil moisture-flow properties will be obtainable from the literature just as they were for the Yolo clay. However, the authors suspect that in the most common situation such properties will need to be measured jointly with the mass-transport characteristics. In this section a method for determining the moisture-flow properties is suggested.

1. **Hydraulic conductivity.** In contrast to the mass-transport case where the transport characteristics are expressed as simple constants such as the distribution coefficient and the longitudinal dispersivity, functional relationships with the independent variable are involved here (see, for example, Fig. 5). A frequently used formula for the hydraulic conductivity is that presented by Gardner [1958]:

$$K(h) = \frac{K_s}{(h/h_0)^d + 1} \tag{34}$$

where $h < 0$ is the pressure head. Parameters K_s, h_o, and d characterize the soil type. From simple mathematical manipulations the significance of these parameters may be determined. Values of conductivity approach that of the saturated conductivity K_s as $h \to 0$. Also, it may be seen that at the critical pressure $K(h_o) = K_s/2$. In addition, the slope of the conductivity curve at $h = h_o$ is directly proportional to the pore-size distribution parameter d. Figure 10 presents curves which, according to Bouwer [1964], are typical of sand, loam, and clay soils.

2. **Moisture characteristic.** King [1965] has shown that a wide range of water content-pressure data (the moisture characteristic) may be fitted with an equation of the form:

$$\theta(h) = \theta_1 \left(\frac{\cosh (h/h_0')^{d'} - \delta \cosh \chi}{\cosh (h/h_0')^{d'} + \delta \cosh \chi} \right) \tag{35}$$

where δ is defined in terms of the residual water content θ_r and the saturated water content (porosity) θ_1:

$$\delta = \frac{\theta_1 - \theta_r}{\theta_1 + \theta_r} \quad . \tag{36}$$

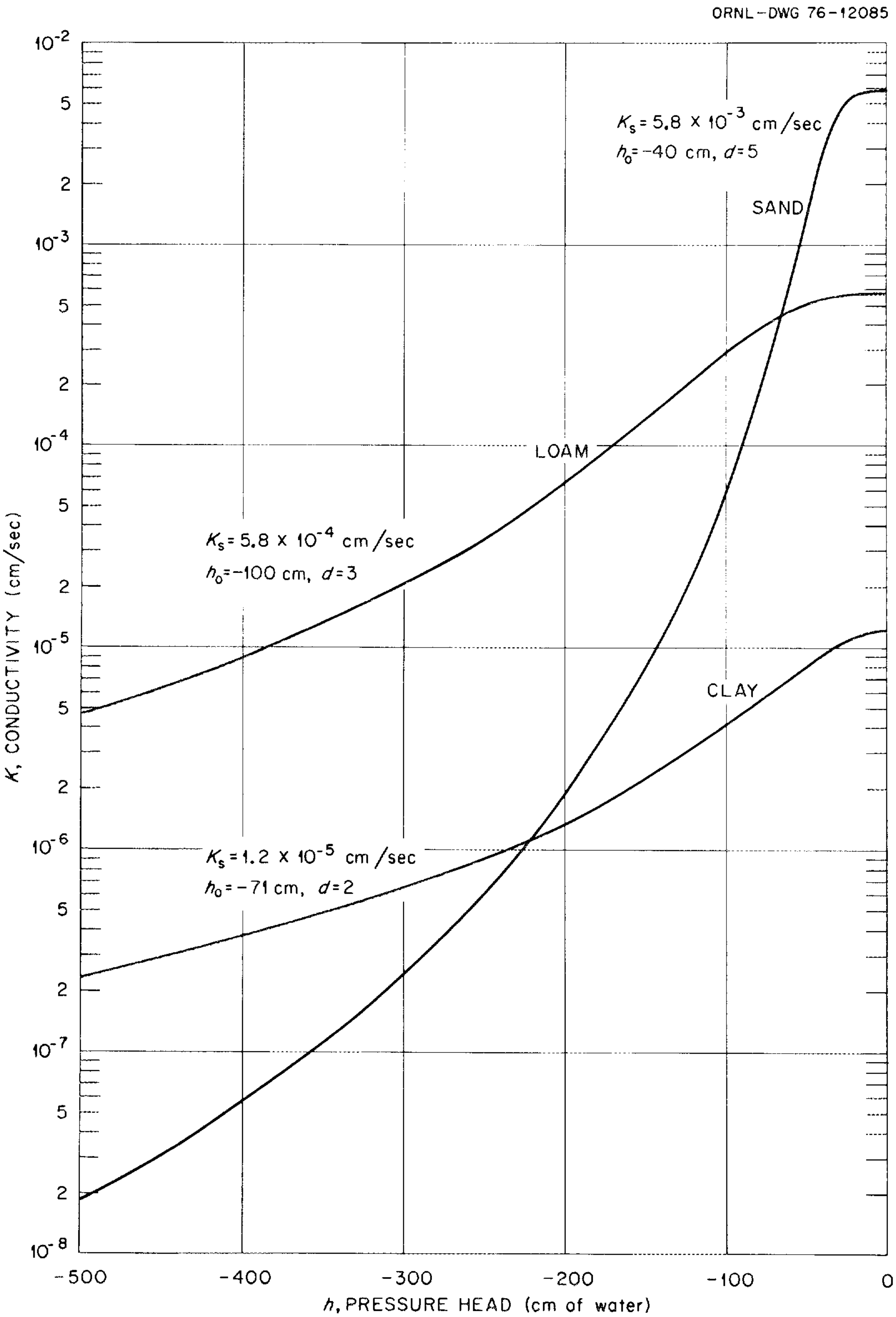

Fig. 10. Representative hydraulic conductivities for sand, clay, and loam soils.

Gillham, et al. [1976] found that parameter χ could be taken as zero without seriously affecting fits to their data, i.e.

$$\theta(h) = \theta_1 \left(\frac{\cosh (h/h_0')^{d'} - \delta}{\cosh (h/h_0')^{d'} + \delta} \right) \quad . \tag{37}$$

This equation may be differentiated

$$\frac{d\theta}{dh} = \frac{(2d'\delta\theta_1/h_0')(h/h_0')^{d'-1} \sinh (h/h_0)^{d'}}{(\cosh (h/h_0')^{d'} + \delta)^2} \tag{38}$$

and inverted

$$h(\theta) = h_0 \left(\ln (\delta/\delta') + [(\delta/\delta')^2 - 1]^{1/2} \right)^{1/d'} \quad . \tag{39}$$

Quantity δ' is defined analogously to that of δ [Eq. (36)]:

$$\delta' = \frac{\theta_1 - \theta}{\theta_1 + \theta} \quad . \tag{40}$$

Parameters θ_1, h_0', and d' have meanings similar to that of their counterparts K_s, h_o, and d in the conductivity parameterization. The water content approaches its saturated value whenever $h \rightarrow 0$ since $d' < 0$. In addition, it may be seen that at the critical pressure $\theta(h_0') \approx \theta_1/5$ provided $\theta_r << \theta_1/5$. At this same pressure the slope is directly proportional to the pore-size distribution parameter d', i.e. $d\theta/dh(h_0') \sim |d'|$. Figure 11 presents three moisture-characteristic curves which might be appropriate for sand, loam, or clay soils. In truth, the curves of Fig. 11 were generated as rather crude fits to the moisture characteristics shown by Hillel and van Bavel [1976]. The intent is merely to show the adaptability of Eq. (37) to different soil textures.

3. **Moisture storage and diffusivity.** The generalized moisture-storage function [Reeves and Duguid, 1975] becomes

$$F(h) = \frac{d\theta(h)}{dh} + \theta(h)\beta' \quad . \tag{41}$$

Strictly speaking, β' is the modified coefficient of compressibility of water. Here, however, this parameter will also be used empirically to characterize the compressibility of the soil medium. The effect of including this quantity in the formulation is to give a nonzero value to the storage function at saturation, i.e. $F(0) = \theta_1\beta'$. Thus the diffusivity

$$Q(h) = \frac{K(h)}{F(h)} \tag{42}$$

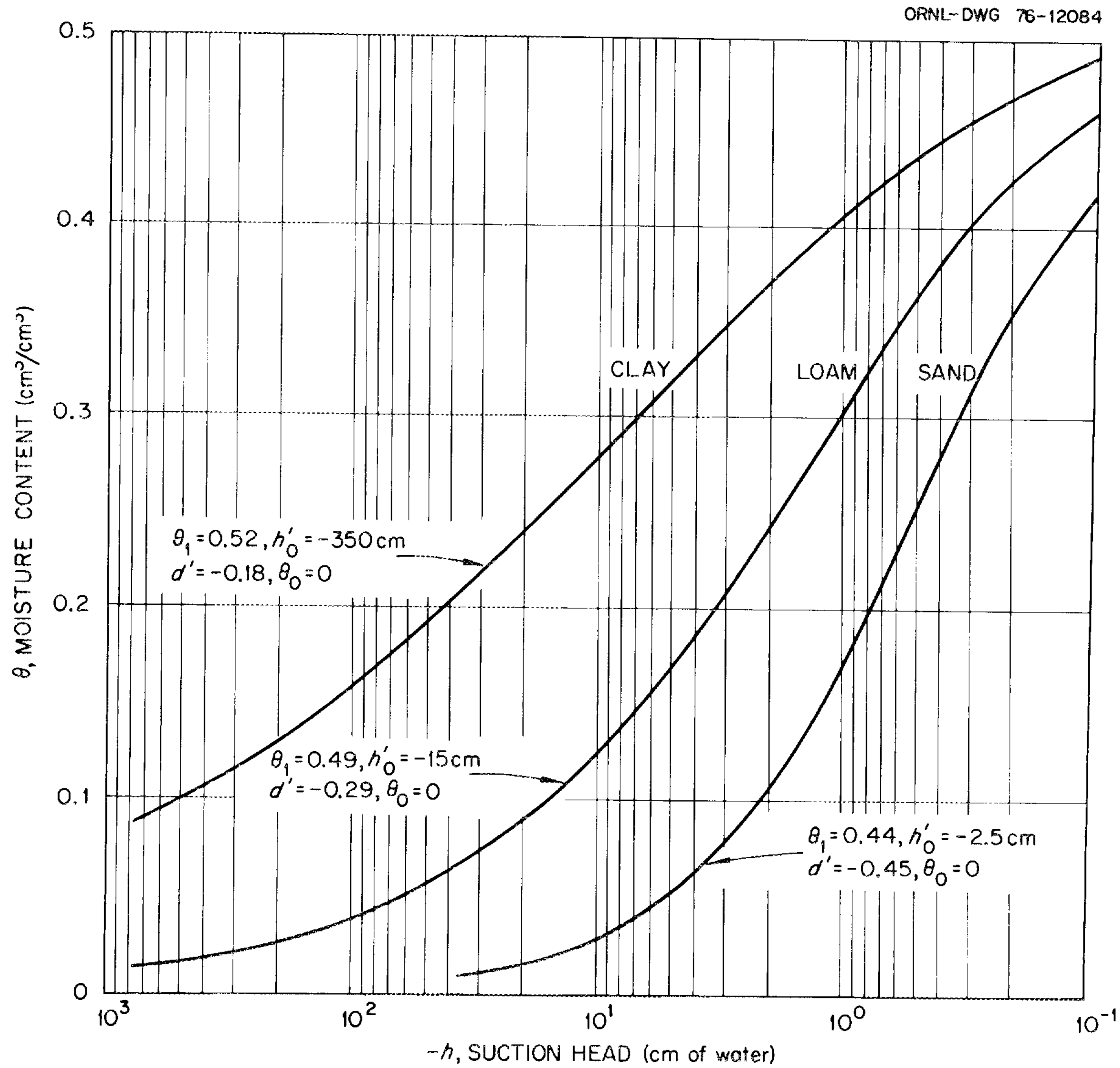

Fig. 11. Representative moisture characteristics for sand, clay, and loam soils.

remains finite at $h = 0$ in accord with the analysis of Phillip [1969]. As was noted previously in connection with Fig. 6, the moisture profiles for water content values approaching saturation are somewhat sensitive to the diffusivity in this water content regime. Hence, such profiles will also be sensitive to the value chosen for β'.

A final demonstration of the efficiency of the parameterizations in this section is presented in Fig. 5. A parameter search, to be described in a later chapter, was performed in order to fit Parlange's capillary-rise results at $t = 10^6$ sec with a moisture profile obtained from the Gardner-King soil-property formulas discussed above. Conductivities and diffusivities, which are given in Eqs. (34) and (42) with supporting Eqs. (37), (38), and (41) as explicit functions of pressure head h are converted to functions of reduced water content θ via Eqs. (6), (39), and (40). The resulting soil properties are presented in Fig. 5, where they may be compared with experimental data.

IV. MASS TRANSPORT

THEORY

In contrast to the water transport, where an approximate analytic solution was appropriate, a fully numerical approach is used here. Such an approach is necessary since the advective flux, Darcy velocity V(x,t), is not, in general, separable in the space-time variables x and t. Also, the variety of initial conditions which are contemplated preclude a perturbative treatment like that used for the water transport. Thus a one-dimensional Galerkin-finite-element implementation similar to the two-dimensional formulation used by Duguid and Reeves [1976] is employed.

1. **Transport equation.** The mass-transport equation may be written as

$$\frac{\partial c_b}{\partial t} - \frac{\partial}{\partial x}\left(\theta D \frac{\partial c}{\partial x}\right) + \frac{\partial}{\partial x}(Vc) + \lambda c_b = 0 \quad . \tag{1}$$

(Symbols which are not defined in the discussion to follow may be found in the notation, Chapter IX.) Variable c_b, the physically measurable quantity, is the bulk concentration and includes both a liquid-phase component c and a solid-phase component s′:

$$c_b = \theta c + \rho s' \tag{2}$$

where θ is the water content and ρ is the bulk density of the solid. If one assumes local equilibrium, i.e. the rate of the adsorptive reaction is fast relative to the rate of transport, then s′ will be a time- and space-independent function of c. If, furthermore, a linear adsorption isotherm is assumed, then

$$s' = \frac{\theta}{n} k_d \, c \tag{3}$$

[Reeves and Duguid, 1976] where n is the porosity. Quantity k_d is the distribution coefficient, whose determination is a primary object of this work. With these assumptions, the bulk concentration becomes

$$c_b = R_d \theta c \tag{4}$$

where

$$R_d = 1 + \frac{\rho k_d}{n} \tag{5}$$

is the retardation factor, and the transport equation, Eq. (1), may be rewritten in terms of one dependent variable:

$$R_d \frac{\partial(\theta c)}{\partial t} - \frac{\partial}{\partial x}\left(\theta D \frac{\partial c}{\partial x}\right) + \frac{\partial}{\partial x}(Vc) + \lambda R_d \theta c = 0 \quad . \tag{6}$$

Adsorption is included above in the first and fourth terms (from the left) of Eq. (6), and the mechanism of dispersion is depicted mathematically by the second term of Eq. (6). Here the equation of Scheideggar [Bear, 1972]

$$\theta D = a_L |V| \tag{7}$$

relates dispersion to the magnitude of the Darcy velocity via the longitudinal dispersivity a_L. Advection by the carrier flux V appears in the third term. Radioactive decay (decay constant λ) is included in the fourth term of Eq. (6) for completeness even though it is expected to play a very minor role in most chromatographic measurements. (A derivation of Eq. (6) may be found in the document by Duguid and Reeves [1976].)

2. **Spatial integration by the Galerkin method.** The basic idea here is quite straightforward and may be seen most transparently if Eq. (6) is rewritten in operator form:

$$\mathscr{L}(c) = 0 \quad . \tag{8}$$

Consider a trial function of the form

$$c' = \sum_{i=1}^{m} N_i(x)\, c_i \tag{9}$$

where the N_i are basis functions spanning the region of interest $0 \leqslant x \leqslant L$, and the m quantities c_i are expansion coefficients. In general, Eq. (8) will not be satisfied by c′ and there will be a residual, i.e.

$$\mathscr{L}(c') \neq 0 \quad . \tag{10}$$

The Galerkin method, however, requires that the weighted averages of this quantity vanish:

$$\int_0^L dx\, N_i(x)\, \mathscr{L}(c') = 0 \quad . \tag{11}$$

(Taking the weighting functions N_i to be identical to the basis functions is the characteristic of the Galerkin method which distinguishes it from among a broad category called weighted-residual techniques [Finlayson, 1972].) The working equations here are found by combining Eqs. (9) and (11). The result

$$\int_0^L dx\, N_i(x)\, \mathscr{L}\left(\sum_j N_j(x)\, c_i\right) = 0 \tag{12}$$

is a matrix equation, which may be solved for the c_i. These coefficients may then be used in Eq. (9) to yield the approximate solution c′ at any position x.

3. Discretization by the finite-element method. In the classical Galerkin method each of the functions N_i extends over the entire domain of integration. Since there is considerable overlapping of the N_i, each integral, Eq. (12), must be carried over its complete extent $0 \leqslant x \leqslant L$, and a full matrix is necessary to depict the coupling of the expansion constants c_i. Such a situation may be alleviated by the use of finite elements. In three-dimensional space these figures would be polyhedra, and in two dimensions they would be polygons. However, for the one-dimensional space considered here they simply constitute segments of a straight line. Each element is spanned by basis functions which are nonzero only in the interior and on the boundaries of the element. Thus each integral of the form of Eq. (12) need be carried only over the region of an individual element, and a sparce matrix results.

To formulate the Galerkin problem for Eq. (6) in terms of finite-element basis functions, it is convenient to introduce the matrix function $\{N(x)\}$. This quantity is a column vector containing two linear functions $N_1(x)$ and $N_2(x)$. These quantities, which are shown in Fig. 12, permit continuity only in the function itself across element boundaries. Hence, first derivatives, are, in general discontinuous, and there will be unavoidably some nonconservation of mass at the nodes. By convention, function N_i is normalized to unity at node i and taken to be zero at the other node so that the expansion constant c_i is identical to the concentration at node i, as anticipated in Eq. (9) by the choice of symbols. In matrix notation this equation becomes, for the r-th finite element

$$ {}_r c\,(x, t) = \{N(x)\}^T \; \{{}_r c(t)\} \tag{13} $$

where the superscript T denotes the transposed matrix. (The prime has been dropped from the notation since only the approximate solution will be considered in the remainder of this work.) Using this notation, both Galerkin integrals [Eq. (12)] for the r-th element become one matrix equation, namely

$$ \int_0^L dx \;\{N\}\mathscr{L}(\{N\}^T \;\{{}_r c\})\, dx = 0 \quad . \tag{14} $$

4. Numerical implementation of the finite-element Galerkin method. To develop working equations from Eq. (14) requires basically the same steps as in document ORNL-4928 [Duguid and Reeves, 1976]. The result is

$$ [{}_r A] \;\{\dot{c}\} + [{}_r B] \;\{c\} + \{{}_r R'\} = 0 \tag{15} $$

where

$$ [{}_r A] = {}_r J \int_{-1}^{1} ds \;\{N\}\,(R_d \theta)\; \{N\}^T \tag{16} $$

$$ [{}_r B] = {}_r J \int_{-1}^{1} ds \left(\frac{\partial}{\partial x} \{N\}\, \theta D \frac{\partial}{\partial x} \{N\}^T \right. \\ \left. - \frac{\partial}{\partial x} \{N\}\; V\; \{N\}^T + \{N\}\; R_d \left(\frac{\partial \theta}{\partial t} + \lambda \theta \right) \{N\}^T \right) \tag{17} $$

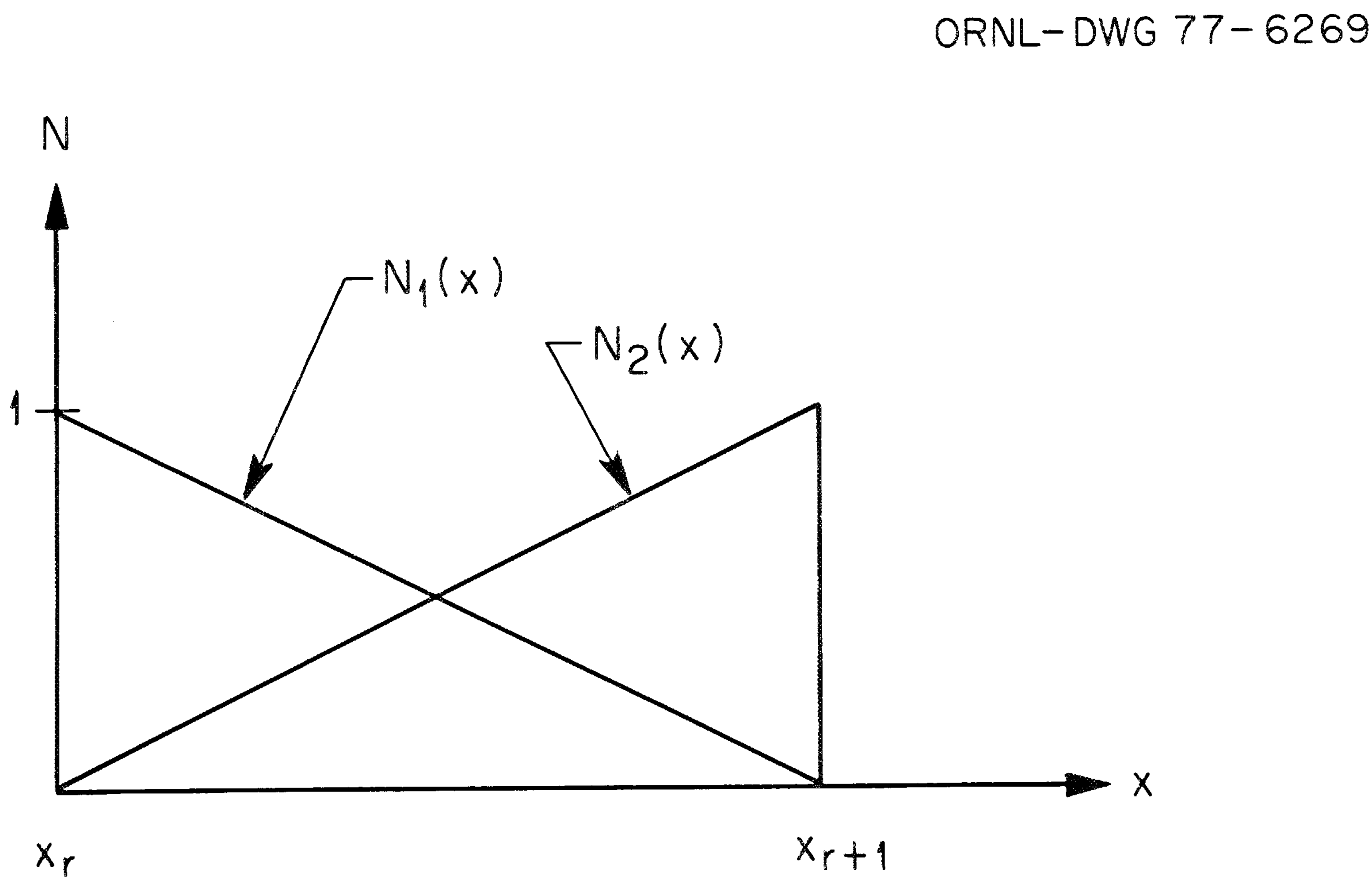

Fig. 12. Basis functions for the r-th finite element.

and

$$\{_rR'\} = \{N\}\, X \Big|_{s=-1}^{s=1} \quad . \tag{18}$$

Quantities $[_rA]$ and $[_rB]$ are 2x2 matrices whereas $\{_rR'\}$ is a 2x1 column vector. The first term on the left-hand side of Eq. (6) contributes both to $[_rA]$ through the term $R_d\theta$ and to $[_rB]$ through the term $R_d(\partial\theta/\partial t)$. The second and third terms on the left-hand side of Eq. (6) contribute, after an integration by parts, both to $[_rB]$ through the term θD and to $\{_rR'\}$. Quantity X in the latter is the mass flux

$$X = -\theta D \frac{\partial c}{\partial x} + cV \quad . \tag{19}$$

Finally the fourth term in Eq. (6), the radioactive decay, gives rise only to the term in $[_rB]$ containing $\lambda\theta$.

For convenience of implementation a new local variable of integration s has been chosen in Eqs. (16) – (18):

$$s = -1 + 2\frac{x - x_1}{x_2 - x_1} \quad . \tag{20}$$

Thus the Jacobian is a simple constant:

$$_rJ = \frac{\partial x}{\partial s} = (x_2 - x_1)/2 \tag{21}$$

and the vector of basis functions may be written:

$$\{N\} = ½\ \{1 + s_j s\}, s_j = s(x_j) \quad . \tag{22}$$

5. **Time integration by the finite-difference technique.** In order to obtain the solution of Eq. (15) at time t + Δt from that at time t, Eq. (15) is written for some intermediate time $t + \omega\Delta t$:

$$[_rA]\ \{_r\dot{c}\}_{t+\omega\Delta t} + [_rB]\ \{c\}_{t+\omega\Delta t} + \{_rR'\} = 0 \tag{23}$$

where $0 \leqslant \omega \leqslant 1$. In the Crank-Nicholson centered-in-time approach $\omega = 1/2$, and in the backward-difference approximation $\omega = 1$. The Crank-Nicholson algorithm has a truncation error of $O(\Delta t^2)$, but its propagation-or-error characteristics frequently lead to oscillatory instabilities. The backward-difference scheme, on the other hand, has a truncation error of $O(\Delta t)$ but is quite resistant to oscillatory instabilities. An arbitrary ω allows an investigation to find the appropriate balance for the problem being considered.

The time derivative of the concentration is expressed as

$$\{_r\dot{c}\}_{t+\omega\Delta t} \approx (\{_rc\}_{t+\Delta t} - \{_rc\}_t)/\Delta t \tag{24}$$

and the value of this quantity at the arbitrary point in time is obtained by linear interpolation:

$$\{_rc\}_{t+\omega\Delta t} = \omega\{_rc\}_{t+\Delta t} + (1-\omega)\{_rc\}_t \quad . \tag{25}$$

Substitution of Eqs. (24) and (25) into Eq. (15) yields the following relationships:

$$[_rC]\ \{_rc\}_{t+\Delta t} = \{_rR\} - \{_rR'\} \tag{26}$$

where

$$[_rC] = [_rA]/\Delta t + \omega[_rB] \tag{27}$$

and

$$\{_rR\} = ([_rA]/\Delta t - (1-\omega)[_rB])\{_rc\}_t \quad . \tag{28}$$

It should be understood that matrices $[_rA]$, $[_rB]$, and $\{_rR'\}$, and, hence, $[_rC]$ and $\{_rR\}$, are evaluated at time $t + \omega\Delta t$. These matrices must therefore be obtained by the interpolation procedure of Eq. (25).

6. **Assembly of elements.** Up to this point the Galerkin-finite-element formulation has been presented only for a typical element r among the collection of finite elements which comprise the region of interest. The result of this analysis is Eq. (26), which is expressed in terms of the 2x2 matrix $[_rC]$ and the two 2x1 vectors $\{_rR\}$ and $\{_rR'\}$. It is now necessary to sum over all m finite elements in order to obtain the corresponding equation for the complete system, namely

$$[C]\ \{c\}_{t+\Delta t} = \{R\} - \{R'\} = \{Y\} \tag{29}$$

where

$$[C] = \sum_e [_rC]$$

$$\{R\} = \sum_e \{_rR\} \tag{30}$$

$$\{R'\} = \sum_e \{_rR'\} \quad .$$

If there are p nodal points in the system, then matrix [C] is p x p and column vectors $\{R\}$, $\{R'\}$, and $\{c\}$ are p x 1. Thus the specialized summation, or assembly, procedure indicated in Eq. (30) converts matrices and vectors of order two into similar quantities of order p. To illustrate how this works, it is convenient to consider the simple two-element system shown in Fig. 13. Each element contains two nodes, which are numbered locally as indicated. By means of the basis functions of Fig. 12, each element contributes both to the diagonal (1,1) and (2,2) matrix elements and to the off-diagonal (1,2) and (2,1) matrix elements of all two-dimensional matrices and to the (1) and (2) matrix elements of all column vectors. As shown in Fig. 13, neighboring elements 1 and 2 contain node 2 (in global notation) in common, and this same node is given different local identification numbers within these elements. Such a circumstance is accounted for in the assembly process, which yields

$$[C] = \begin{bmatrix} {}_1C_{11} & {}_1C_{12} & 0 \\ {}_1C_{12} & ({}_1C_{22} + {}_2C_{11}) & {}_2C_{12} \\ 0 & {}_2C_{21} & {}_2C_{22} \end{bmatrix} \tag{31}$$

and

$$\{R\} = \begin{Bmatrix} {}_1R_1 \\ {}_1R_2 + {}_2R_1 \\ {}_2R_2 \end{Bmatrix} \tag{32}$$

with similar expressions for $\{c\}$ and $\{R'\}$. Matrix [C] is tridiagonal due to the sequential (global) numbering of the nodes. Equations (31) and (32) demonstrate both the index-shifting and summation properties of the assembly process.

7. **Application of boundary conditions.** Two types of boundary conditions are considered here, namely Neumann constant-flux and Dirichlet constant-concentration specifications. The former condition is imposed through column vector $\{R'\}$ [see Eqs. (18) and (30)]. If a flux X_i is imposed at node i, then $R'_i = X_i$ is prescribed. (The appropriate basis function N_i of Eq. (13) has a value of unity at node i.) Conversely if there is no externally applied flux at node i, then it follows that $R'_i = 0$.

At nodes where Dirichlet constant-concentration boundary conditions are applied, an identity equation is generated for each such node and included in the matrices of Eq. (29). As an example, take the two-element system of Fig. 13 with the concentration at node 1 constrained to the value of b at all times, i.e.

$$c_1 = b \qquad \text{and} \qquad b \neq b(t) \ . \tag{33}$$

Equation (29) then takes the form

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & C_{22} & C_{23} \\ 0 & C_{32} & C_{33} \end{bmatrix} \begin{Bmatrix} c_1 \\ c_2 \\ c_3 \end{Bmatrix} = \begin{Bmatrix} b \\ Y_2 - C_{21}b \\ Y_3 \end{Bmatrix} \tag{34}$$

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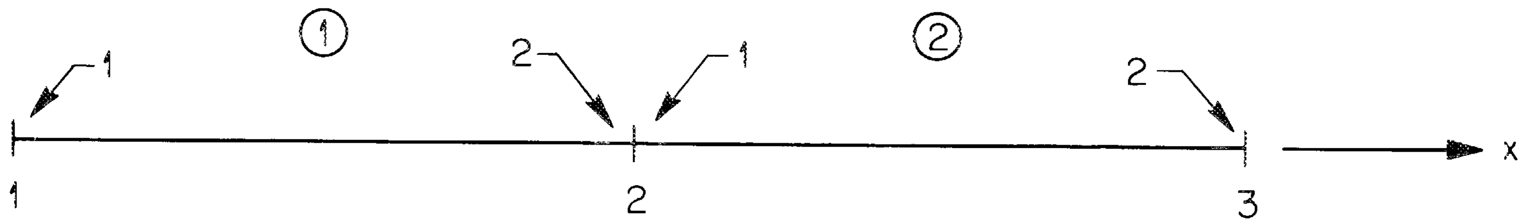

Fig. 13. A two-element system. Element numbers are circled. Local node numbers appear above the x axis, and global node numbers appear below the x axis.

in which the tridiagonal structure of matrix [C] [Eq. (31)] has been taken into account. This result may easily be generalized to an arbitrary number of equations with one or two Dirichlet boundary nodes.

8. Solution of the assembled equations. In solving the assembled equations expressed in Eq. (29), the matrix [C] is decomposed into the product of upper and lower triangular matrices using the Gauss technique. The lower triangular matrix is used to modify the right-hand side of $\{Y\}$ for back-substitution into the upper triangular matrix to obtain a solution. If the matrix [C] and the time step Δt do not change with time, the decomposition needs to be performed only once.

SAMPLE CALCULATIONS

In this section the results of three sample calculations are presented. Each of these hypothetical cases are based on a chromatographic column of length $L = 40$ cm with boundary-initial conditions

$$\begin{aligned} &c(x = 0, t) = 1 \\ &c(x = L, t) = 0 \\ &c(0 < x < L, t = 0) = 0 \quad . \end{aligned} \tag{35}$$

Whenever a temporally and spatially variable Darcy velocity $V(x,t)$ is used, it is taken to be that for horizontal flow in Yolo clay as described in the previous chapter.

1. Numerical results. The objective here is threefold. Firstly, we would like to typify the time development of a concentration profile for the variable advective velocity. This is done in Fig. 14. Using the curve $c(x,t = 1 \text{ day})$ as "experimental data," a parameter search (see next chapter) is made in order to define an equivalent constant Darcy velocity subject to the proviso $\theta = n$. Concentrations for this velocity are also shown in Fig. 14 for comparison.

Secondly, we would like to demonstrate the effects of both the distribution coefficient k_d and the dispersivity a_L and to distinguish one from the other. Figure 15 shows concentration profiles $c(x,t)$ at $t = 1$ day corresponding to several different values of the dispersivity a_L. Figure 16 exhibits similar curves for several different values of the distribution coefficient k_d. Obviously the effects on fluid concentration c of changing values of a_L are quite similar to those attributable to changing values of k_d. If only fluid concentrations were measured in a chromatograph, there would be little hope for distinguishing the two. Fortunately, however, the chromatographic method measures the bulk concentration

$$c_b = R_d \theta c \tag{4}$$

where

$$R_d = 1 + \frac{\rho k_d}{n} \quad . \tag{5}$$

The water-content factor $\theta(x,t)$ serves to modify the shape of the fluid concentration profile, as shown by the plots of $c_b/R_d n$ in Fig. 16. Nevertheless, it provides no distinction between a_L and k_d. The normalization R_d does provide such a distinction since it depends only on k_d [Eq.(5)]. As indicated by the quoted values of $R_d n$ in Fig. 16, this normalization can be quite large, compared to the maximum fluid concentration of unity, and quite variable, changing by over three orders of magnitude as k_d changes from zero to 1000 cm^3/gm.

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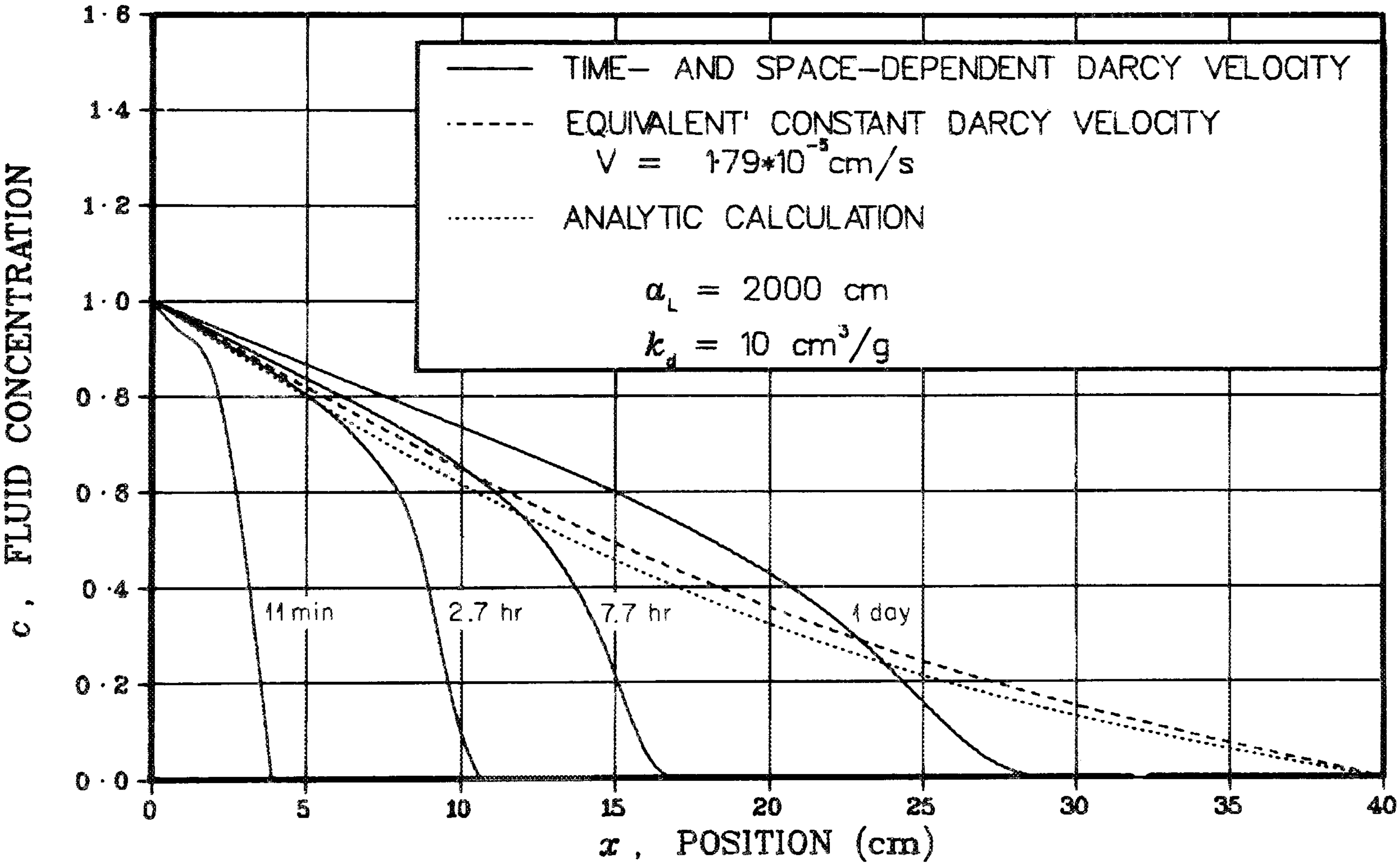

Fig. 14. Development of concentration profiles as a function of time for a variable advective velocity.

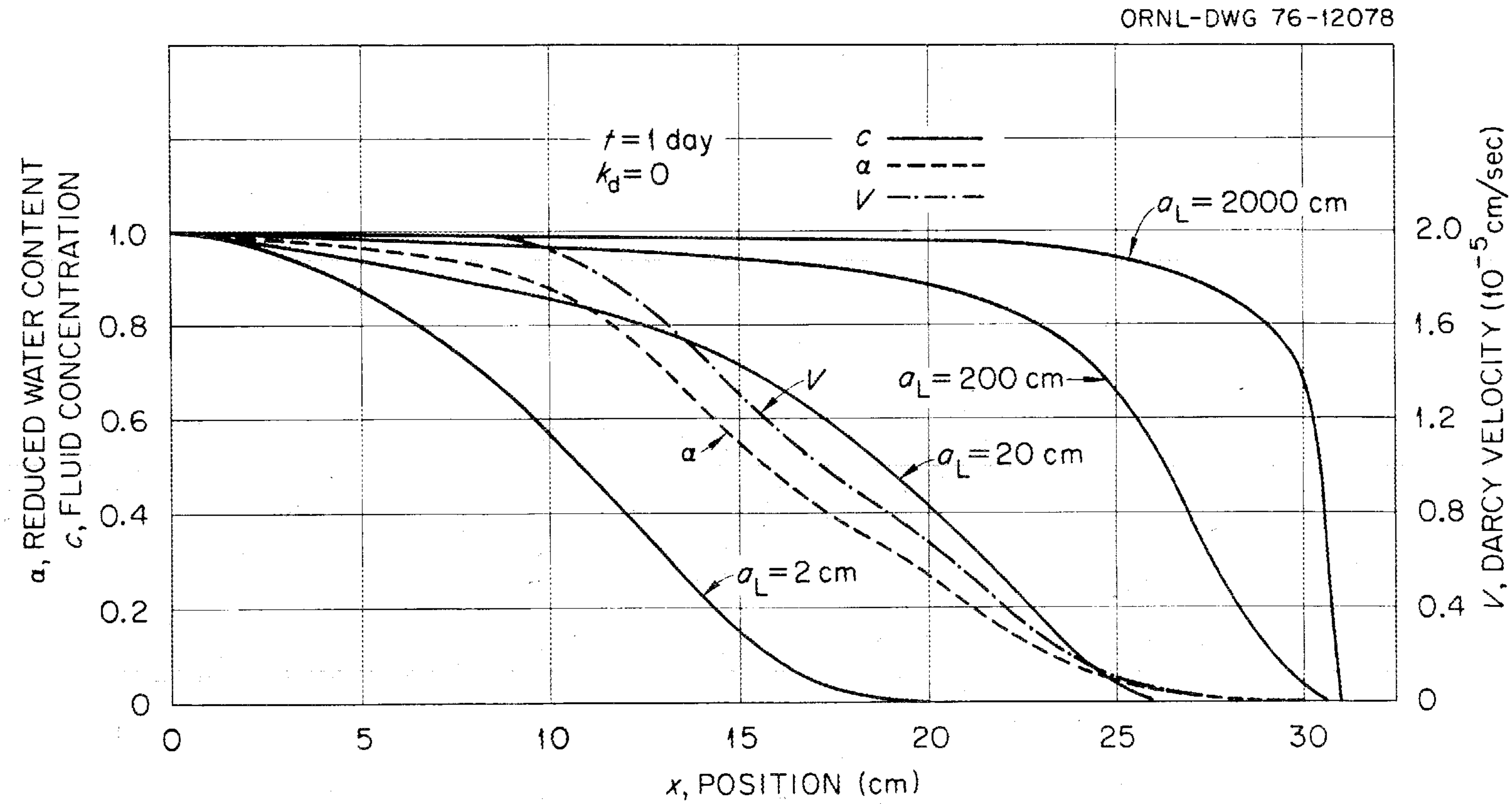

Fig. 15. Effect of the dispersivity parameters on profile development.

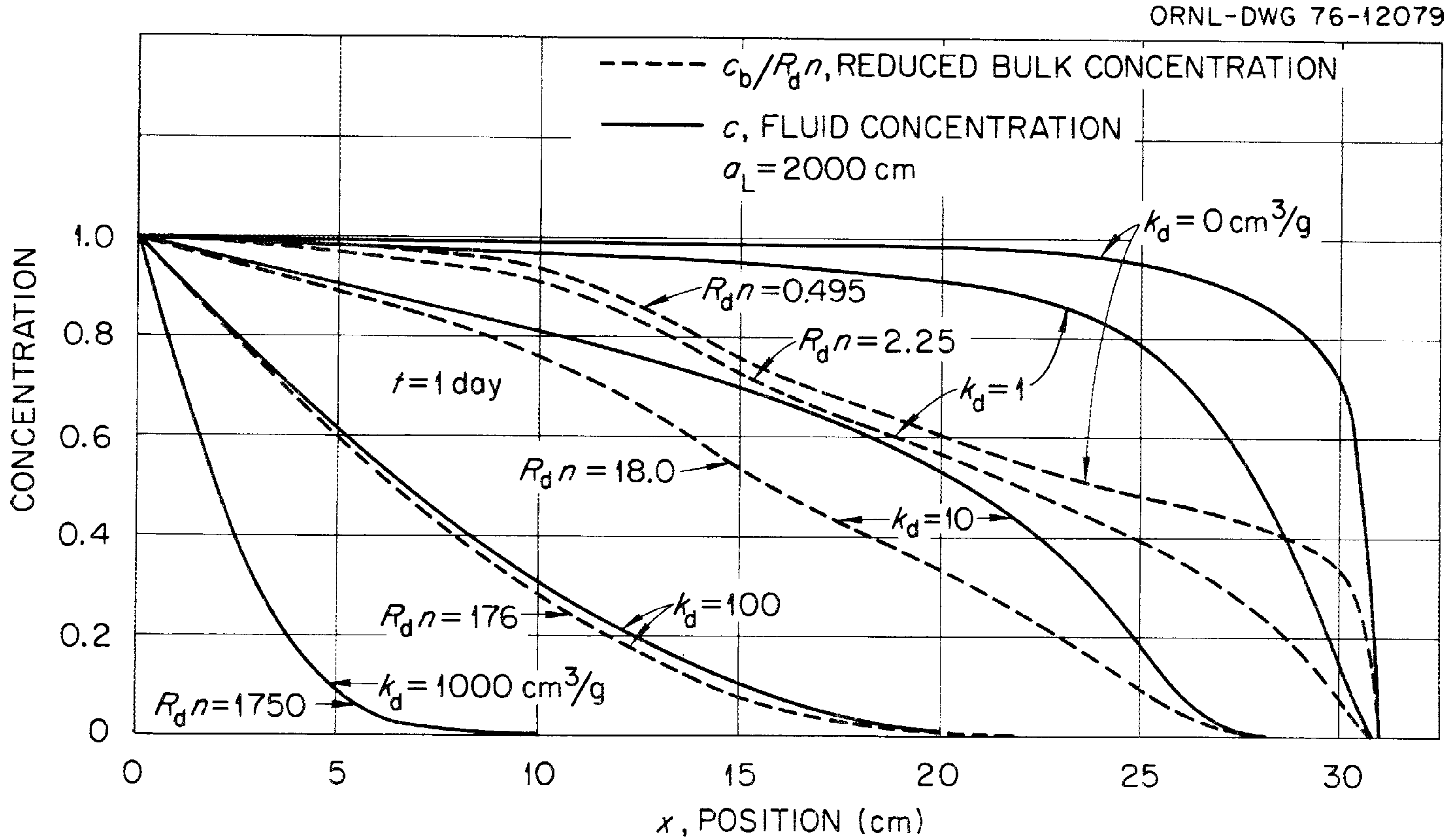

Fig. 16. Effect of the distribution coefficient on profile development.

2. **Analytical comparison.** The third and final objective of this section is to test the numerical results of Fig. 14 for the constant-velocity case against analytical results. To sketch briefly the analytic solution process we cast Eq. (6) into the form

$$\frac{\partial c}{\partial t} = q^2 \frac{\partial^2 c}{\partial x^2} - v \frac{\partial c}{\partial x} \quad . \tag{36}$$

Here

$$q^2 = a_L V/\theta R_d \tag{37a}$$

and

$$v = V/\theta R_d \tag{37b}$$

where quantity θ like V is assumed to be a constant. For convenience the assumption $\lambda = 0$ is made.
The transformation

$$c = e^{\mu x}\, g \qquad \mu = v/2q^2 \tag{38}$$

removes the first-derivative term in Eq. (36) to yield the form

$$\frac{\partial g}{\partial t} = q^2 \left(\frac{\partial^2 g}{\partial x^2} - \mu^2 g \right) \quad . \tag{39}$$

The solution of this equation, subject to the boundary-initial conditions of Eq. (35), may be expressed [Berg and McGregor, 1966] as an expansion over the eigenfunctions of Eq. (39). The result is

$$c(x, t) = e^{-\mu x} \left(\frac{\sinh \mu (L - x)}{\sinh \mu L} + \frac{2}{L} \sum_{m=1}^{\infty} \frac{\omega_m}{\mu^2 + \omega_m{}^2}\, e^{-\lambda_m q^2 t} \sin \omega_m x \right) \tag{40}$$

where

$$\omega_m = \frac{m\pi}{L} \tag{41a}$$

$$\lambda_m = \left(\frac{m\pi}{L} \right)^2 + \mu^2 \quad . \tag{41b}$$

Results obtained from Eq. (40) are plotted alongside the corresponding numerical results in Fig. 14. The variation, about 5% on the average, is acceptable for the space mesh used here for which $\delta x = 0.5$ cm.

V. OPTIMIZATION

INTRODUCTION

In contrast to the water-transport and mass-transport developments of previous sections, no improvements or modifications have been added in this chapter to existing numerical procedures. Thus the objective here is to present those basic concepts which permit use of the computer program listed in Appendix B. Additional technical information may be obtained from the references to be cited.

The optimization problem for chromatographic analysis is twofold. Firstly, given the experimentally determined water contents $\theta^x(x,t)$, it is required to find soil parameters for the best-fitting theoretical function $\theta(x,t,K_s,h_o,d,\beta'_o,h'_o,d')$ so that the corresponding Darcy velocities may be determined. Secondly, given these velocities and the experimentally determined concentrations $c_b^x(x,t)$, it is required to find mass-transport parameters for the best fitting theoretical function $c_b(x,t,k_d,a_L,\rho,n)$. It is, of course, desirable independently to measure parameters a_L, ρ, and n whenever possible in order to reduce numerical error in the determination of k_d.

The best fit of a theoretical function $f(x,t,\bar{p})$ is defined as that set of parameter values $\bar{p}$ (in vector notation) which minimizes the quantity

$$X^2(\bar{p}) = \sum_{i=1}^{N_t} \sum_{j=1}^{N_x(i)} \left(\left(f(x_j, t_i, \bar{p}) - f^x(x_j, t_i)\right) / \sigma^x(x_j, t_i)\right)^2 \quad . \tag{1}$$

Symbol f may be identified with either θ or c_b, and σ^x is the experimental error. The number of position variables N_x will, in general, be a function of the time t_i at which the measurements were taken, as indicated by the argument. Integer N_t represents the total number of such time steps. Formally $\bar{p}$ may be viewed as a vector in an N_p-dimensional parameter space with components p_1, p_2, ..., p_{N_p}, and $X^2(\bar{p})$ is a hypersurface in an $(N_p + 1)$-dimensional space. The problem is to locate the point $\bar{p}$ at which X^2 is minimized.

OPTIMAL SEARCH

One of the simplest methods for minimizing X^2 is the *direct search*. This technique involves sequential evaluation of this dependent variable and subsequent comparison with the best previously determined value together with a strategy for determining where the next trial will be made. One particular strategy characterizes the *pattern-search method* [Hooke and Jeeves, 1961]. When this technique is generalized to the case of constrained parameters, it is called the *optimal-search method* [Weissman and Wood, 1966]. The latter is chosen here since it permits the user to impose physical restrictions by specifying an allowable range for any parameter. The computer implementation used here is that of Westley [Westley and Watts, 1970].

The optimal-search strategy may be explained as follows. Initially a *base point* $\bar{p}_o$ is chosen arbitrarily. Then *exploration* begins about this point. First the *exploratory trial point* $\bar{p}_+ = \bar{p}_o + \bar{e}_1\Delta p_1$ is chosen where $\bar{e}_1$ is a unit vector parallel to the p_1 axis. If a *success* is obtained, i.e. $X^2(p_1) < (1 - T_x)X^2(p_o)$, then an *exploratory move* is made to $\bar{p}' = \bar{p}_+$, where T_x is an acceptance factor for function improvement and $\bar{p}'$ is the current estimate for the next base point $\bar{p}_1$. If a failure is obtained, i.e. $X^2(p) > (1 - T_x)X^2(p_o)$, then a new trial point $\bar{p}_- = \bar{p}_o - \bar{e}_1\Delta p_1$ is chosen. If success is achieved at $\bar{p}_-$ then an exploratory move is made to $\bar{p}' = \bar{p}_-$. Here and in the case of incrementation, whenever there is a success, the step is accelerated in preparation for the next exploration, i.e. $\Delta p_i \rightarrow A\Delta p_i$ where $A > 1$ is an acceleration factor. If this possibility is also exhausted, then there is no exploratory move, i.e. $\bar{p}' = \bar{p}_o$. The step size is then reduced in preparation for the next exploration, i.e. $\Delta p_i \rightarrow B\Delta p_i$ where $B < 1$ is a reduction factor. The next step is to increment, decrement, or leave unchanged parameter p_2 in the same manner as for parameter p_1. After taking each parameter, in turn, a new base point $\bar{p}_1$ will most likely be obtained. Figure 17 presents an example for a two-dimensional parameter space.

The next step is to take a pattern trial move to $\bar{p}' = 2\bar{p}_1 - \bar{p}_0$ followed by exploratory trial moves. (Trial moves are indicated as dashed lines in Fig. 17.) If this series of moves is successful, i.e. $X^2(\bar{p}') < (1 - T_x)X^2(\bar{p}_1)$, then a pattern move is made to $\bar{p}_2 = \bar{p}'$. It should be noted here that the sequence of trial moves outlined above continues even if $X^2(2\bar{p}_1 - \bar{p}_0) > (1 - T_x)X^2(\bar{p}_1)$. In addition, there is no acceleration or reduction of the step sizes in such a trial-point exploration. Similar pattern moves are taken until there is a failure. Then a return is effected to the base point, say $\bar{p}_i$, from which the trial moves emanated. A *base-point exploration* then follows, in which step-size reductions are permitted.

At this point all the distinctions between a base-point exploration and a *pattern exploration* should be clarified. Basically there are three differences. Firstly, for the former a base-point move, in effect, is made each time there is a successful exploratory move. For a pattern exploration, on the other hand, a base-point move is made only after the inclusion of exploratory moves of all parameters have been made, and there has been a successful comparison with the previous base point, rather than the origin of the exploration. Such was the case in the example of Fig. 17, where a base-point exploration was employed about the initial guess $\bar{p}_0$. Secondly, as noted earlier, step-size modification is allowed only during a base-point exploration. Finally, normal termination of the search may only follow a base-point exploration. This happens when there are failures in all parameters p_i and all increments are less than or equal to their lower limits, i.e. $\Delta p_i \leqslant T_p p_i$ where T_p is a step-size tolerance factor. Pattern exploration, since it occurs about a trial point rather than an established base point, is not deemed to be sufficiently reliable to justify either step-size modification or normal termination. (Nonnormal termination occurs whenever the prescribed maximum number of function evaluations of $f(x,t,\bar{p})$ has been exceeded.)

The above strategy is identical to that of the pattern-search method. The only additional feature required by the optimal-search strategy is to test after each incrementation (or decrementation) to see whether the parameter is within the prescribed range of allowable values. If not, then the parameter value is simply set equal to the nearest bound.

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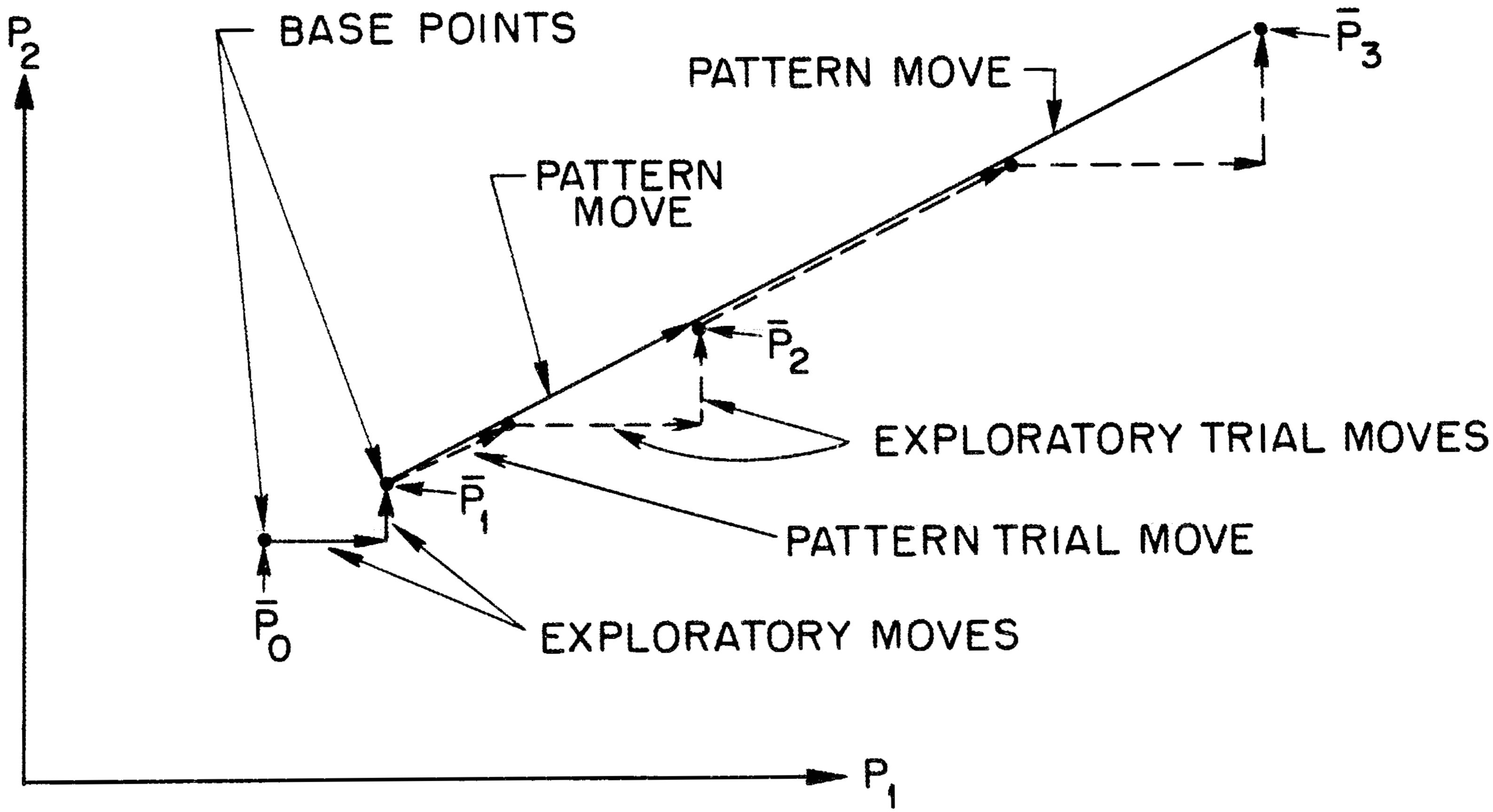

Fig. 17. Examples of base-point exploration, pattern moves, and of successful pattern-point explorations.

VI. COMPUTER IMPLEMENTATION

The computer program is divided into three functional units pertaining to (1) the water transport, (2) the mass transport, and (3) the automatic search procedures, all of which were described formally in preceding chapters. Routine MAIN controls the operation of these units as prescribed by the user (see Fig. 18). The individual units are structured as shown in Figs. 19, 20, and 21. In all, there are 34 separate subprograms, listings of which may be found in Appendix B.

WATER TRANSPORT

For the water-transport procedures the control function is performed by WTR (see Fig. 19). Using input data obtained by DATAW, routine WTR directs its supporting routines so as to obtain both position $x(\theta,t)$ and Darcy velocity $V(\theta,t)$ as functions of both time t and the water content variable, which may be either θ or its reduced counterpart α. If desired, these results may be printed (PRINTW) or stored (STRW) on an auxiliary storage device.

The quantities which determine the moisture-flow characteristics of the soil are the soil properties $Q(\theta)$ and $K(\theta)$. These functions may either be read in as tabular functions or be generated from the Gardner and King form factors, as described in the last section of Chapter II. In the former case semi-logarithmic Lagrangian interpolation by routine YLAG [Westley and Watts, 1970] is used in order to obtain soil properties appropriate for subsequent Gauss integration. In the latter case the diffusivities and conductivities are calculated directly by SPROP on such a grid. Since a given set of soil properties is independent of both position and time, and since these values are required only for the Gauss-quadrature grid of water-content values, they are calculated only once.

Initially the soil properties are used to determine the time function $t(W_l)$ for selected values of the reduced end-point Darcy velocity W_l. This is done by applying the Gauss quadrature algorithm (subroutine GAUSS) to evaluate the integral in Eq. (III.26). By sorting (routine DSORT) the results into ascending order in the time variable, the tabular function is placed in a form suitable for interpolation. This is necessary since calculation of $x(\alpha,t)$ and $W(\alpha,t)$ require the end-point velocity $W_l(t)$, as indicated by Eqs. (III.31) and (III.32). Double logarithmic Lagrangian interpolation (YLAG) is used for this purpose.

Dependent variables $x(\alpha,t)$ and $W(\alpha,t)$ are evaluated by either the first-order formulas, Eqs. (III.17) and (III.18), or the second-order formulas, Eqs. (III.31) and (III.32), as specified by the user. Integrals in the above-mentioned equations are evaluated by subroutine GAUSS with the various integrands supplied by the function routine FUNS. The unreduced velocity V is obtained from the reduced velocity W through application of Eq. (III.9). In addition, when coupling with the mass transport is required, functions $x(\theta,t)$ and $V(\theta,t)$ are transformed to the functions $\theta(x,t)$ and $V(x,t)$ by WTR, and then Lagrangian interpolation is performed to yield the moisture transport variables θ and V on the spatial grid specified by the mass-transport calculation.

Obviously, the Lagrange-interpolation and Gauss-quadrature techniques play important roles in the water-transport determination. For this reason the order parameters, which govern the accuracy of each method, are separately identified as input quantities. (Appendices C and D give a complete description of the input.)

MASS TRANSPORT

When the moisture-transport variables θ and V are obtained, either as results of the above-mentioned calculation or as input quantities, the mass-transport equation, Eq. (IV.6), is solved numerically as depicted by Fig. 20. As indicated by its central location, subroutine MTR performs the control function here. Using input data obtained by DATAM, routine MTR directs its supporting routines so as to obtain fluid concentration $c(x,t)$ and its bulk counterpart $c_b(x,t)$ as functions of both position x and time t. Results may be printed (PRINTM) or stored (STRM).

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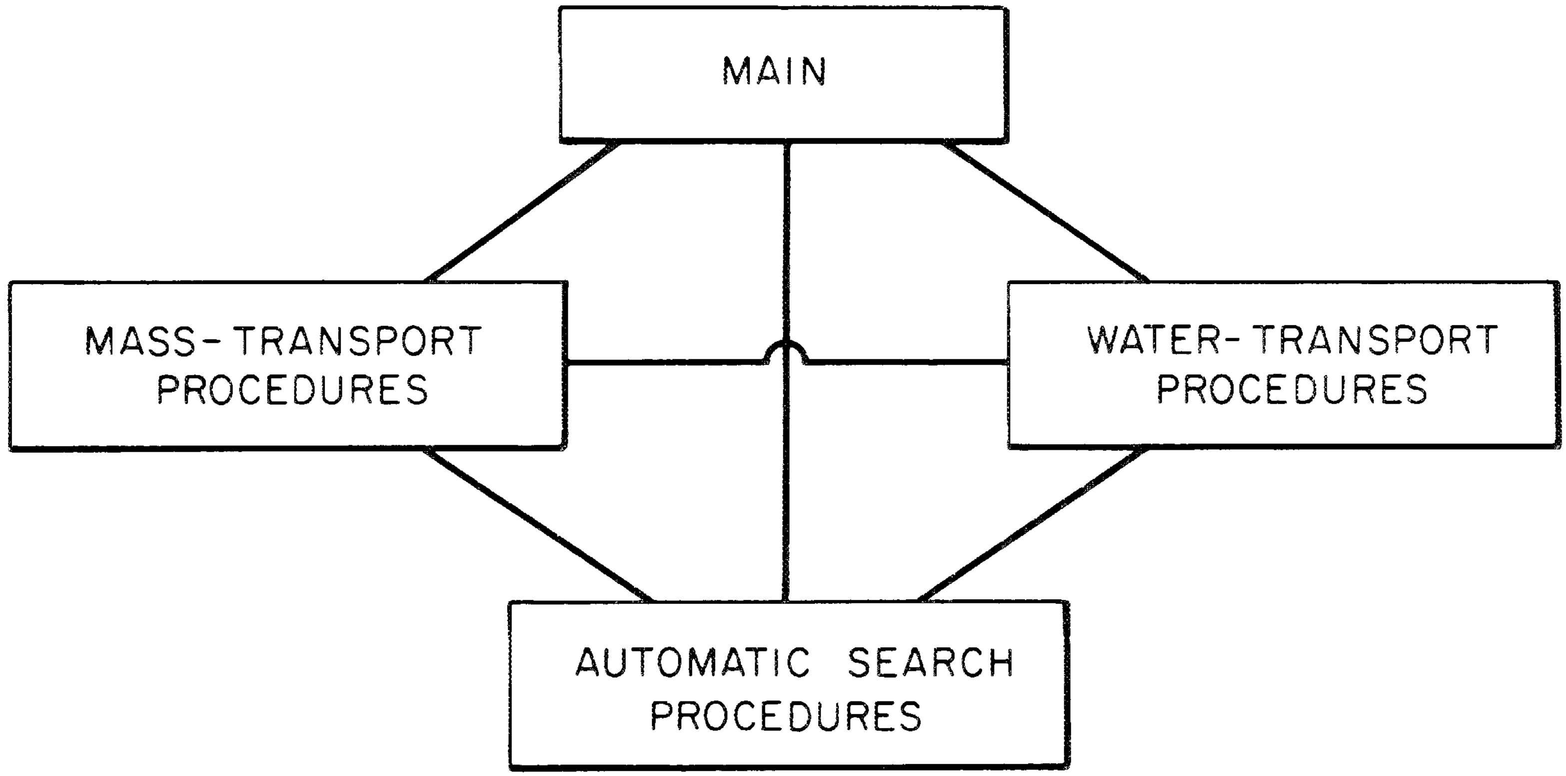

Fig. 18. Flow chart connecting the functional units of the program.

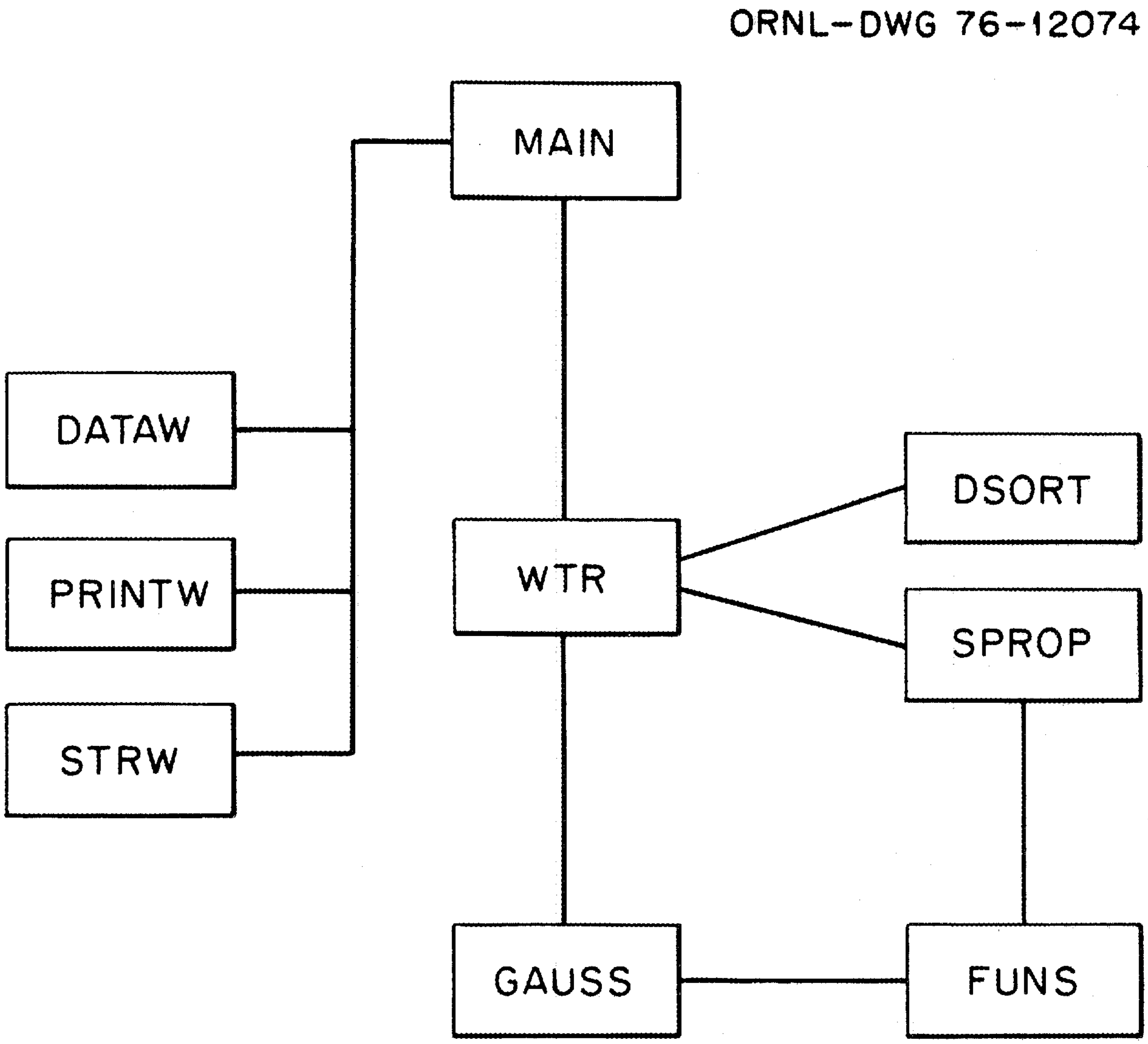

Fig. 19. Flow chart specifying the water-transport routines.

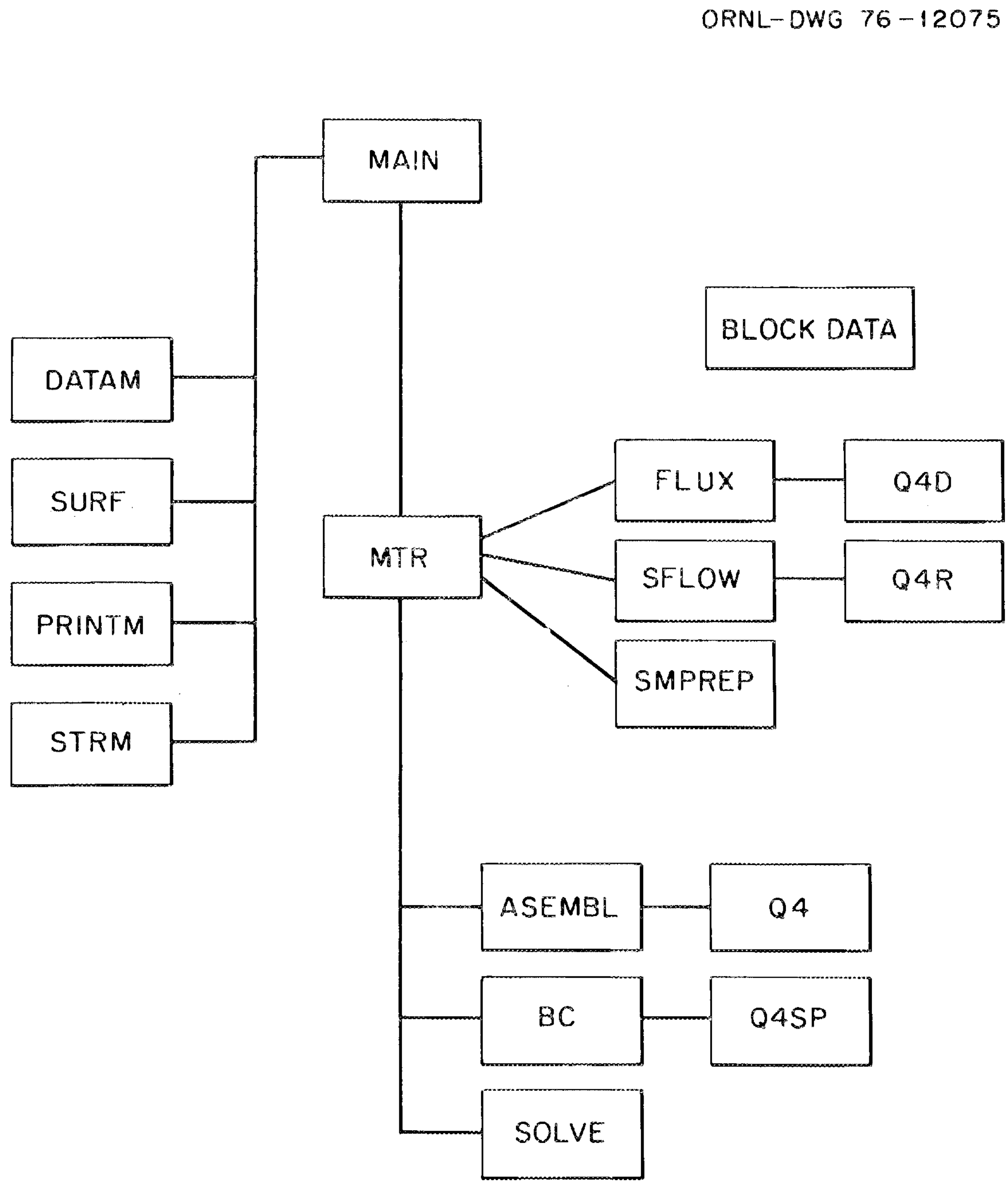

Fig. 20. Flow chart specifying the mass-transport routines.

The primary computations for the mass transport are carried out in routines Q4, ASEMBL, BC, and SOLVE. Subroutine Q4 generates the linear basis functions N_i [Eq. (IV.22)] and the Jacobian $_rJ$ and, using known (or assumed) soil-solution properties, performs the integrations necessary to obtain element matrices $[_rA]$ and $[_rB]$. The Gauss quadrature algorithm of order two is employed here. Subroutine ASEMBL has two functions. First, it applies the finite-difference discretization for the time variable to obtain matrices $[_rC]$ and $\{_rR\}$ from $[_rA]$ and $[_rB]$ as prescribed in Eqs. (IV.27) and (IV.28). Secondly, it assembles these quantities via Eqs. (IV.30) to obtain the global matrices [C] and $\{R\}$. Routine BC applies the boundary conditions as discussed in Chapter IV, Theory Section 7, and SOLVE solves the resulting asymmetric banded matrix system by Gaussian elimination.

Supporting calculations are carried out in SURF, FLUX, Q4D, SFLOW, and Q4R. Subroutine SURF identifies boundary nodes and elements. Routine FLUX and Q4D determine the mass flux at each node from the predetermined concentration distribution. To determine the mass balance, end-point mass fluxes are integrated over time by SFLOW, and concentration distributions are integrated over space by Q4R.

OPTIMIZATION

The optimal-search technique, which was described briefly in Chapter V, is implemented as shown in Fig. 21. Using search parameters and experimental data input through DATAS, routine SEARCH produces a set of physical parameters $\bar{p}$ which minimize $X^2(\bar{p})$, Eq. (V.1). This set of parameters and the corresponding best fits to the experimental data are then printed by PRINTS.

One of the four different X^2 evaluators, MEVAL, MWEVAL, MWVAL2, or WEVAL, is chosen depending on user specifications. For example, WEVAL is used whenever the experimental water contents $\theta^x(x,t)$ are to be fitted, whereas MWEVAL is used whenever experimental concentrations $c_b^x(x,t)$ are to be optimally approximated. In the latter case it is understood that the water transport is to be calculated simultaneously from known soil parameters.

The material-transport and water-transport procedures here assume the role of providing theoretical functions for the X^2 evaluators. There are necessarily, however, some linkage routines. Parameter linkage is accomplished by BUFFM and BUFFW. Subroutine BUFFM establishes the correspondence between various elements of the parameter array $\bar{p}$ and the material-transport parameters k_d, a_L, ρ, and n. Routine BUFFW performs this same function for the water-transport parameters. Nodal-point linkage is accomplished by YLAG, SWPREP, and DSORT. Calculational space grids must, in general, differ from experimental space grids. The former is chosen from considerations to achieve computation efficiency, whereas the latter is dictated by the experimental techniques. This disparity is rectified by simply interpolating with YLAG to obtain the theoretical functions at the experimental positions.

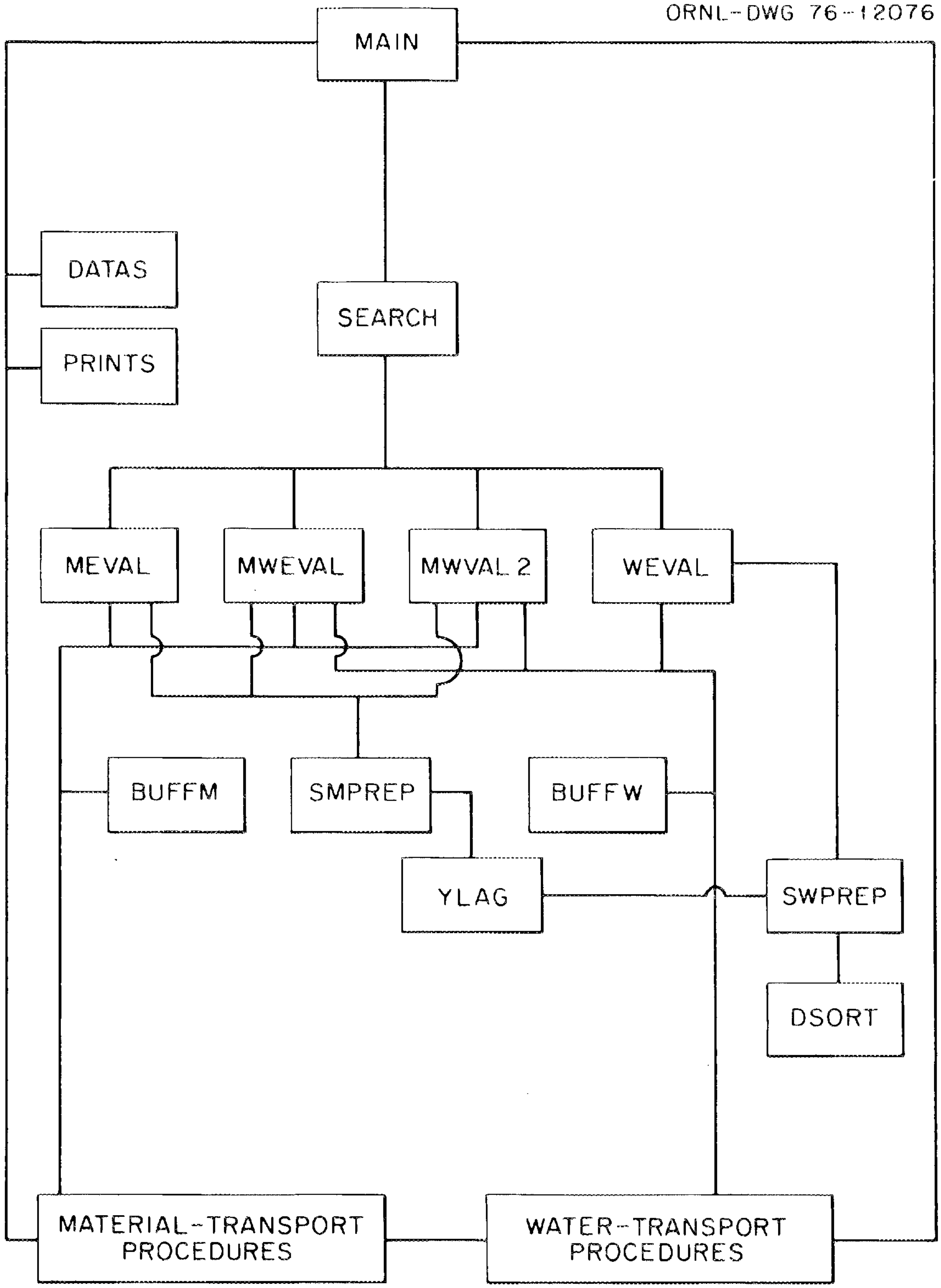

Fig. 21. Flow chart specifying the optimization routines.

VII. ANALYSIS OF EXPERIMENTAL DATA

Correspondence of theory and experiment is the subject of this chapter. More precisely, the optimization procedure of Chapter V is used to automatically adjust parameters of both the water-transport theory (Chapter III) and the mass-transport theory (Chapter IV) so as to "best fit" the experimental data (Chapter II). One of the mass-transport parameters, namely the distribution coefficient k_d, is of special interest.

Before proceeding, however, certain general remarks should be made regarding the work presented in this chapter. In the first place, it is somewhat fragmentary since it represents our first attempt to analyze experimental data. Even so, feasibility is demonstrated by the Sr and Pu analyses presented. Finally the need for further refinement of two different aspects of our analysis, namely the water-transport and the migration of multiple species, can be seen.

WATER TRANSPORT

The purpose here is to determine both the water content $\theta(x,t)$ and the Darcy velocity $V(x,t)$. These quantities are necessary since they characterize the carrier fluid and thereby control the mass transport. To calculate the latter, a space-time grid must be superposed on the region of integration (x,t). The spacings within this grid are governed by convergence and stability criteria of the numerical algorithms, and, in general, are much finer than the corresponding experimental grid. Thus the need for an interpolating procedure arises. The strategy adopted here is to fit the experimental data at the selected points at which it is measured. One thereby determines parametrically an interpolation function which may be used at space-time points other than those for which measurements are taken.

Another consideration concerns the experimental observable, which is simply the relative radioactivity. In the case of tritium, which is not adsorbed, this radioactivity is taken to be proportional to the water content. Thus the fitting function must be more than a simple interpolation function. It must have sufficient theoretical foundation that Darcy velocities may be extracted from it. The formal development of such a function is the subject of Chapter III.

Figures 22 and 23 present two different radioactivity profiles for the movement of tritiated water in Fuquay sand corresponding to two different values of the eluting time. (The radionuclide here is placed in the feed solution rather than being spotted directly onto the soil.) Parameter values for the theoretical fits are given in Table 1. These fits are not extremely good. There is a plateau in the experimental data for the lower values of the position x which is not present in the theory. Secondly, the experimental wetting front is steeper than that of the theoretical fit. The problem here appears to be experimental. The relatively weak beta (0.018 MeV) coming from ^{3}H permits observation of only the topmost layer of soil, where evaporation, inhomogeneity, and two-dimensional effects are the greatest. A different experimental technique appears to be called for. Perhaps dissection followed by weighing the increments before and after drying would be more satisfactory.

MASS TRANSPORT

The best fits obtained to date are shown in Figs. 24–26. Figures 24 and 25 pertain to ^{85}Sr transport in Fuquay sand and Figs. 26 and 27 pertain to ^{237}Pu transport in the same soil. In each case the radionuclide is spotted directly onto the soil. (Figures 28 and 29 show the corresponding initial conditions.)

The soil is then wetted for approximately 17 hours using water as the eluting solution and counted to obtain the radionuclide profiles. Figures 24 and 26 exhibit the resulting profiles. After drying, the soil is wetted for a second time and counted. Figures 25 and 27 pertain to this wetting, again for Sr and Pu, respectively.

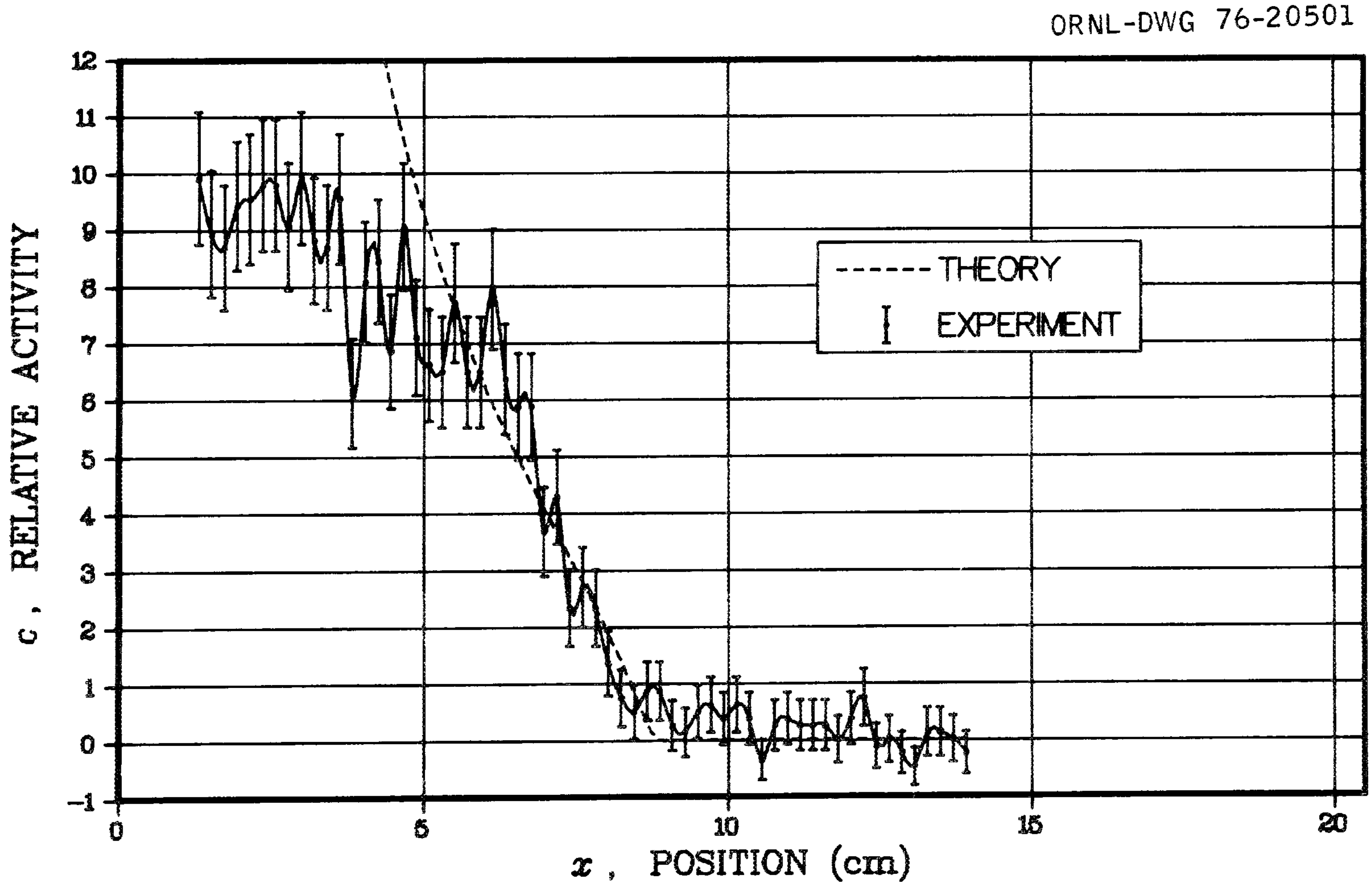

Fig. 22. ^{3}H distribution in Fuquay sand at t = 1 min.

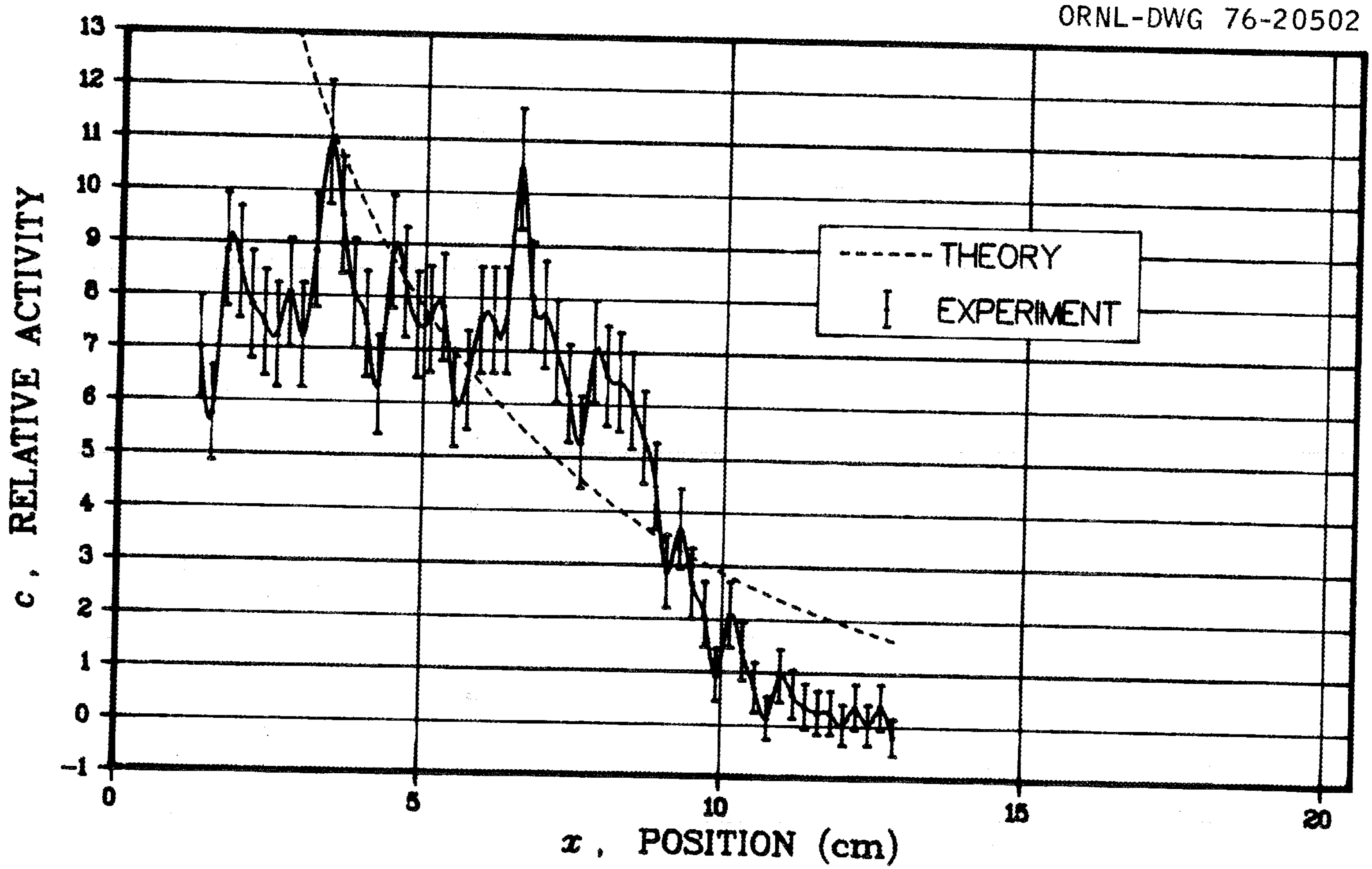

Fig. 23. ^{3}H distribution in Fuquay sand at t = 4 min.

Table 1. Moisture-Transport Parameters for Fuquay Sand

Conductivity Parameters	K_s	7.57×10^{-5} cm/sec
	h_o	−49.9 cm
	d	1.78
Moisture-Content Parameters	β'	3.97×10^{-4}
	h'_o	−23.2 cm
	d′	−0.419
	θ_r, θ_o	0.00625
	θ_l, n	0.625

Table 2. Mass-Transport Parameters for Fuquay Sand

Parameter	^{85}Sr		^{237}Pu	
	1⁺	2⁺	1⁺	2⁺
k_d (cm^3/g)	25.9⁺	36.3⁺	44.0	42.3⁺
ρ (g/cm^3)	1.75	1.75	1.75	1.75
a_L (cm)	0.150⁺	0.333⁺	0.446⁺	0.126⁺

⁺These numbers refer either to the first or second wetting.

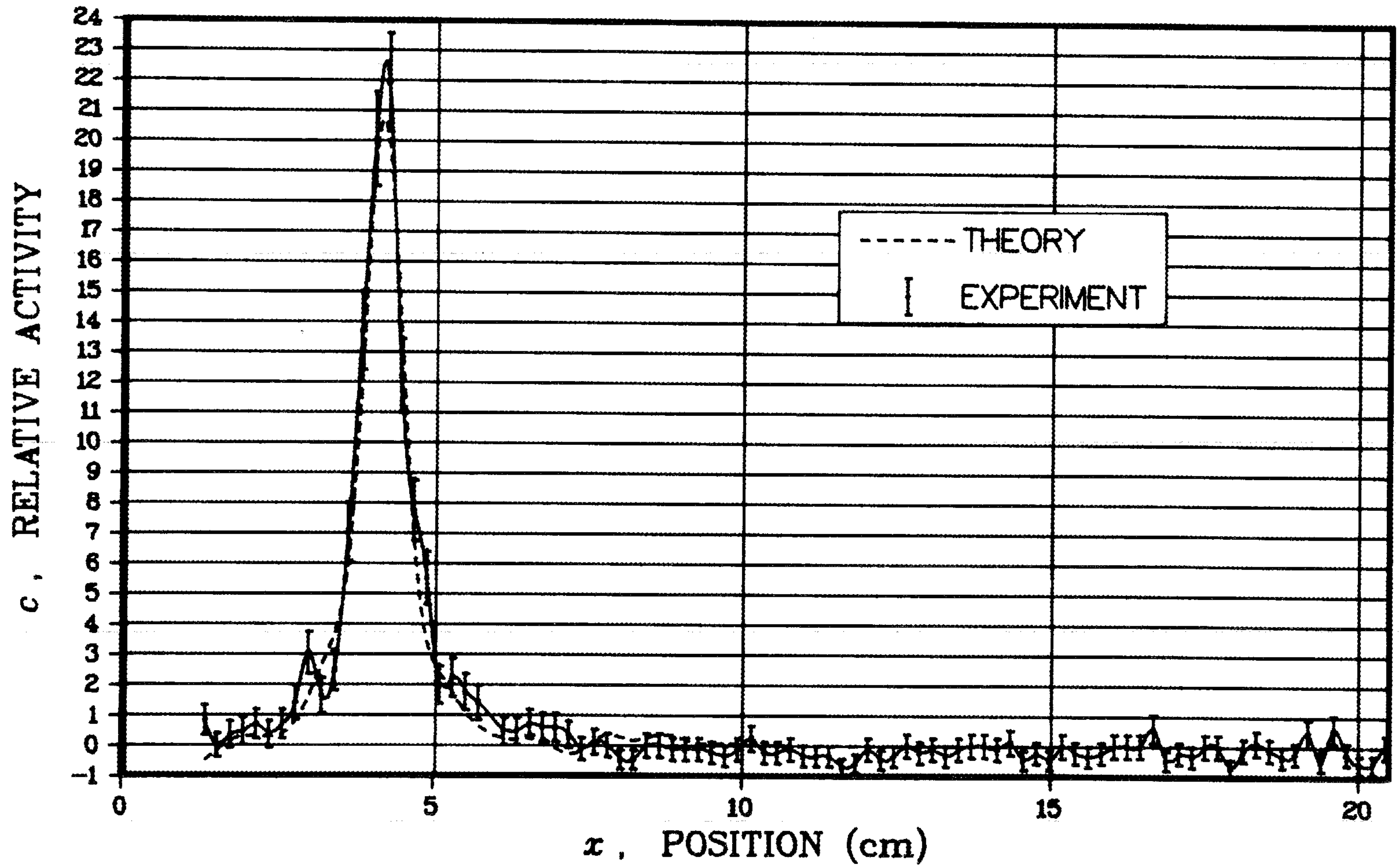

Fig. 24. ^{85}Sr distribution in Fuquay sand after one wetting with water.

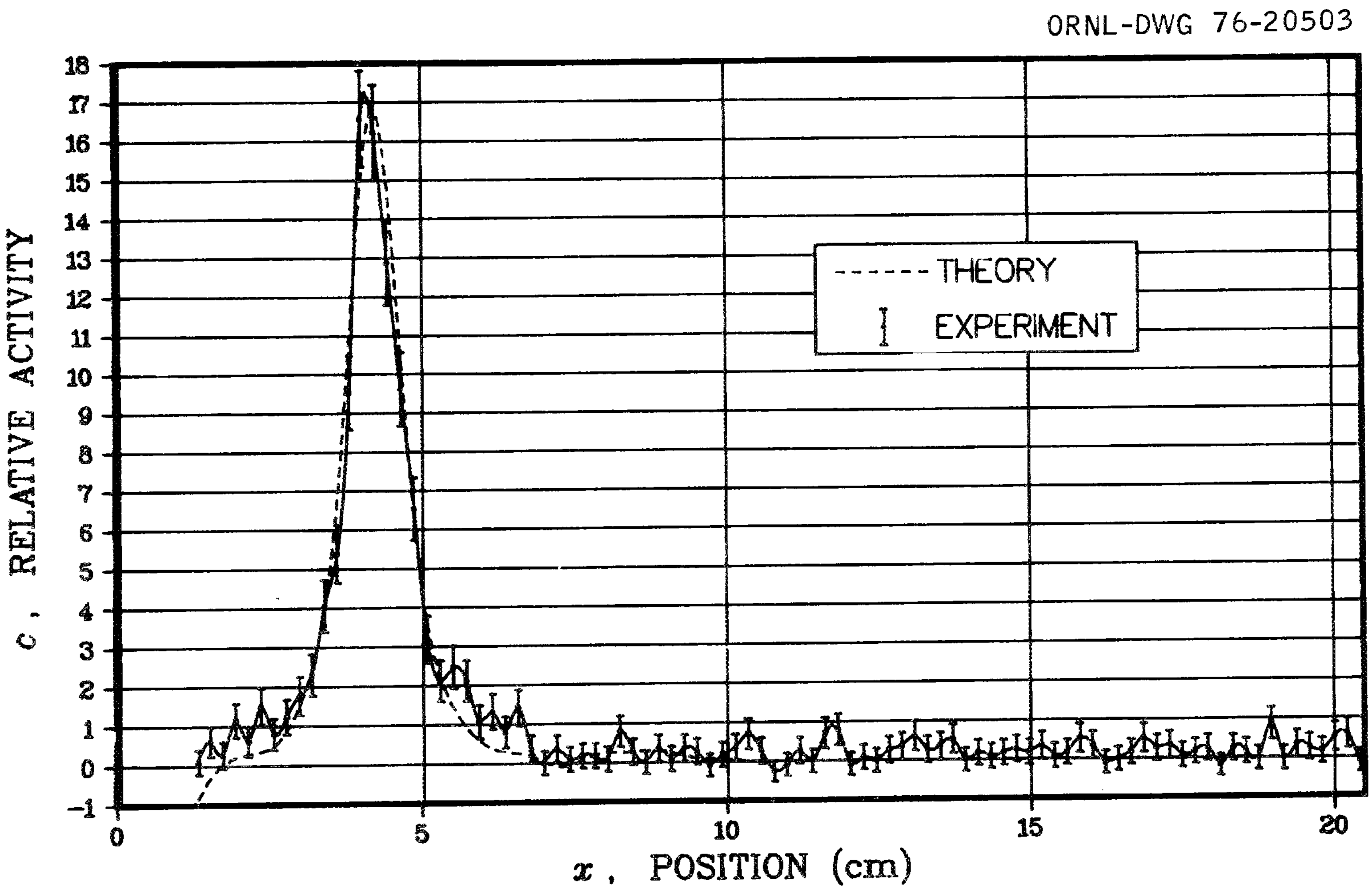

Fig. 25. ^{85}Sr distribution in Fuquay sand after two wettings with water.

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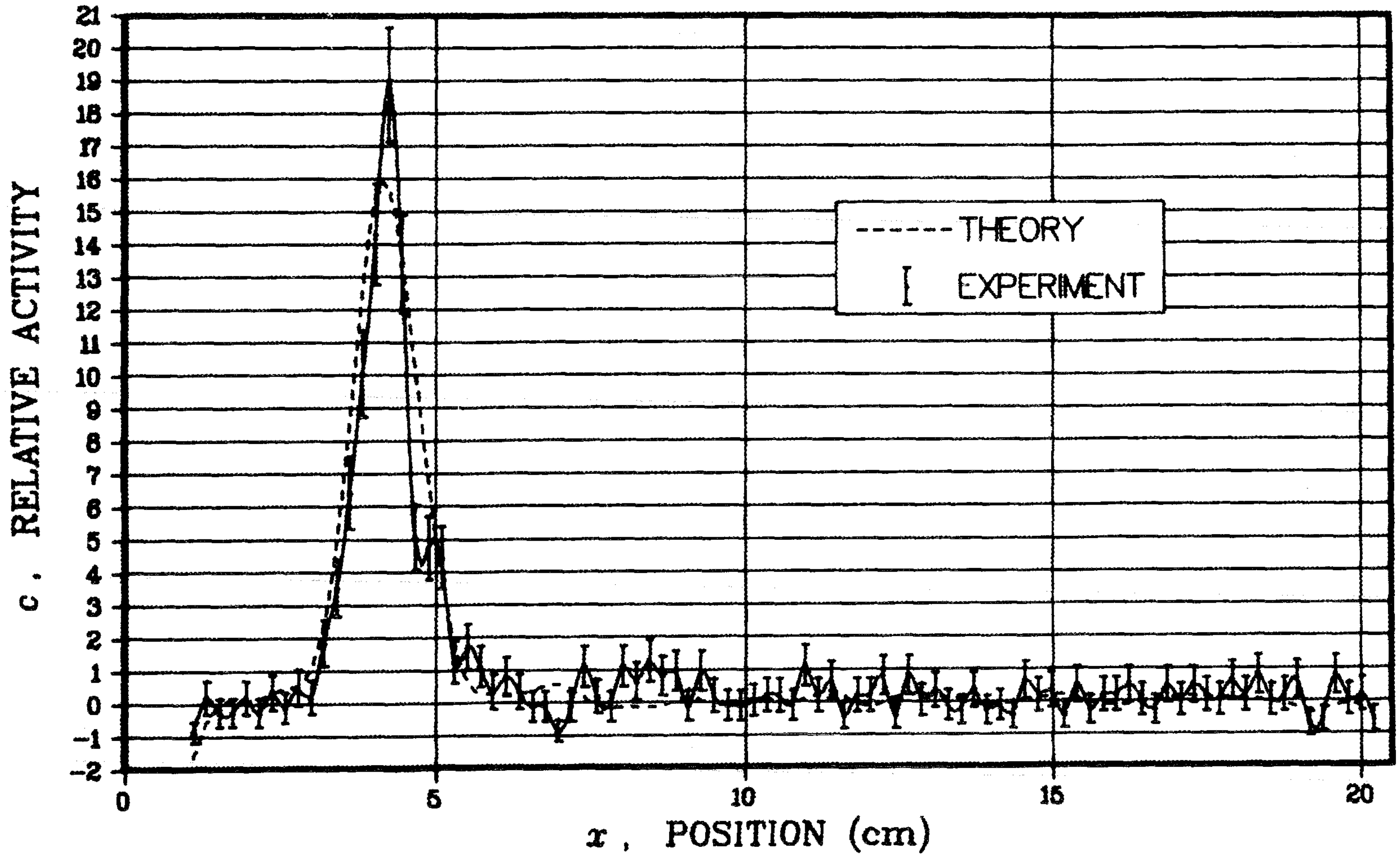

Fig. 26. ^{237}Pu distribution in Fuquay sand after one wetting with water.

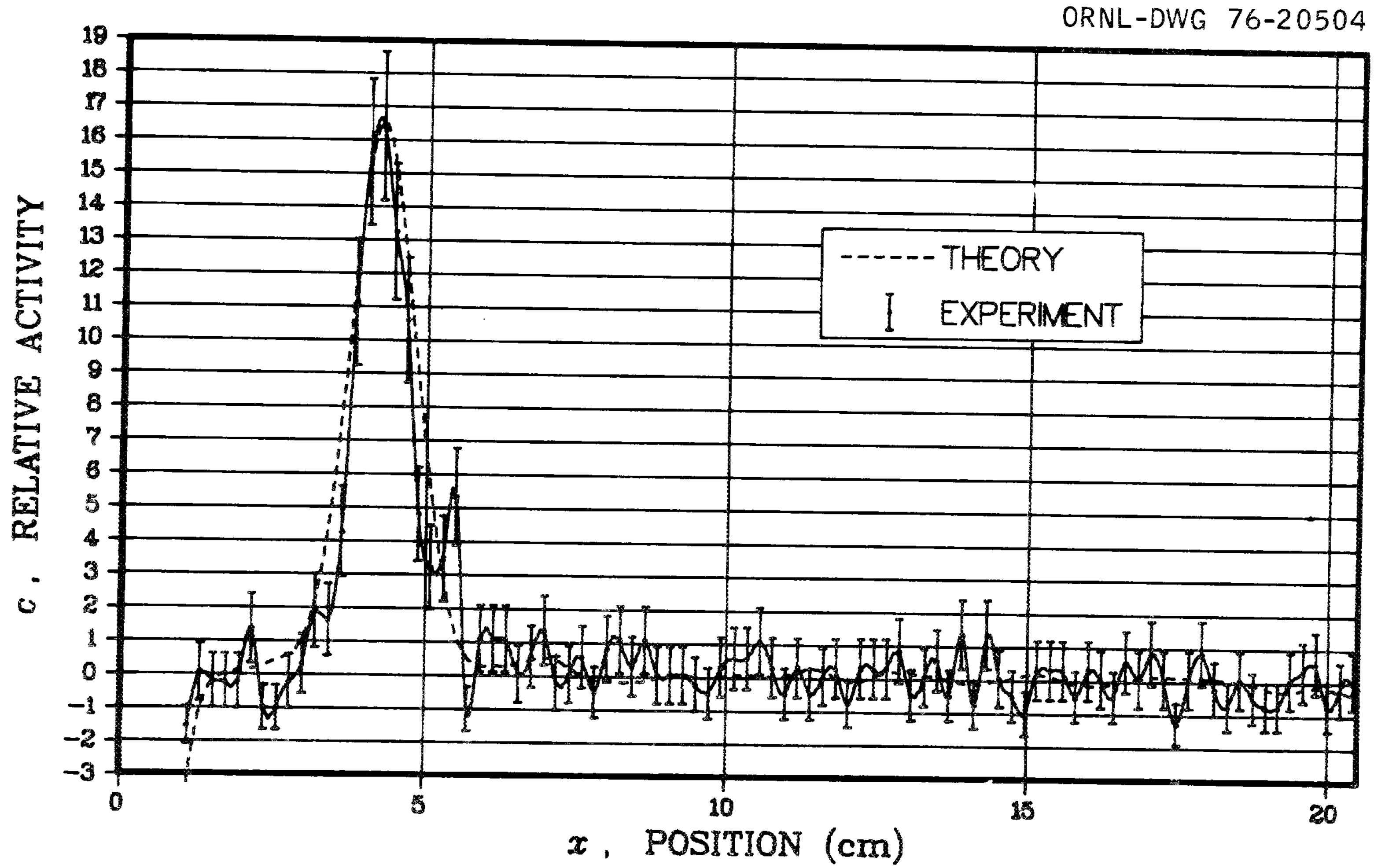

Fig. 27. ^{237}Pu distribution in Fuquay sand after two wettings with water.

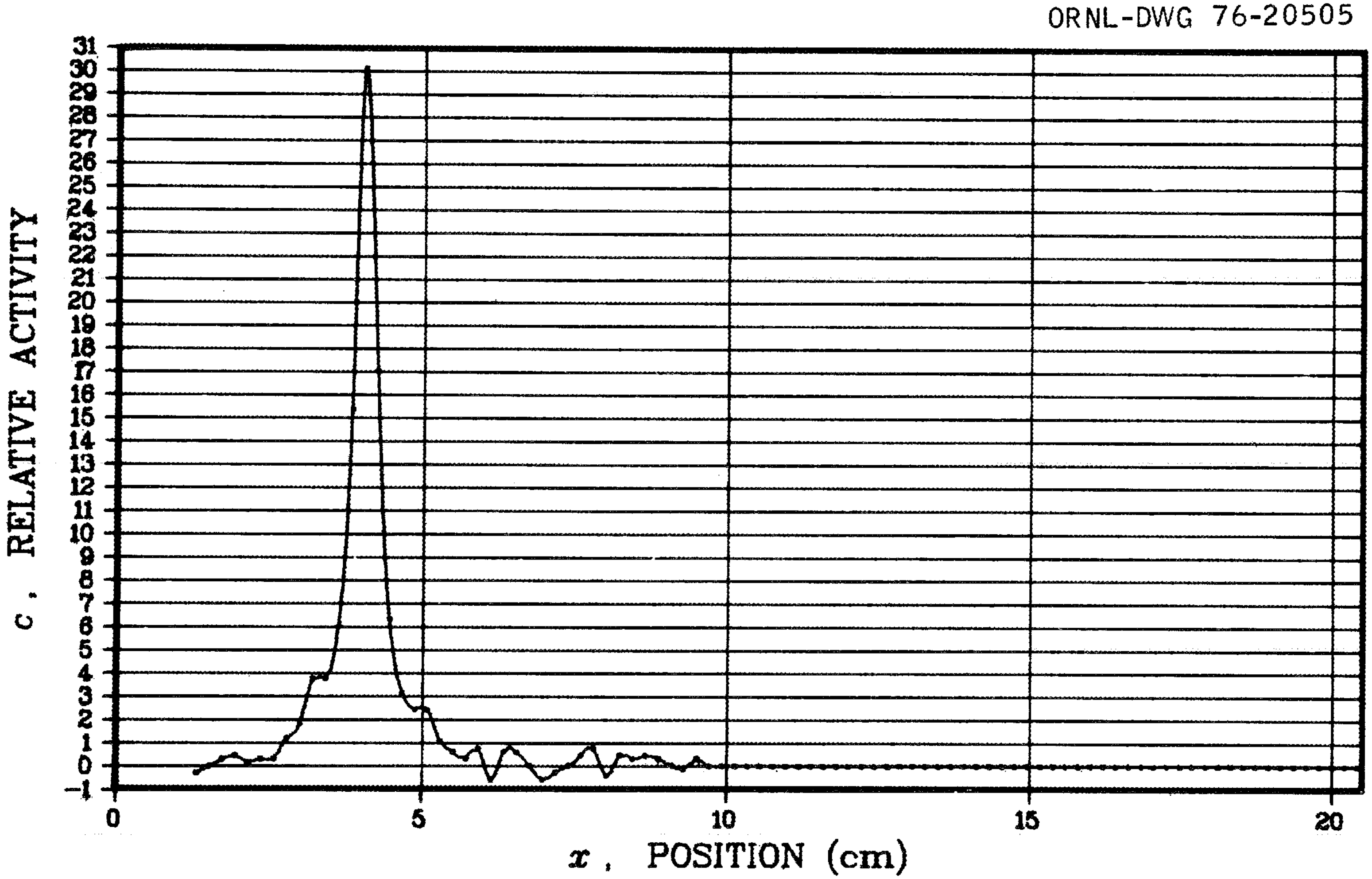

Fig. 28. ^{85}Sr distribution in Fuquay sand directly after spotting.

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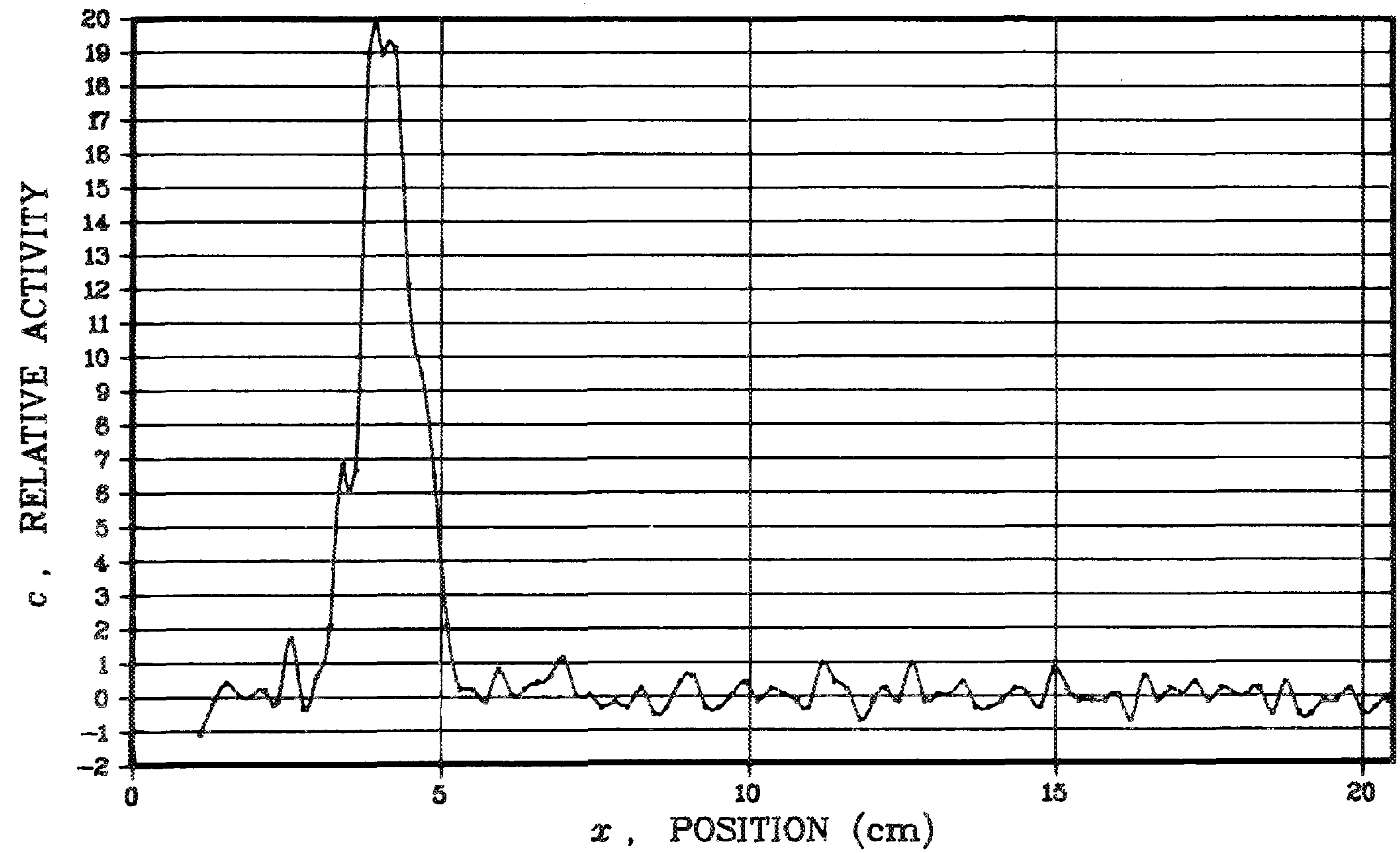

Fig. 29. ^{237}Pu distribution in Fuquay sand directly after spotting.

Mass-transport parameters obtained from our least-squares fitting procedure are shown in Table 2. Perhaps the most striking things about the values given pertain to the R_d determinations for ^{237}Pu. First, there is excellent agreement between the two wettings. Secondly, the magnitudes of these numbers is rather small compared to the value $k_d \sim 10^4$ cm^3/gm, which has appeared frequently in the literature. [See, for example, Prout, 1958.] Speciation, however, plays an important role in determining Pu mobilities [Bondietti, 1976] and appears to be a partial explanation of the phenomena observed here. Our suspension measurement of $k_d = 83$ cm^3/gm seems to confirm this explanation. However, it does raise another question regarding the difference between our chromatographic measurement of about 43 cm^3/gm and our suspension measurement reported above. The latter is larger than the former by a factor of about two. The explanation here appears to be that of reduced exchange between soil and soil solution in the chromatographic method relative to the suspension method.

A similar point may be made regarding the chromatographic measurements for ^{85}Sr reported in Table 2. The average value of the two distribution coefficients reported there is $k_d = 31$ cm^3/gm, which is substantially lower than our suspension measurement of $k_d = 85$ cm^3/gm. Here the latter is greater than the former by a factor of about three. Again the reduced exchange in the chromatographic measurement appears to be the reason. Prokhorov [1962] compared a flow-type determination to a suspension determination for the case of ^{90}Sr. He got 21 cm^3/gm for the former and 490 cm^3/gm for the latter with the numbers differing by a factor of about 23.

Figure 30 exhibits experimental and theoretical results for a 0.01 N $Ca(NO_3)_2$ eluting solution. Experimentally the peak moves rather than being distorted, as was the case when water was the eluting agent. The theory, however, is unable to account for this moving peak, as may be seen by comparing Fig. 30 with the initial condition shown in Fig. 28. The explanation pertains to the fact that there are here two competing ions, Ca^{++} and Sr^{++}. Calcium ions are exchanged with Sr ions, forcing the latter to move to a region in which Ca concentrations are weaker. A more general theory, like that of Rubin and James [1973], is called for here.

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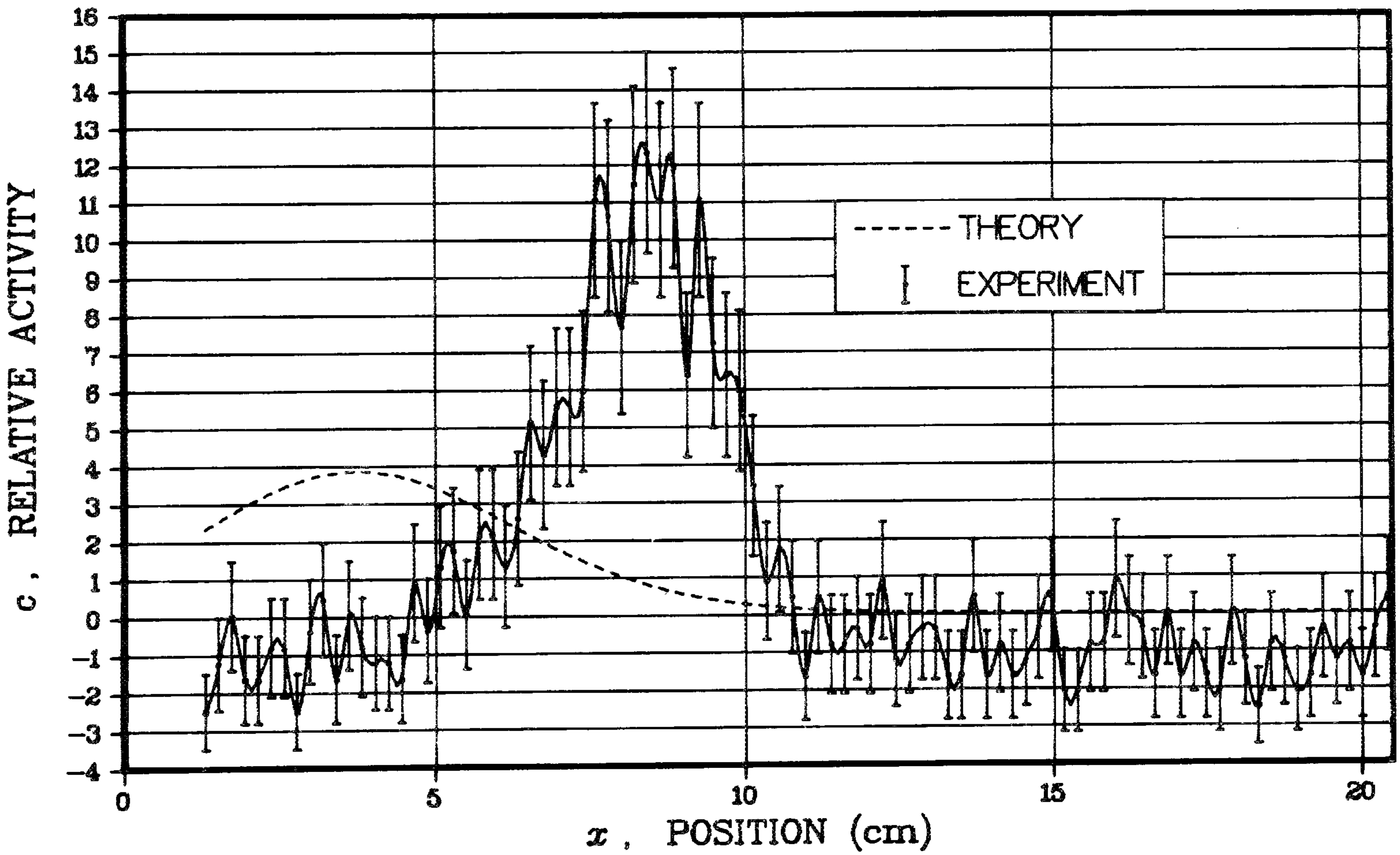

Fig. 30. ^{85}Sr distribution in Fuquay sand after one wetting with 0.01 N $Ca(NO_3)_2$.

VIII. CONCLUSIONS

This report documents our initial effort to quantify soil chromatography. Experimentally, a radiochromatographic scanner coupled to a multichannel analyzer is employed. These instruments provide the resolution, the sensitivity, and the numeric output necessary for computer analysis of the chromatographic profiles.

Theoretically, the chromatographic eluting process is perceived as a coupled flow of water and a dissolved constituent through a soil matrix. Solution procedures for solving the appropriate transport equations are developed and implemented. The end product here is a computer code capable of automatically analyzing the experimental data. This analysis consists in fitting the chromatographic profiles to determine several water- and mass-transport parameters, one of which is the distribution coefficient k_d.

The merit of the chromatographic method is that it simulates field conditions more accurately than do other techniques. This is very important for the determination of the distribution coefficient. Our results for ^{85}Sr and ^{237}Pu show that the reduced exchange inherent in a flow-type situation leads to k_d values which are lower than conventional suspension measurements by factors of three and two, respectively.

Finally the need for two refinements is noted. One pertains to experimental determination of the water transport. From a preliminary investigation it appears that a dissection method is the answer here. The other pertains to theoretical assessment of competing cations. In addition, a wider variety of soils, including slabs of porous rocks, is desired. Future research will focus on these areas.

IX. NOTATION

A	Acceleration parameter (dimensionless).
$[_rA]$	(2x2) matrix of integrals for r-th finite element (L).
a_L	Longitudinal dispersivity (L).
B	Reduction parameter (dimensionless).
$[_rB]$	(2x2) matrix of integrals for r-th finite element (L/T).
b	Dirichlet boundary condition for the concentration (M/L^3).
$[_rC]$	(2x2) matrix of integrals for r-th finite element (L/T).
$[C]$	Assembly of all $[_rC]$ (L/T).
c	Concentration of the dissolved constituent (M/L^3).
c'	Numerical approximation to c (M/L^3).
c_b	Bulk concentration including both dissolved and adsorbed constituents (M/L^3).
c_i	Concentration at node i (M/L^3).
$\{_rc\}$	(2x1) vector of concentration values at nodes of r-th element (M/L^3).
$\{c\}$	Vector of concentrations value at all nodes of the system (M/L^3).
D	Hydrodynamic dispersion (L^2/T).
d	Pore-size distribution index of the Gardner conductivity relation (dimensionless).
d'	Pore-size distribution index of the King moisture-characteristic function (dimensionless).
F	Moisture-storage function (L^{-1}).
f	Theoretical prediction either of water content (L^3/L^3) or concentration (M/L^3).
f^x	Experimental data either for water content (L^3/L^3) or concentration (M/L^3).
g	Transformed concentration (M/L^3).
h	Pressure head (L).
h_o	Critical-pressure parameter of the Gardner conductivity relation (L).
h'_o	Critical-pressure parameter of the King moisture-characteristic function (L).
I	Integral encountered in the relation $t(W_1)$ (T^2/L^2).
J	Integral encountered in the second-order solution of the water-transport equation (T).
$_rJ$	Jacobian for transformation to local coordinates (L).
K	Hydraulic conductivity (L/T).
K_s	Saturated conductivity parameter of the Gardner conducitvity relation (L/T).
K_0	$K(\theta = \theta_o)$ (L/T).

k_d	Saturated distribution coefficient (L^3/M).
L	Length of chromatographic column (L).
$\mathcal{L}$	Differential operator for mass-transport (dimensionless).
$\{N\}, N_i$	Basis functions (dimensionless).
N_t	Number of experimental times (dimensionless).
N_x	Number of experimental positions (dimensionless).
n	Porosity (L^3/L^3).
p_i	Theoretical parameter. May represent either moisture-transport or mass-transport parameter with its associated dimension (variable dimension).
$p, \bar{p}_i, \bar{p}'$	Vector of theoretical parameters (variable dimension).
Q	Diffusivity (L^2/T).
q^2	$a_L V/\theta R_d$, the effective diffusivity (L^2/T).
$\{R\}$	Vector obtained in numerical solution of mass-transport equation ($M/L^2/T$).
$\{_r R'\}$	(2x1) vector of values of the mass flux at the boundaries of the r-th element ($M/L^2/T$).
$\{R'\}$	Vector of mass-transport boundary flows ($M/L^2/T$).
R_d	Retardation factor (dimensionless).
S	Length of soil column (L).
s	Local variable of integration (dimensionless).
s_j	Value of s at j-th node, i.e. $s_1 = -1$ and $s_2 = 1$ (dimensionless).
s'	Solid-phase concentration of the adsorbed constituent (M/M).
T_p	Parameter step-size tolerance factor (dimensionless).
T_x	X^2 acceptance factor (dimensionless).
t	Time (T).
V	Darcy velocity (L/T).
v	$V/\theta R_d$, the effective velocity (L/T).
W	Reduced Darcy velocity (L/T).
$W^{(n)}$	The n-th approximation to the velocity solution of the water-transport equation (L/T).
W_1	$W(\alpha = 1)$ (L/T).
W_0	$W(\alpha = 0)$ (L/T).
X	Mass flux ($M/L^2/T$).
x	Position coordinate (L).

$x^{(n)}$	The n-th approximation to the position solution of the water-transport equation (L).
$\{Y\}$	$\{R\} - \{R'\}$, vector obtained in the numerical solution of the mass-transport equation ($M/L^2/T$).
α,β,γ	Reduced water content (dimensionless).
β'	Modified coefficient of compressibility (L^{-1}).
Δp_i	Parameter increment (variable dimension).
Δt	Time increment (T).
δ	$(\theta_1 - \theta_r)/(\theta_1 + \theta_r)$ (dimensionless).
ϵ	Angle of inclination of the chromatographic column (°).
θ	Moisture content (L^3/L^3).
θ_r	Residual moisture-content parameter (L^3/L^3).
θ_0	Initial moisture content (L^3/L^3).
θ_1	Boundary moisture content, equal to the porosity n in this document (L^3/L^3).
θ^x	Experimental water content (L^3/L^3).
κ	Reduced hydraulic conductivity (L/T).
λ	Decay constant (T^{-1}).
λ_m	Eigenvalues of transformed mass-transport equation (L^{-2}).
μ	Transformation parameter (L^{-1}).
δ'	$(\theta_1 - \theta)/(\theta_1 + \theta)$ (dimensionless).
ρ	Bulk density of the medium (M/L^3).
σ^x	Experimental measurement error either in water content (L^3/L^3) or in concentration (M/L^3).
X^2	Sum of weighted squares of residuals between experimental and theoretical points (dimensionless).
χ	Parameter of the King moisture-characteristic function, taken to be zero in this document (dimensionless).
ω	Time-integration parameter (dimensionless).
ω_m	Spatial frequency for eigenfunctions of concentrations (L^{-1}).

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APPENDIX A

EXAMPLE CALCULATION: ^{237}Pu IN FUQUAY SAND

INPUT

```
    7     1 PU, FUQUAY SAND, 1W
  101  100     1     0  150     2     0     0     0     1     1     0     0     3     1     2
     .075         0.5    3600.     1.00E5         .5          0.          20.          0.
      .5          0.
1000000000100000000010000000001000000000 100000000010000000000000100000001000000000
1000000000100000000 001000000000100000000 00100000000010000000001000000000100000000 0
0.         0.         0.         0.         0.
     1.105       1.315       1.525       1.735       1.945       2.155       2.365       2.575
     2.785       2.995       3.205       3.415       3.625       3.835       4.045       4.255
     4.465       4.675       4.885       5.095       5.305       5.515       5.725       5.935
     6.145       6.355       6.565       6.775       6.985       7.195       7.405       7.615
     7.825       8.035       8.245       8.455       8.665       8.875       9.085       9.295
     9.505       9.715       9.925      10.135      10.345      10.555      10.765      10.975
    11.185      11.395      11.605      11.815      12.025      12.235      12.445      12.655
    12.865      13.075      13.285      13.495      13.705      13.915      14.125      14.335
    14.545      14.755      14.965      15.175      15.385      15.595      15.805      16.015
    16.225      16.435      16.645      16.855      17.065      17.275      17.485      17.695
    17.905      18.115      18.325      18.535      18.745      18.955      19.165      19.375
    19.585      19.795      20.005      20.215      20.425      20.635      20.845      21.055
    21.265      21.475      21.685      21.895          0.
    -5.810      -0.810       2.190       0.190       0.190       1.190      -0.810       9.190
    -1.810       3.190      11.190      36.190      35.190     100.190     100.190     101.190
    64.190      50.190      34.190      11.190       1.190       1.190      -0.810       4.190
     0.190       1.190       2.190       3.190       6.190       0.190       0.190      -1.810
    -0.810      -1.810       1.190      -2.810      -1.810       2.190       3.190      -1.810
    -1.810       0.190       2.190      -0.810       1.190       0.190      -0.810      -1.810
     5.190       2.190       1.190      -3.810      -0.810       1.190      -0.810       5.190
    -0.810       0.190       0.190       2.190      -1.810      -1.810      -0.810       1.190
     0.190      -1.810       4.190       1.190      -0.810      -0.810      -0.810       0.190
    -3.810       3.190      -0.810       1.190       0.190       2.190      -0.810       1.190
     0.190       0.190       1.190      -2.810       2.190      -2.810      -2.810      -0.810
    -0.810       1.190      -2.810      -1.810      -0.810      -3.810      -3.810      -5.810
    -5.810      -5.810      -5.810      -5.810          0.
    1     0.
  101     0.
    0    37     0    41     3     3     4     8     2     0     1     1
.00625     .671       68.        .01
.000100    -49.9      1.78
.000397    -23.2      -.419
10.        20.        30.        40.        50.        60.        70.        80.
90.        .1         .2         .3         .4         .5         .6         .7
.8         .9         1.         2.         3.         4.         5.         6.
7.         8.         9.         10.        200.       300.       400.       500.
600.       700.       800.       900.       1000.
   11     3    30     3     1     1     1     0
1.5        0.25       1.E-10     1.E-10 0.1            1.
43.875     1.75       0.44191    .00625     0.625      .757E-4 -49.9     1.78
0.000397   -23.2      -0.419
    1     0     1     0     0     0     0     0     0     0     0
    1.E50      1.E50      1.E50 1.      1.                1.E50 -1.       5.0
    1.E50 -1.         -.1
1.         .5         .01        0.         0.                1.E-6 -150.      .5
   -1.E50 -500.       -.45
2400.
   92
     1.105       1.315       1.525       1.735       1.945       2.155       2.365       2.575
     2.785       2.995       3.206       3.415       3.625       3.835       4.045       4.255
     4.465       4.675       4.885       5.095       5.305       5.515       5.725       5.935
     6.145       6.355       6.565       6.775       6.985       7.195       7.405       7.615
     7.825       8.035       8.245       8.455       8.665       8.875       9.085       9.295
     9.505       9.715       9.925      10.135      10.345      10.555      10.765      10.975
    11.185      11.395      11.605      11.815      12.025      12.235      12.445      12.655
    12.865      13.075      13.286      13.495      13.705      13.915      14.125      14.335
    14.545      14.755      14.965      15.175      15.385      15.595      15.805      16.015
    16.225      16.435      16.646      16.855      17.065      17.275      17.485      17.695
    17.905      18.115      18.325      18.535      18.745      18.955      19.165      19.375
    19.585      19.795      20.005      20.215
    -5.810       1.190      -1.810      -1.810       1.190      -1.810       2.190      -0.810
     3.190       1.190      12.190      23.190      42.190      66.190      94.190     124.190
    88.190      33.190      31.190      29.190       8.190      11.190       7.190       2.190
     5.190       2.190      -0.810      -0.810      -5.810      -0.810       7.190       1.190
    -0.810       7.190       4.190       8.190       5.190       6.190      -0.810       6.190
     1.190      -0.810      -0.810       0.190       1.190       1.190      -0.810       7.190
     1.190       4.190      -2.810       1.190       1.190       5.190      -2.810       5.190
```

0.190	2.190	-0.810	-1.810	2.190	-1.810	-0.810	-2.810
4.190	1.190	2.190	-2.810	3.190	-1.810	1.190	1.190
3.190	0.190	-1.810	3.190	0.190	3.190	1.190	0.190
4.190	1.190	5.190	0.190	1.190	4.190	-4.810	-3.810
5.190	0.190	1.190	-3.810				
2.175	3.425	2.955	2.955	3.425	2.955	3.568	3.119
3.705	3.425	4.768	5.808	7.262	8.760	10.234	11.607
9.936	6.613	6.460	6.303	4.328	4.662	4.211	3.568
3.966	3.568	3.119	3.119	2.175	3.119	4.211	3.425
3.119	4.211	3.838	4.328	3.966	4.090	3.119	4.090
3.425	3.119	3.119	3.276	3.425	3.425	3.119	4.211
3.425	3.838	2.780	3.425	3.425	3.966	2.780	3.966
3.276	3.568	3.119	2.955	3.568	2.955	3.119	2.780
3.838	3.425	3.568	2.780	3.705	2.955	3.425	3.425
3.705	3.276	2.955	3.705	3.276	3.705	3.425	3.276
3.838	3.425	3.966	3.276	3.425	3.838	2.394	2.594
3.966	3.276	3.425	2.594				

2. 6.

OUTPUT

CALCULATION.. TYPE 7.. PROBLEM 1.. PU, FUQUAY SAND, IW

MATERIAL-TRANSPORT INPUT TABLE 1.. BASIC PARAMETERS

NUMBER OF NODAL POINTS.	101
NUMBER OF ELEMENTS.	100
NUMBER OF DIFFERENT MATERIALS	1
NUMBER OF CORRECTION MATERIALS.	0
NUMBER OF TIME INCREMENTS	150
NUMBER OF BOUNDARY CONDITIONS	2
NUMBER OF SURFACE TERMS	0
VELOCITY INPUT CONTROL.	0
AUXILIARY STORAGE CONTROL	0
STEADY-STATE CONTROL.	1
TIME-STEP CONTROL	1
NUMBER OF LOWER VARIABLY SIZED ELEMENTS	0
NUMBER OF UPPER VARIABLY SIZED ELEMENTS	0
NORSETT TIME INTEGRATION INDEX.	3
INITIAL-CONDITION CONTROL	1
MESH CONTROL.	2
TIME INCREMENT.	0.7500D-01
MULTIPLIER FOR INCREASING DELT.	0.500000
MAXIMUM VALUE OF DELT	0.3600D 04
MAXIMUM VALUE OF TIME	0.1000D 51
TIME-INTEGRATION PARAMETER.	0.500000
ORIGIN OF MESH GENERATION	0.0
MAXIMUM X-VALUE	20.0000
LOWER FIRST X-INCREMENT	0.0
UPPER FIRST X-INCREMENT	0.5000
CONSTANT DARCY VELOCITY	0.0

OUTPUT CONTROL

1000000000100000000010000000001000000000100000000010000000000001000000100000000010000000001000000001
00000000010000000001000000000100000000001000000001

MATERIAL-TRANSPORT INPUT TABLE 2.. MATERIAL PROPERTIES

MAT. NO.	KD	RHOB	AL	THETAR	POR
1	0.0	0.0	0.0	0.0	0.0

MATERIAL-TRANSPORT TABLE 3.. NODAL-POINT DATA

NODE	X
1	0.0
2	0.1105D 01
3	0.1315D 01
4	0.1525D 01
5	0.1735D 01
6	0.1945D 01
7	0.2155D 01
8	0.2365D 01
9	0.2575D 01
10	0.2785D 01
11	0.2995D 01
12	0.3205D 01
13	0.3415D 01
14	0.3625D 01
15	0.3835D 01
16	0.4045D 01
17	0.4255D 01
18	0.4465D 01

19	0.4675D 01
20	0.4885D 01
21	0.5095D 01
22	0.5305D 01
23	0.5515D 01
24	0.5725D 01
25	0.5935D 01
26	0.6145D 01
27	0.6355D 01
28	0.6565D 01
29	0.6775D 01
30	0.6985D 01
31	0.7195D 01
32	0.7405D 01
33	0.7615D 01
34	0.7825D 01
35	0.8035D 01
36	0.8245D 01
37	0.8455D 01
38	0.8665D 01
39	0.8875D 01
40	0.9085D 01
41	0.9295D 01
42	0.9505D 01
43	0.9715D 01
44	0.9925D 01
45	0.1014D 02
46	0.1035D 02
47	0.1056D 02
48	0.1077D 02
49	0.1098D 02
50	0.1119D 02
51	0.1140D 02
52	0.1161D 02
53	0.1182D 02
54	0.1203D 02
55	0.1224D 02
56	0.1245D 02
57	0.1266D 02
58	0.1287D 02
59	0.1308D 02
60	0.1329D 02
61	0.1350D 02
62	0.1371D 02
63	0.1392D 02
64	0.1413D 02
65	0.1434D 02
66	0.1455D 02
67	0.1476D 02
68	0.1497D 02
69	0.1518D 02
70	0.1539D 02
71	0.1560D 02
72	0.1581D 02
73	0.1602D 02
74	0.1623D 02
75	0.1644D 02
76	0.1665D 02
77	0.1686D 02
78	0.1707D 02
79	0.1728D 02
00	0.1749D 02
81	0.1770D 02
82	0.1791D 02
83	0.1812D 02
84	0.1833D 02
85	0.1854D 02
86	0.1875D 02
87	0.1896D 02
88	0.1917D 02
89	0.1938D 02
90	0.1959D 02
91	0.1980D 02
92	0.2001D 02
93	0.2022D 02

94	0.2043D 02
95	0.2064D 02
96	0.2085D 02
97	0.2106D 02
98	0.2127D 02
99	0.2148D 02
100	0.2169D 02
101	0.2190D 02

MATERIAL-TRANSPORT TABLE 4.. ELEMENT DATA

	GLOBAL INDICES OF ELEMENT NODES			
ELEMENT	1	2	MATERIAL	NODE DIFF.
1	1	2	1	1
2	2	3	1	1
3	3	4	1	1
4	4	5	1	1
5	5	6	1	1
6	6	7	1	1
7	7	8	1	1
8	8	9	1	1
9	9	10	1	1
10	10	11	1	1
11	11	12	1	1
12	12	13	1	1
13	13	14	1	1
14	14	15	1	1
15	15	16	1	1
16	16	17	1	1
17	17	18	1	1
18	18	19	1	1
19	19	20	1	1
20	20	21	1	1
21	21	22	1	1
22	22	23	1	1
23	23	24	1	1
24	24	25	1	1
25	25	26	1	1
26	26	27	1	1
27	27	28	1	1
28	28	29	1	1
29	29	30	1	1
30	30	31	1	1
31	31	32	1	1
32	32	33	1	1
33	33	34	1	1
34	34	35	1	1
35	35	36	1	1
36	36	37	1	1
37	37	38	1	1
38	38	39	1	1
39	39	40	1	1
40	40	41	1	1
41	41	42	1	1
42	42	43	1	1
43	43	44	1	1
44	44	45	1	1
45	45	46	1	1
46	46	47	1	1
47	47	48	1	1
48	48	49	1	1
49	49	50	1	1
50	50	51	1	1
51	51	52	1	1
52	52	53	1	1
53	53	54	1	1
54	54	55	1	1
55	55	56	1	1
56	56	57	1	1
57	57	58	1	1
58	58	59	1	1
59	59	60	1	1

60	60	61	1	1
61	61	62	1	1
62	62	63	1	1
63	63	64	1	1
64	64	65	1	1
65	65	66	1	1
66	66	67	1	1
67	67	68	1	1
68	68	69	1	1
69	69	70	1	1
70	70	71	1	1
71	71	72	1	1
72	72	73	1	1
73	73	74	1	1
74	74	75	1	1
75	75	76	1	1
76	76	77	1	1
77	77	78	1	1
78	78	79	1	1
79	79	80	1	1
80	80	81	1	1
81	81	82	1	1
82	82	83	1	1
83	83	84	1	1
84	84	85	1	1
85	85	86	1	1
86	86	87	1	1
87	87	88	1	1
88	88	89	1	1
89	89	90	1	1
90	90	91	1	1
91	91	92	1	1
92	92	93	1	1
93	93	94	1	1
94	94	95	1	1
95	95	96	1	1
96	96	97	1	1
97	97	98	1	1
98	98	99	1	1
99	99	100	1	1
100	100	101	1	1

MATERIAL-TRANSPORT INPUT TABLE 5.. BOUNDARY CONDITIONS OF FORM R=BB

NODE	BB
1	0.0
101	0.0

WATER-TRANSPORT INPUT TABLE 8.. BASIC PARAMETERS

FUNCTION TYPE	2
NUMBER OF TABULAR TIME NODES.	37
NUMBER OF TIME NODES FOR STAND-ALONE OPERATION.	0
NUMBER OF THETA VALUES.	41
NUMBER OF CONDUCTIVITY SOIL PARAMETERS.	3
NUMBER OF CAPACITY OR DIFFUSIVITY SOIL PARAMETERS . . .	3
ORDER OF LEGENDRE-GAUSS INTEGRATION	4
ORDER NEAR ALPHA = 1.	8
NUMBER OF POINTS IN INTERPOLATING POLYNOMIAL.	2
AUXILIARY STORAGE CONTROL	0
VARIABLE-MESH CONTROL	1
ANALYTIC SOIL-PROPERTIES CONTROL.	1
INITIAL CONDITION ON WATER CONTENT THETA.	0.6250D-02
BOUNDARY CONDITION ON WATER CONTENT THETA	0.6710D 00
INCLINATION IN DEGREES.	0.6800D 02
ALPHA INCREMENT NEAR ALPHA = 1.	0.1000D-01

AKPAR:
0.1000000D-03 -0.4990000D 02 0.1780000D 01

```
CDPAR:
 0.3970000D-03 -0.2320000D 02 -0.4190000D 00

V1/AKSAT:
 0.1000000D 02  0.2000000D 02  0.3000000D 02  0.4000000D 02  0.5000000D 02  0.6000000D 02  0.7000000D 02  0.8000000D 02
 0.9000000D 02  0.1000000D 00  0.2000000D 00  0.3000000D 00  0.4000000D 00  0.5000000D 00  0.6000000D 00  0.7000000D 00
 0.8000000D 00  0.9000000D 00  0.1000000D 01  0.2000000D 01  0.3000000D 01  0.4000000D 01  0.5000000D 01  0.6000000D 01
 0.7000000D 01  0.8000000D 01  0.9000000D 01  0.1000000D 02  0.2000000D 03  0.3000000D 03  0.4000000D 03  0.5000000D 03
 0.6000000D 03  0.7000000D 03  0.8000000D 03  0.9000000D 03  0.1000000D 04


SEARCH INPUT TABLE 1.. BASIC PARAMETERS

     NUMBER OF SEARCH PARAMETERS . . . . . . . . . . . . . . .   11
     DIAGNOSTIC PRINTER CONTROL. . . . . . . . . . . . . . . .    3
     MAXIMUM CHI-SQUARED EVALUATIONS . . . . . . . . . . . . .   30
     WEIGHT-CONTROL INTEGER. . . . . . . . . . . . . . . . . .    3
     NUMBER OF EXPERIMENTAL TIME NODES . . . . . . . . . . . .    1
     PARAMETER BOUNDS CONTROL. . . . . . . . . . . . . . . . .    1
     NUMBER OF SEARCH CYCLES . . . . . . . . . . . . . . . . .    1
     AUXILIARY STORAGE CONTROL . . . . . . . . . . . . . . . .    0
     ACCELERATION PARAMETER. . . . . . . . . . . . . . . 0.1500D 01
     REDUCTION PARAMETER . . . . . . . . . . . . . . . . 0.2500D 00
     STEP-SIZE TOLERANCE . . . . . . . . . . . . . . . . 0.1000D-09
     CHI-SQUARE ACCEPTANCE FACTOR. . . . . . . . . . . . 0.1000D-09
     PARAMETER STEP-LENGTH FRACTION. . . . . . . . . . . 0.1000D 00
     WEIGHTING CONSTANT. . . . . . . . . . . . . . . . . 0.1000D 01


SEARCH INPUT TABLE 3.. EXPERIMENTAL DATA

     TABLE AT TIME =0.2400D 04
```

IX	XX	YX	WX
1	0.11050D 01	-0.10076D 01	0.0
2	0.13150D 01	0.20638D 00	0.0
3	0.15250D 01	-0.31390D 00	0.0
4	0.17350D 01	-0.31390D 00	0.0
5	0.19450D 01	0.20638D 00	0.0
6	0.21550D 01	-0.31390D 00	0.38076D 01
7	0.23650D 01	0.37981D 00	0.26116D 01
8	0.25750D 01	-0.14048D 00	0.34177D 01
9	0.27850D 01	0.55323D 00	0.24221D 01
10	0.29950D 01	0.20638D 00	0.28343D 01
11	0.32050D 01	0.21141D 01	0.14625D 01
12	0.34150D 01	0.40218D 01	0.98562D 00
13	0.36250D 01	0.73169D 01	0.63045D 00
14	0.38350D 01	0.11479D 02	0.43327D 00
15	0.40450D 01	0.16335D 02	0.31745D 00
16	0.42550D 01	0.21538D 02	0.24679D 00
17	0.44650D 01	0.15295D 02	0.33678D 00
18	0.46750D 01	0.57561D 01	0.76027D 00
19	0.48850D 01	0.54092D 01	0.79671D 00
20	0.50950D 01	0.50623D 01	0.83689D 00
21	0.53050D 01	0.14204D 01	0.17750D 01
22	0.55150D 01	0.19407D 01	0.15297D 01
23	0.57250D 01	0.12469D 01	0.18750D 01
24	0.59350D 01	0.37981D 00	0.26116D 01
25	0.61450D 01	0.90009D 00	0.0
26	0.63550D 01	0.37981D 00	0.0
27	0.65650D 01	-0.14048D 00	0.0
28	0.67750D 01	-0.14048D 00	0.0
29	0.69850D 01	-0.10076D 01	0.0
30	0.71950D 01	-0.14048D 00	0.0
31	0.74050D 01	0.12469D 01	0.0
32	0.76150D 01	0.20638D 00	0.0
33	0.78250D 01	-0.14048D 00	0.0
34	0.80350D 01	0.12469D 01	0.0
35	0.82450D 01	0.72666D 00	0.0
36	0.84550D 01	0.14204D 01	0.0

37	0.86650D 01	0.90009D 00	0.0
38	0.88750D 01	0.10735D 01	0.0
39	0.90850D 01	-0.14048D 00	0.0
40	0.92950D 01	0.10735D 01	0.0
41	0.95050D 01	0.20638D 00	0.0
42	0.97150D 01	-0.14048D 00	0.0
43	0.98250D 01	-0.14048D 00	0.0
44	0.10135D 02	0.32951D-01	0.0
45	0.10345D 02	0.20638D 00	0.0
46	0.10555D 02	0.20638D 00	0.0
47	0.10765D 02	-0.14048D 00	0.0
48	0.10975D 02	0.12469D 01	0.0
49	0.11185D 02	0.20638D 00	0.0
50	0.11395D 02	0.72666D 00	0.0
51	0.11605D 02	-0.48733D 00	0.0
52	0.11815D 02	0.20638D 00	0.0
53	0.12025D 02	0.20638D 00	0.0
54	0.12235D 02	0.90009D 00	0.0
55	0.12445D 02	-0.48733D 00	0.0
56	0.12655D 02	0.90009D 00	0.0
57	0.12865D 02	0.32951D-01	0.0
58	0.13075D 02	0.37981D 00	0.0
59	0.13285D 02	-0.14048D 00	0.0
60	0.13495D 02	-0.31390D 00	0.0
61	0.13705D 02	0.37981D 00	0.0
62	0.13915D 02	-0.31390D 00	0.0
63	0.14125D 02	-0.14048D 00	0.0
64	0.14335D 02	-0.48733D 00	0.0
65	0.14545D 02	0.72666D 00	0.0
66	0.14755D 02	0.20638D 00	0.0
67	0.14965D 02	0.37981D 00	0.0
68	0.15175D 02	-0.48733D 00	0.0
69	0.15385D 02	0.55323D 00	0.0
70	0.15595D 02	-0.31390D 00	0.0
71	0.15805D 02	0.20638D 00	0.0
72	0.16015D 02	0.20638D 00	0.0
73	0.16225D 02	0.55323D 00	0.0
74	0.16435D 02	0.32951D-01	0.0
75	0.16645D 02	-0.31390D 00	0.0
76	0.16855D 02	0.55323D 00	0.0
77	0.17065D 02	0.32951D-01	0.0
78	0.17275D 02	0.55323D 00	0.0
79	0.17485D 02	0.20638D 00	0.0
80	0.17695D 02	0.32951D-01	0.0
81	0.17905D 02	0.72666D 00	0.0
82	0.18115D 02	0.20638D 00	0.0
83	0.18325D 02	0.90009D 00	0.0
84	0.18535D 02	0.32951D-01	0.0
85	0.18745D 02	0.20638D 00	0.0
86	0.18955D 02	0.72666D 00	0.0
87	0.19165D 02	-0.83419D 00	0.0
88	0.19375D 02	-0.66076D 00	0.0
89	0.19585D 02	0.90009D 00	0.0
90	0.19795D 02	0.32951D-01	0.0
91	0.20005D 02	0.20638D 00	0.0
92	0.20215D 02	-0.66076D 00	0.0

SEARCH INPUT TABLE 2.. INITIAL VALUES OF PARAMETERS, LIMITS, AND INCREMENTS

IP	P	PH	PL	DP
1	0.43875D 02	0.10000D 51	0.10000D 01	0.43875D 01
2	0.17500D 01	0.17500D 01	0.17500D 01	0.17500D 00
3	0.44191D 00	0.10000D 51	0.10000D-01	0.44191D-01
4	0.62500D-02	0.62500D-02	0.62500D-02	0.62500D-03
5	0.62500D 00	0.62500D 00	0.62500D 00	0.62500D-01
6	0.75700D-04	0.75700D-04	0.75700D-04	0.75700D-05
7	-0.49900D 02	-0.49900D 02	-0.49900D 02	-0.49900D 01
8	0.17800D 01	0.17800D 01	0.17800D 01	0.17800D 00
9	0.39700D-03	0.39700D-03	0.39700D-03	0.39700D-04
10	-0.23200D 02	-0.23200D 02	-0.23200D 02	-0.23200D 01
11	-0.41900D 00	-0.41300D 00	-0.41900D 00	-0.41900D-01

```
NP      NFUN                 ACC        RED        TOLSTP        TOLFUN
11       30                1.5000     0.2500     0.100D-09     0.100D-09
         PH                  P                    PL
     0.1000000D 51     0.4387500D 02     0.1000000D 01
     0.1750000D 01     0.1750000D 01     0.1750000D 01
     0.1000000D 51     0.4419100D 00     0.1000000D-01
     0.6250000D-02     0.6250000D-02     0.6250000D-02
     0.6250000D 00     0.6250000D 00     0.6250000D 00
     0.7570000D-04     0.7570000D-04     0.7570000D-04
    -0.4990000D 02    -0.4990000D 02    -0.4990000D 02
     0.1780000D 01     0.1780000D 01     0.1780000D 01
     0.3970000D-03     0.3970000D-03     0.3970000D-03
    -0.2320000D 02    -0.2320000D 02    -0.2320000D 02
    -0.4190000D 00    -0.4190000D 00    -0.4190000D 00
NFUN=     1
*    0.3916939D 02     0.4387500D 02  0.1750000D 01  0.4419100D 00  0.6250000D-02  0.6250000D 00  0.7570000D-04 -0.4990000D 02
                      0.1780000D 01  0.3970000D-03 -0.2320000D 02 -0.4190000D 00
DELP                   0.4387500D 01  0.0             0.4419100D-01  0.0             0.0             0.0             0.0
                      0.0            0.0             0.0             0.0
BEGIN EXPLORATORY LOOP
INCREMENT THE I-TH VARIABLE
F 1  0.3834348D 02     0.4826250D 02  0.1750000D 01  0.4419100D 00  0.6250000D-02  0.6250000D 00  0.7570000D-04 -0.4990000D 02
                       0.1780000D 01  0.3970000D-03 -0.2320000D 02 -0.4190000D 00
ACCELERATE THE STEP SIZE
INCREMENT THE I-TH VARIABLE
F 3  0.3936946D 02     0.4826250D 02  0.1750000D 01  0.4861010D 00  0.6250000D-02  0.6250000D 00  0.7570000D-04 -0.4990000D 02
                       0.1780000D 01  0.3970000D-03 -0.2320000D 02 -0.4190000D 00
DECREMENT THE I-TH VARIABLE
R 3  0.3740409D 02     0.4826250D 02  0.1750000D 01  0.3977190D 00  0.6250000D-02  0.6250000D 00  0.7570000D-04 -0.4990000D 02
                       0.1780000D 01  0.3970000D-03 -0.2320000D 02 -0.4190000D 00
DECREMENT THE I-TH VARIABLE
ACCEPT NEW POINT
AFTER     4 NFUN A NEW BASE PT. - START PATTERN MOVE
RESULT OF PATTERN MOVE
P    0.3629755D 02     0.5265000D 02  0.1750000D 01  0.3535280D 00  0.6250000D-02  0.6250000D 00  0.7570000D-04 -0.4990000D 02
                       0.1780000D 01  0.3970000D-03 -0.2320000D 02 -0.4190000D 00
NFUN=     5
*    0.3740409D 02     0.4826260D 02  0.1750000D 01  0.3977190D 00  0.6250000D-02  0.6250000D 00  0.7570000D-04 -0.4990000D 02
                      0.1780000D 01  0.3970000D-03 -0.2320000D 02 -0.4190000D 00
DELP                   0.6581250D 01  0.0            -0.6628650D-01  0.0             0.0             0.0             0.0
                      0.0            0.0             0.0             0.0
BEGIN EXPLORATORY LOOP
INCREMENT THE I-TH VARIABLE
F 1  0.3619816D 02     0.5923125D 02  0.1750000D 01  0.3535280D 00  0.6250000D-02  0.6250000D 00  0.7570000D-04 -0.4990000D 02
                       0.1780000D 01  0.3970000D-03 -0.2320000D 02 -0.4190000D 00
INCREMENT THE I-TH VARIABLE
F 3  0.3567872D 02     0.5923125D 02  0.1750000D 01  0.2872415D 00  0.6250000D-02  0.6250000D 00  0.7570000D-04 -0.4990000D 02
                       0.1780000D 01  0.3970000D-03 -0.2320000D 02 -0.4190000D 00
ACCEPT NEW POINT
AFTER     7 NFUN A NEW BASE PT. - START PATTERN MOVE
RESULT OF PATTERN MOVE
P    0.3776559D 02     0.7020000D 02  0.1750000D 01  0.1767640D 00  0.6250000D-02  0.6250000D 00  0.7570000D-04 -0.4990000D 02
                       0.1780000D 01  0.3970000D-03 -0.2320000D 02 -0.4190000D 00
NFUN=     8
*    0.3567872D 02     0.5923125D 02  0.1750000D 01  0.2872415D 00  0.6250000D-02  0.6250000D 00  0.7570000D-04 -0.4990000D 02
                      0.1780000D 01  0.3970000D-03 -0.2320000D 02 -0.4190000D 00
DELP                   0.6581250D 01  0.0            -0.6628650D-01  0.0             0.0             0.0             0.0
                      0.0            0.0             0.0             0.0
BEGIN EXPLORATORY LOOP
INCREMENT THE I-TH VARIABLE
F 1  0.3874343D 02     0.7678125D 02  0.1750000D 01  0.1767640D 00  0.6250000D-02  0.6250000D 00  0.7570000D-04 -0.4990000D 02
                       0.1780000D 01  0.3970000D-03 -0.2320000D 02 -0.4190000D 00
DECREMENT THE I-TH VARIABLE
R 1  0.3681042D 02     0.6361875D 02  0.1750000D 01  0.1767640D 00  0.6250000D-02  0.6250000D 00  0.7570000D-04 -0.4990000D 02
                       0.1780000D 01  0.3970000D-03 -0.2320000D 02 -0.4190000D 00
INCREMENT THE I-TH VARIABLE
F 3  0.3974768D 02     0.6361875D 02  0.1750000D 01  0.1104775D 00  0.6250000D-02  0.6250000D 00  0.7570000D-04 -0.4990000D 02
                       0.1780000D 01  0.3970000D-03 -0.2320000D 02 -0.4190000D 00
DECREMENT THE I-TH VARIABLE
R 3  0.3596435D 02     0.6361875D 02  0.1750000D 01  0.2430505D 00  0.6250000D-02  0.6250000D 00  0.7570000D-04 -0.4990000D 02
                       0.1780000D 01  0.3970000D-03 -0.2320000D 02 -0.4190000D 00
PATTERN MODE EXPLORATORY FAILURE RESTORE BASE PT.
```

```
NFUN=    12
*     0.3567872D 02     0.5923125D 02  0.1750000D 01  0.2872415D 00  0.6250000D-02  0.6250000D 00  0.7570000D-04 -0.4990000D 02
                        0.1780000D 01  0.3970000D-03 -0.2320000D 02 -0.4190000D 00
DELP                    0.6581250D 01  0.0           -0.6628650D-01  0.0            0.0            0.0            0.0
                        0.0            0.0            0.0            0.0
BEGIN EXPLORATORY LOOP
INCREMENT THE I-TH VARIABLE
F 1  0.3605899D 02      0.6581250D 02  0.1750000D 01  0.2872415D 00  0.6250000D-02  0.6250000D 00  0.7570000D-04 -0.4990000D 02
                        0.1780000D 01  0.3970000D-03 -0.2320000D 02 -0.4190000D 00
DECREMENT THE I-TH VARIABLE
R 1  0.3549282D 02      0.5265000D 02  0.1750000D 01  0.2872415D 00  0.6250000D-02  0.6250000D 00  0.7570000D-04 -0.4990000D 02
                        0.1780000D 01  0.3970000D-03 -0.2320000D 02 -0.4190000D 00
DECREMENT THE I-TH VARIABLE
INCREMENT THE I-TH VARIABLE
F 3  0.3515897D 02      0.5265000D 02  0.1750000D 01  0.2209550D 00  0.6250000D-02  0.6250000D 00  0.7570000D-04 -0.4990000D 02
                        0.1780000D 01  0.3970000D-03 -0.2320000D 02 -0.4190000D 00
ACCELERATE THE STEP SIZE
ACCEPT NEW POINT
AFTER    15 NFUN A NEW BASE PT. - START PATTERN MOVE
RESULT OF PATTERN MOVE
P     0.3508262D 02     0.4606875D 02  0.1750000D 01  0.1546685D 00  0.6250000D-02  0.6250000D 00  0.7570000D-04 -0.4990000D 02
                        0.1780000D 01  0.3970000D-03 -0.2320000D 02 -0.4190000D 00
NFUN=    16
*     0.3515897D 02     0.5265000D 02  0.1750000D 01  0.2209550D 00  0.6250000D-02  0.6250000D 00  0.7570000D-04 -0.4990000D 02
                        0.1780000D 01  0.3970000D-03 -0.2320000D 02 -0.4190000D 00
DELP                   -0.9871875D 01  0.0           -0.9942975D-01  0.0            0.0            0.0            0.0
                        0.0            0.0            0.0            0.0
BEGIN EXPLORATORY LOOP
INCREMENT THE I-TH VARIABLE
F 1  0.3512234D 02      0.3619688D 02  0.1750000D 01  0.1546685D 00  0.6250000D-02  0.6250000D 00  0.7570000D-04 -0.4990000D 02
                        0.1780000D 01  0.3970000D-03 -0.2320000D 02 -0.4190000D 00
DECREMENT THE I-TH VARIABLE
R 1  0.3625620D 02      0.5594062D 02  0.1750000D 01  0.1546685D 00  0.6250000D-02  0.6250000D 00  0.7570000D-04 -0.4990000D 02
                        0.1780000D 01  0.3970000D-03 -0.2320000D 02 -0.4190000D 00
INCREMENT THE I-TH VARIABLE
F 3  0.4202390D 02      0.4606875D 02  0.1750000D 01  0.5523875D-01  0.6250000D-02  0.6250000D 00  0.7570000D-04 -0.4990000D 02
                        0.1780000D 01  0.3970000D-03 -0.2320000D 02 -0.4190000D 00
DECREMENT THE I-TH VARIABLE
R 3  0.3522319D 02      0.4606875D 02  0.1750000D 01  0.2540983D 00  0.6250000D-02  0.6250000D 00  0.7570000D-04 -0.4990000D 02
                        0.1780000D 01  0.3970000D-03 -0.2320000D 02 -0.4190000D 00
ACCEPT NEW POINT
AFTER    20 NFUN A NEW BASE PT. - START PATTERN MOVE
RESULT OF PATTERN MOVE
P     0.3665806D 02     0.3948750D 02  0.1750000D 01  0.8838200D-01  0.6250000D-02  0.6250000D 00  0.7570000D-04 -0.4990000D 02
                        0.1780000D 01  0.3970000D-03 -0.2320000D 02 -0.4190000D 00
NFUN=    21
*     0.3508262D 02     0.4606875D 02  0.1750000D 01  0.1546685D 00  0.6250000D-02  0.6250000D 00  0.7570000D-04 -0.4990000D 02
                        0.1780000D 01  0.3970000D-03 -0.2320000D 02 -0.4190000D 00
DELP                   -0.9871875D 01  0.0           -0.9942975D-01  0.0            0.0            0.0            0.0
                        0.0            0.0            0.0            0.0
BEGIN EXPLORATORY LOOP
INCREMENT THE I-TH VARIABLE
F 1  0.3722692D 02      0.2961562D 02  0.1750000D 01  0.8838200D-01  0.6250000D-02  0.6250000D 00  0.7570000D-04 -0.4990000D 02
                        0.1780000D 01  0.3970000D-03 -0.2320000D 02 -0.4190000D 00
DECREMENT THE I-TH VARIABLE
R 1  0.3843772D 02      0.4935937D 02  0.1750000D 01  0.8838200D-01  0.6250000D-02  0.6250000D 00  0.7570000D-04 -0.4990000D 02
                        0.1780000D 01  0.3970000D-03 -0.2320000D 02 -0.4190000D 00
DECREMENT THE I-TH VARIABLE
R 3  0.3494490D 02      0.3948750D 02  0.1750000D 01  0.1878118D 00  0.6250000D-02  0.6250000D 00  0.7570000D-04 -0.4990000D 02
                        0.1780000D 01  0.3970000D-03 -0.2320000D 02 -0.4190000D 00
ACCEPT NEW POINT
AFTER    24 NFUN A NEW BASE PT. - START PATTERN MOVE
RESULT OF PATTERN MOVE
P     0.3678156D 02     0.3290625D 02  0.1750000D 01  0.2209550D 00  0.6250000D-02  0.6250000D 00  0.7570000D-04 -0.4990000D 02
                        0.1780000D 01  0.3970000D-03 -0.2320000D 02 -0.4190000D 00
NFUN=    25
*     0.3494490D 02     0.3948750D 02  0.1750000D 01  0.1878118D 00  0.6250000D-02  0.6250000D 00  0.7570000D-04 -0.4990000D 02
                        0.1780000D 01  0.3970000D-03 -0.2320000D 02 -0.4190000D 00
DELP                   -0.9871875D 01  0.0            0.9942975D-01  0.0            0.0            0.0            0.0
                        0.0            0.0            0.0            0.0
BEGIN EXPLORATORY LOOP
INCREMENT THE I-TH VARIABLE
F 1  0.4473127D 02      0.2303437D 02  0.1750000D 01  0.2209550D 00  0.6250000D-02  0.6250000D 00  0.7570000D-04 -0.4990000D 02
                        0.1780000D 01  0.3970000D-03 -0.2320000D 02 -0.4190000D 00
DECREMENT THE I-TH VARIABLE
```

```
R 1  0.3501327D 02    0.4277812D 02  0.1750000D 01  0.2209550D 00  0.6250000D-02  0.6250000D 00  0.7570000D-04 -0.4990000D 02
                      0.1780000D 01  0.3970000D-03 -0.2320000D 02 -0.4190000D 00
INCREMENT THE I-TH VARIABLE
F 3  0.3655449D 02    0.4277812D 02  0.1750000D 01  0.3203848D 00  0.6250000D-02  0.6250000D 00  0.7570000D-04 -0.4990000D 02
                      0.1780000D 01  0.3970000D-03 -0.2320000D 02 -0.4190000D 00
DECREMENT THE I-TH VARIABLE
R 3  0.3549111D 02    0.4277812D 02  0.1750000D 01  0.1215253D 00  0.6250000D-02  0.6250000D 00  0.7570000D-04 -0.4990000D 02
                      0.1780000D 01  0.3970000D-03 -0.2320000D 02 -0.4190000D 00
PATTERN MODE EXPLORATORY FAILURE RESTORE BASE PT.
NFUN=     29
*    0.3494490D 02    0.3948760D 02  0.1750000D 01  0.1878118D 00  0.6250000D-02  0.6250000D 00  0.7570000D-04 -0.4990000D 02
                     0.1780000D 01  0.3970000D-03 -0.2320000D 02 -0.4190000D 00
DELP                 -0.9871875D 01  0.0            0.9942975D-01  0.0            0.0            0.0            0.0
                     0.0             0.0            0.0            0.0
BEGIN EXPLORATORY LOOP
INCREMENT THE I-TH VARIABLE
F 1  0.3757823D 02    0.2961562D 02  0.1750000D 01  0.1878118D 00  0.6250000D-02  0.6250000D 00  0.7570000D-04 -0.4990000D 02
                      0.1780000D 01  0.3970000D-03 -0.2320000D 02 -0.4190000D 00
DECREMENT THE I-TH VARIABLE
R 1  0.3502854D 02    0.4935937D 02  0.1750000D 01  0.1878118D 00  0.6250000D-02  0.6250000D 00  0.7570000D-04 -0.4990000D 02
                      0.1780000D 01  0.3970000D-03 -0.2320000D 02 -0.4190000D 00
REDUCE STEP SIZE
INCREMENT THE I-TH VARIABLE
F 3  0.3642456D 02    0.3948750D 02  0.1750000D 01  0.2872415D 00  0.6250000D-02  0.6250000D 00  0.7570000D-04 -0.4990000D 02
                      0.1780000D 01  0.3970000D-03 -0.2320000D 02 -0.4190000D 00
DECREMENT THE I-TH VARIABLE
R 3  0.3665806D 02    0.3948750D 02  0.1750000D 01  0.8838200D-01  0.6250000D-02  0.6250000D 00  0.7570000D-04 -0.4990000D 02
                      0.1780000D 01  0.3970000D-03 -0.2320000D 02 -0.4190000D 00
REDUCE STEP SIZE
BASE PT. EXPLORATORY MODE FAILURE
THE NUMBER OF FUNCTION EVALUATIONS  EXCEEDED    33
*    0.3494490D 02    0.3948750D 02  0.1750000D 01  0.1878118D 00  0.6250000D-02  0.6250000D 00  0.7570000D-04 -0.4990000D 02
                     0.1780000D 01  0.3970000D-03 -0.2320000D 02 -0.4190000D 00
```

WATER-TRANSPORT INPUT TABLE 8.. BASIC PARAMETERS

THP:

0.6250000D-02	0.3100000D-01	0.5527404D-01	0.7907212D-01	0.1023942D 00	0.1252404D 00	0.1476106D 00	0.1695048D 00
0.1909231D 00	0.2118654D 00	0.2323317D 00	0.2523221D 00	0.2718365D 00	0.2908750D 00	0.3094375D 00	0.3275240D 00
0.3451346D 00	0.3622692D 00	0.3789279D 00	0.3951106D 00	0.4108173D 00	0.4260481D 00	0.4408029D 00	0.4550817D 00
0.4688846D 00	0.4822115D 00	0.4950625D 00	0.5074375D 00	0.5193365D 00	0.5307596D 00	0.5417067D 00	0.5521779D 00
0.5621731D 00	0.5716923D 00	0.5807356D 00	0.5893029D 00	0.5973942D 00	0.6050096D 00	0.6121490D 00	0.6188125D 00
0.6250000D 00							

ALP:

0.0	0.4000000D-01	0.7923077D-01	0.1176923D 00	0.1553846D 00	0.1923077D 00	0.2284615D 00	0.2638462D 00
0.2984615D 00	0.3323077D 00	0.3653846D 00	0.3976923D 00	0.4292308D 00	0.4600000D 00	0.4900000D 00	0.5192308D 00
0.5476923D 00	0.5753846D 00	0.6023077D 00	0.6284615D 00	0.6538462D 00	0.6784615D 00	0.7023077D 00	0.7253846D 00
0.7476923D 00	0.7692308D 00	0.7900000D 00	0.8100000D 00	0.8292308D 00	0.8476923D 00	0.8653846D 00	0.8823077D 00
0.8984615D 00	0.9138462D 00	0.9284615D 00	0.9423077D 00	0.9553846D 00	0.9676923D 00	0.9792308D 00	0.9900000D 00
0.1000000D 01							

****

SYSTEM-FLOW TABLE 11.. AT TIME = 4.1263D 00 ,(DELT = 1.0494D 00)

TYPE OF FLOW	RATE	INC. FLOW	TOTAL FLOW
CONSTANT-CONCENTRATION NODE FLOW. . . .	0.5720D-02	0.6575D-02	0.4728D-01
CONSTANT-FLUX-NODE FLOW	0.0	0.0	0.0
SEEPAGE FLUX-NODE FLOW.	0.0	0.0	0.0
NUMERICAL LOSSES.	0.0	0.0	0.0
NET FLOW.	0.5720D-02	0.6575D-02	0.4728D-01
INCREASE IN MATERIAL CONTENT (LIQUID) .	-0.1969D-02	-0.2067D-02	0.1572D-01
INCREASE IN MATERIAL CONTENT (SOLID). .	-0.2177D 00	-0.2285D 00	0.1738D 01
RADIOACTIVE LOSSES (LIQUID AND SOLID) .	0.0	0.0	0.0

SYSTEM-FLOW TABLE 21.. AT TIME = 3.5177D 01 ,(DELT = 5.4876D 00)

TYPE OF FLOW	RATE	INC. FLOW	TOTAL FLOW
CONSTANT-CONCENTRATION NODE FLOW. . . .	0.1515D-02	0.8787D-02	0.1260D 00
CONSTANT-FLUX-NODE FLOW	0.0	0.0	0.0
SEEPAGE FLUX-NODE FLOW.	0.0	0.0	0.0
NUMERICAL LOSSES.	0.0	0.0	0.0
NET FLOW.	0.1515D-02	0.8787D-02	0.1260D 00
INCREASE IN MATERIAL CONTENT (LIQUID) .	-0.3440D-03	-0.1888D-02	0.8962D-02
INCREASE IN MATERIAL CONTENT (SOLID). .	-0.3804D-01	-0.2087D 00	0.9909D 00
RADIOACTIVE LOSSES (LIQUID AND SOLID) .	0.0	0.0	0.0

SYSTEM-FLOW TABLE 31.. AT TIME = 1.4442D 02 ,(DELT = 1.6622D 01)

TYPE OF FLOW	RATE	INC. FLOW	TOTAL FLOW
CONSTANT-CONCENTRATION NODE FLOW. . . .	0.5936D-03	0.1028D-01	0.2226D 00
CONSTANT-FLUX-NODE FLOW	0.0	0.0	0.0
SEEPAGE FLUX-NODE FLOW.	0.0	0.0	0.0
NUMERICAL LOSSES.	0.0	0.0	0.0
NET FLOW.	0.5936D-03	0.1028D-01	0.2226D 00
INCREASE IN MATERIAL CONTENT (LIQUID) .	-0.5278D-04	-0.8774D-03	-0.1687D-02
INCREASE IN MATERIAL CONTENT (SOLID). .	-0.5836D-02	-0.9701D-01	-0.1865D 00
RADIOACTIVE LOSSES (LIQUID AND SOLID) .	0.0	0.0	0.0

SYSTEM-FLOW TABLE 41.. AT TIME = 4.1926D 02 ,(DELT = 3.8283D 01)

TYPE OF FLOW	RATE	INC. FLOW	TOTAL FLOW
CONSTANT-CONCENTRATION NODE FLOW. . . .	0.1973D-03	0.9586D-02	0.3295D 00
CONSTANT-FLUX-NODE FLOW	0.0	0.0	0.0
SEEPAGE FLUX-NODE FLOW.	0.0	0.0	0.0
NUMERICAL LOSSES.	0.0	0.0	0.0
NET FLOW.	0.1973D-03	0.9586D-02	0.3295D 00
INCREASE IN MATERIAL CONTENT (LIQUID) .	-0.1628D-04	-0.6231D-03	-0.8988D-02
INCREASE IN MATERIAL CONTENT (SOLID). .	-0.1799D-02	-0.6889D-01	-0.9938D 00
RADIOACTIVE LOSSES (LIQUID AND SOLID) .	0.0	0.0	0.0

SYSTEM-FLOW TABLE 51.. AT TIME = 9.9123D 02 ,(DELT = 7.5576D 01)

TYPE OF FLOW	RATE	INC. FLOW	TOTAL FLOW
CONSTANT-CONCENTRATION NODE FLOW. . . .	-0.3871D-05	-0.1067D-03	0.3546D 00
CONSTANT-FLUX-NODE FLOW	0.0	0.0	0.0
SEEPAGE FLUX-NODE FLOW.	0.0	0.0	0.0
NUMERICAL LOSSES.	0.0	0.0	0.0
NET FLOW.	-0.3871D-05	-0.1067D-03	0.3546D 00
INCREASE IN MATERIAL CONTENT (LIQUID) .	-0.3799D-05	-0.2871D-03	-0.1296D-01
INCREASE IN MATERIAL CONTENT (SOLID). .	-0.4200D-03	-0.3174D-01	-0.1432D 01
RADIOACTIVE LOSSES (LIQUID AND SOLID) .	0.0	0.0	0.0

SYSTEM-FLOW TABLE 64.. AT TIME = 2.4000D 03 ,(DELT = 4.4510D 01)

TYPE OF FLOW	RATE	INC. FLOW	TOTAL FLOW
CONSTANT-CONCENTRATION NODE FLOW.	-0.2011D-04	-0.8952D-03	0.3301D 00
CONSTANT-FLUX-NODE FLOW	0.0	0.0	0.0
SEEPAGE FLUX-NODE FLOW.	0.0	0.0	0.0
NUMERICAL LOSSES.	0.0	0.0	0.0
NET FLOW.	-0.2011D-04	-0.8952D-03	0.3301D 00
INCREASE IN MATERIAL CONTENT (LIQUID) .	-0.4195D-06	-0.1867D-04	-0.1494D-01
INCREASE IN MATERIAL CONTENT (SOLID). .	-0.4638D-04	-0.2064D-02	-0.1652D 01
RADIOACTIVE LOSSES (LIQUID AND SOLID) .	0.0	0.0	0.0

SEARCH OUTPUT TABLE 1.. FINAL VALUE OF PARAMETERS, BOUNDS, AND INCREMENTS

IP	P	PH	PL	DP
1	0.39487D 02	0.10000D 51	0.10000D 01	-0.24680D 01
2	0.17500D 01	0.17500D 01	0.17500D 01	0.0
3	0.18781D 00	0.10000D 51	0.10000D-01	0.24857D-01
4	0.62500D-02	0.62500D-02	0.62500D-02	0.0
5	0.62500D 00	0.62500D 00	0.62500D 00	0.0
6	0.75700D-04	0.75700D-04	0.75700D-04	0.0
7	-0.49900D 02	-0.49900D 02	-0.49900D 02	0.0
8	0.17600D 01	0.17800D 01	0.17800D 01	0.0
9	0.39700D-03	0.39700D-03	0.39700D-03	0.0
10	-0.23200D 02	-0.23200D 02	-0.23200D 02	0.0
11	-0.41900D 00	-0.41900D 00	-0.41900D 00	0.0

SEARCH OUTPUT TABLE 2.. EXPERIMENTAL DATA AND THEORETICAL FIT

TABLE AT TIME =0.2400D 04

IX	XX	YX	YT	DYX
1	0.11050D 01	-0.10076D 01	-0.18238D 01	0.37720D 00
2	0.13150D 01	0.20638D 00	-0.49805D 00	0.59399D 00
3	0.15250D 01	-0.31390D 00	0.10680D 00	0.51248D 00
4	0.17350D 01	-0.31390D 00	0.14870D 00	0.51248D 00
5	0.19450D 01	0.20638D 00	0.84781D-01	0.59399D 00
6	0.21550D 01	-0.31390D 00	0.80579D-01	0.51248D 00
7	0.23650D 01	0.37981D 00	0.27110D 00	0.61879D 00
8	0.25750D 01	-0.14048D 00	0.61266D 00	0.54092D 00
9	0.27850D 01	0.55323D 00	0.47621D 00	0.64255D 00
10	0.29950D 01	0.20638D 00	0.59136D 00	0.59399D 00
11	0.32050D 01	0.21141D 01	0.19570D 01	0.82690D 00
12	0.34150D 01	0.40218D 01	0.43638D 01	0.10073D 01
13	0.36250D 01	0.73169D 01	0.77534D 01	0.12594D 01
14	0.38350D 01	0.11479D 02	0.12882D 02	0.15192D 01
15	0.40450D 01	0.16335D 02	0.16803D 02	0.17749D 01
16	0.42550D 01	0.21538D 02	0.17006D 02	0.20130D 01
17	0.44650D 01	0.15295D 02	0.14005D 02	0.17232D 01
18	0.46750D 01	0.57561D 01	0.10280D 02	0.11469D 01
19	0.48850D 01	0.54092D 01	0.69613D 01	0.11203D 01
20	0.50950D 01	0.50623D 01	0.38095D 01	0.10931D 01
21	0.53050D 01	0.14204D 01	0.14120D 01	0.75059D 00
22	0.55150D 01	0.19407D 01	0.32545D 00	0.80852D 00
23	0.57250D 01	0.12469D 01	0.13590D 00	0.73030D 00
24	0.59350D 01	0.37981D 00	0.27256D 00	0.61879D 00
25	0.61450D 01	0.90009D 00	0.28682D 00	0.68781D 00
26	0.63550D 01	0.37981D 00	0.23338D 00	0.61879D 00
27	0.65650D 01	-0.14048D 00	0.32435D 00	0.54092D 00
28	0.67750D 01	-0.14048D 00	0.54959D 00	0.54092D 00
29	0.69850D 01	-0.10076D 01	0.68346D 00	0.37720D 00
30	0.71950D 01	-0.14048D 00	0.45641D 00	0.54092D 00
31	0.74050D 01	0.12469D 01	0.93658D-01	0.73030D 00
32	0.76150D 01	0.20638D 00	-0.13945D 00	0.59399D 00
33	0.78250D 01	-0.14048D 00	-0.21530D 00	0.54092D 00
34	0.80350D 01	0.12469D 01	-0.18025D 00	0.73030D 00
35	0.82450D 01	0.72666D 00	-0.12027D 00	0.66561D 00
36	0.84550D 01	0.14204D 01	-0.21150D 00	0.75059D 00

37	0.86650D 01	0.90009D 00	-0.21564D 00	0.68781D 00
38	0.88750D 01	0.10735D 01	0.80973D-01	0.70932D 00
39	0.90850D 01	-0.14048D 00	0.27708D 00	0.54092D 00
40	0.92950D 01	0.10735D 01	0.57440D-01	0.70932D 00
41	0.95050D 01	0.20638D 00	-0.17340D 00	0.59399D 00
42	0.97150D 01	-0.14048D 00	-0.73988D-01	0.54092D 00
43	0.99250D 01	-0.14048D 00	0.11287D 00	0.54092D 00
44	0.10135D 02	0.32951D-01	0.11362D 00	0.56815D 00
45	0.10345D 02	0.20638D 00	0.84011D-01	0.59399D 00
46	0.10555D 02	0.20638D 00	0.44903D-01	0.59399D 00
47	0.10765D 02	-0.14048D 00	-0.75358D-01	0.54092D 00
48	0.10975D 02	0.12469D 01	-0.36002D-01	0.73030D 00
49	0.11185D 02	0.20638D 00	0.31527D 00	0.59399D 00
50	0.11395D 02	0.72666D 00	0.47754D 00	0.66561D 00
51	0.11605D 02	-0.48733D 00	0.20802D 00	0.48213D 00
52	0.11815D 02	0.20638D 00	-0.19082D 00	0.59399D 00
53	0.12025D 02	0.20638D 00	-0.24674D 00	0.59399D 00
54	0.12235D 02	0.90009D 00	-0.49126D-01	0.68781D 00
55	0.12445D 02	-0.48733D 00	0.14252D 00	0.48213D 00
56	0.12655D 02	0.90009D 00	0.33600D 00	0.68781D 00
57	0.12865D 02	0.32951D-01	0.24579D 00	0.56815D 00
58	0.13075D 02	0.37981D 00	0.57310D-01	0.61879D 00
59	0.13285D 02	-0.14048D 00	0.69976D-01	0.54092D 00
60	0.13495D 02	-0.31390D 00	0.12780D 00	0.51248D 00
61	0.13705D 02	0.37981D 00	-0.48527D-01	0.61879D 00
62	0.13915D 02	-0.31390D 00	-0.23443D 00	0.51248D 00
63	0.14125D 02	-0.14048D 00	-0.16814D 00	0.54092D 00
64	0.14335D 02	-0.48733D 00	0.16100D-01	0.48213D 00
65	0.14545D 02	0.72666D 00	0.26071D-01	0.66561D 00
66	0.14755D 02	0.20638D 00	0.81720D-02	0.59399D 00
67	0.14965D 02	0.37981D 00	0.24486D 00	0.61879D 00
68	0.15175D 02	-0.48733D 00	0.29657D 00	0.48213D 00
69	0.15385D 02	0.55323D 00	0.51895D-01	0.64255D 00
70	0.15595D 02	-0.31390D 00	-0.11800D 00	0.51248D 00
71	0.15805D 02	0.20638D 00	-0.12202D 00	0.59399D 00
72	0.16015D 02	0.20638D 00	-0.15029D 00	0.59399D 00
73	0.16225D 02	0.55323D 00	-0.20882D 00	0.64255D 00
74	0.16435D 02	0.32951D-01	-0.69098D-04	0.56815D 00
75	0.16645D 02	-0.31390D 00	0.10804D 00	0.51248D 00
76	0.16855D 02	0.55323D 00	0.97914D-01	0.64255D 00
77	0.17065D 02	0.32951D-01	0.13288D 00	0.56815D 00
78	0.17275D 02	0.55323D 00	0.17784D 00	0.64255D 00
79	0.17485D 02	0.20638D 00	0.10189D 00	0.59399D 00
80	0.17695D 02	0.32951D-01	0.77889D-01	0.56815D 00
81	0.17905D 02	0.72666D 00	0.79439D-01	0.66561D 00
82	0.18115D 02	0.20638D 00	0.76037D-01	0.59399D 00
83	0.18325D 02	0.90009D 00	0.30470D-01	0.68781D 00
84	0.18535D 02	0.32951D-01	-0.90951D-01	0.56815D 00
85	0.18745D 02	0.20638D 00	-0.50399D-01	0.59399D 00
86	0.18955D 02	0.72666D 00	-0.20899D 00	0.66561D 00
87	0.19165D 02	-0.83419D 00	-0.39127D 00	0.41519D 00
88	0.19375D 02	-0.66076D 00	-0.29263D 00	0.44987D 00
89	0.19585D 02	0.90009D 00	-0.10646D 00	0.68781D 00
90	0.19795D 02	0.32951D-01	-0.27923D-01	0.56815D 00
91	0.20005D 02	0.20638D 00	-0.21790D 00	0.59399D 00
92	0.20215D 02	-0.66076D 00	-0.32141D 00	0.44987D 00

AVERAGE POINT RESIDUAL = 0.1356D 01

APPENDIX B

LISTING OF THE COMPUTER PROGRAM

```
      BLOCK DATA
C
C  FUNCTION OF ROUTINE--TO INITIALIZE THE COMMON BLOCKS.
C
      IMPLICIT REAL*8(A-H,O-Z)
      REAL*4 PMAT
      COMMON/MIVAR/KPRO,KPR(1000),MAXDIF,MAXEL,MAXNP,MAXMAT,MAXBW,
     1 MAXNTI,NMPPM
      COMMON/MRVAR/ A(101,2),B(101,3),R(101),RP(101),RI(101),RB(101),
     1 DP(101),R1(101),RT(101),XTMP(101),BFLX(101),BFLXP(101), FX(100,2)
     1 ,FRATE(10),FLOW(10),TFLOW(10),W,PMAT(3,5)
      DATA MAXEL,MAXNP,MAXMAT,MAXBW,MAXNTI,NMPPM/100,101,1,3,1000,5/
      DATA PMAT/4H    ,4H  KD,4H    ,4H    ,4HRHOB,4H    ,4H    ,
     1 4H  AL,4H    ,4H   T,4HHETA,4HR   ,4H    , 4HPOR ,4H    /
      END
C
C
C  FUNCTION OF PROGRAM--TO SIMULATE TRANSIENT ONE-DIMENSIONAL
C  MATERIAL AND MOISTURE FLOW IN A THIN-LAYER CHANNEL CHROMATOGRAPH.
C  THE GALERKIN-FINITE-ELEMENT METHOD IS USED FOR THE MATERIAL
C  TRANSPORT, AND THE PARLANGE PERTABATIVE METHOD IS USED FOR
C  THE MOISTURE TRANSPORT.
C
C
C  DIMENSIONING FORMAT--
C
C     COMMON/PROBID/TITLE(8),NPROB
C
C     COMMON/CRVAR/TIME,TH(MAXEL,2),THM(MAXEL,2),THW(MAXEL,2),
C    1 DTH(MAXEL,2),VX(MAXEL,2),VXP(MAXEL,2),VXW(MAXEL,2)
C     COMMON/GEOM/X(MAXNP),BB(2),DCOSB(2),DCOS(2),DELT,CHNG,
C    1 DELMAX,TMAX,IPX(MAXNP),IE(MAXEL,3),NPN(2),NPST(2),NPTST(2),
C    1 NBE(2),NTSE(2),ISB(2,2),IS(2,2),NNP,NEL,NMAT,IBAND,NBC,
C    1 NST,NTST,NBEL,NTI,NNOR
C     COMMON/MIVAR/KPRO,KPR(MAXNTI),MAXDIF,MAXEL,MAXNP,MAXMAT,
C    1 MAXBW,MAXNTI,NMPPM
C     COMMON/MPROP/PROP(MAXMAT,NMPPM),VXI
C     COMMON/MRVAR/ C(MAXNP,MAXBW),R(MAXNP),RP(MAXNP),RI(MAXNP),
C    1 RB(MAXNP),DP(MAXNP),XTMP(MAXNP),BFLX(MAXNP),BFLXP(MAXNP),
C    1 FX(MAXEL,2),FRATE(10),FLOW(10),TFLOW(10),W,PMAT(3,NMPPM)
C
C     COMMON/NUMITG/ NORDR1,NORDER,NITP,ITHMIN,IGSS,ITMIN,
C    1 IGSSV(3)
C     COMMON/TFLX/TTAB(MXTTAB),V1N(MXTTAB),V1TAB(MXTTAB),
C    1 W1TAB(MXTTAB),UTAB(MXTTAB),TTABL(MXTTAB),W1TABL(MXTTAB),
C    1 TEMP(MXTTAB),IPTTAB(MXTTAB),NTTAB
C     COMMON/TWTR/T(MAXNTW),NT
C     COMMON/WPROP/AKPAR(MXSLP),CDPAR(MXSLP),AKSN(MXSLP2),
C    1 ALPK(MXSLP2),D(MXSLP2),ALPD(MXSLP2),AKSAT,AKSNO,NKPAR,
C    1 NKSP,NCDPAR,NDSP
C     COMMON/XVAR/XSUP1(MAXTHP),XSUP2(MAXTHP),THP(MAXTHP),
C    1 ALP(MAXTHP),VSUP1(MAXTHP),VSUP2(MAXTHP),F(MAXTHP),QGA(MAXTHP),
C    1 QG(MAXTHP),THTMP(MAXTHP),AKGSS((MAXTHP-1)*MXGSS+MXGSS1),
C    1 DGSS((MAXTHP-1)*MXGSS+MXGSS1),IPTTH(MAXTHP),NTH,JTH,NGSS
C
C     COMMON/SIP/NP,KPRS,MXFUN,ICONV,NSCY,IPA(MAXSCY,MAXSHP)
C     COMMON/SRP/ DELTO,CHISO,ACC,RED,TOLSTP,TOLFUN,PO(MAXSHP),
C    1 PH(MAXSHP),PL(MAXSHP),DELP(MAXSHP),PLO(MAXSHP),PHO(MAXSHP)
C     COMMON/XIV/MYXL(MXTMEX),MYXU(MXTMEX),NYX(MXTMEX),NTX,NXT
C     COMMON/XRV/XX(MXNPEX,MXTMEX),WX(MXNPEX,MXTMEX),YX(MXNPEX,
C    1 MXTMEX),DYX(MXNPEX,MXTMEX),YT(MXNPEX),TX(MXTMEX),XWTL(MXTMEX),
C    1 XWTU(MXTMEX)
C
C        WHERE    MAXBW IS THE MAXIMUM BAND WIDTH,
C                 MAXEL IS THE MAXIMUM NUMBER OF ELEMENTS,
C                 MAXMAT IS THE MAXIMUM NUMBER OF MATERIALS,
C                 MAXNP IS THE MAXIMUM NUMBER OF NODAL POINTS,
C                 MAXNTI IS THE MAXIMUM NUMBER OF TIME INTERVALS,
C                 NMPPM IS THE MAXIMUM NUMBER OF MATERIAL PROPERTIES PER
C                         MATERIAL,
C
C                 MAXNTW IS THE MAXIMUM NUMBER OF TIME VALUES USED IN THE
C                         UNCOUPLED WATER TRANSPORT CALCULATION,
C                 MAXTHP IS THE MAXIMUM NUMBER OF THETA POINTS,
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C                 MXGSS IS THEMAXIMUM NUMBER OF GAUSS POINTS USED ON ALL
C                         INTERVALS EXCEPT THE ONE NEAREST ALPHA = 1,
C                 MXGSS1 IS THE MAXIMUM NUMBER OF GAUSS POINTS USED ON THE
C                         INTERVAL NEAREST ALPHA = 1,
C                 MXSLP IS THE MAXIMUM NUMBER OF SOIL PROPERTIES,
C                 MXSLP2 IS 2*MXSLP,
C                 MXTTAB IS THE MAXIMUM NUMBER OF ENTRIES IN THE TIME
C                         TABLE,
C
C                 MAXSCY IS THE MAXIMUM NUMBER OF SEARCH CYCLES,
C                 MAXSHP IS THE MAXIMUM NUMBER OF SEARCH PARAMETERS,
C                 MXNPEX IS THE MAXIMUM NUMBER OF EXPERIMENTAL POINTS,
C                 MXTMEX IS THE MAXIMUM NUMBER OF EXPERIMENTAL TIMES.
C
      IMPLICIT REAL*8(A-H,O-Z)
      REAL*8 MEVAL,MWEVAL,MWVAL2
      REAL*4 PMAT
      COMMON/CTRL/KPGM,KWTR,KWI,KSTRM,KSTRW,ISTOP,KSS,KDIG,KMOUT, KWOUT,
     1 KTSTP,KSOUT,KSRCH,KBUFF,KANL,KIC,KSTRS
      COMMON/PROBID/TITLE(8),NPROB
      COMMON/CRVAR/TIME,TH(100,2),THM(100,2),THW(100,2),DTH(100,2),
     1 VX(100,2),VXP(100,2),VXW(100,2)
      COMMON/GEOM/X(101),BB(2),DCOSB(2),DCOS(2),DELT,CHNG,DELMAX,TMAX,
     1 IPX(101),IE(100,3),NPN(2),NPST(2),NPTST(2),NBE(2),NTSE(2), ISB(2,
     1 2),IS(2,2),NNP,NEL,NMAT,IBAND,NBC,NST,NTST,NBEL,NTI,NNOR
      COMMON/MIVAR/KPRQ,KPR(1000),MAXDIF,MAXEL,MAXNP,MAXMAT,MAXBW,
     1 MAXNTI,NMPPM
      COMMON/MRVAR/ A(101,2),B(101,3),R(101),RP(101),RI(101),RB(101),
     1 DP(101),RI(101),RT(101),XTMP(101),BFLX(101),BFLXP(101), FX(100,2)
     1 ,FRATE(10),FLOW(10),TFLOW(10),W,PMAT(3,5)
      COMMON/CW1/ W1,V1
      COMMON/NUMITG/ NORDR1,NORDER,NITP,ITHMIN,IGSS,ITMIN, IGSSV(3)
      COMMON/TWTR/T(50),NT
      COMMON/SIP/NP,KPRS,MXFUN,ICONV,NSCY,IPA(5,20)
      COMMON/SRP/ DELTO,CHIS,ACC,RED,TOLSTP,TOLFUN,P(20), PH(20),PL(20),
     1 DELP(20),PLO(20),PHO(20)
      EXTERNAL WEVAL,MEVAL,MWEVAL,MWVAL2
C
C   INPUT PROGRAM-CONTROL PARAMETER AND PROBLEM IDENTIFICATION.
C
   10 READ 10000,KPGM,NPROB,(TITLE(I),I=1,8)
      PRINT 10100,KPGM,NPROB,(TITLE(I),I=1,8)
      KBUFF=0
      KSRCH=0
      IF (KPGM.GT.3) KSRCH=1
      GO TO (20,50,80,130,160,190,220),KPGM
C
C   DETERMINE MATERIAL TRANSPORT ONLY.
C
   20 CALL DATAM
   30 CALL MINL
      TIME=0.
      CALL PRINTM(0)
      IF (KSTRM.EQ.1) CALL STRMI
      TIME=DELT
      DO 40 ITM=1,NTI
         CALL MTRAN
         CALL PRINTM(ITM)
         IF (KSTRM.EQ.1.AND.KPR(ITM).GT.0) CALL STRMT
         IF (KSS.EQ.0) GO TO 10
         IF (TIME.EQ.TMAX) GO TO 10
         DELT=DELT*(1.+CHNG)
         DELT=DMIN1(DELT,DELMAX)
         TIME=TIME+DELT
         IF (TIME.LT.TMAX) GO TO 40
         DELT=DELT-(TIME-TMAX)
         TIME =TMAX
   40    CONTINUE
      GO TO 10
C
C   CALCULATE WATER TRANSPORT ONLY.
C
   50 CALL DINW
   60 CALL PWCAL
      CALL WINL
```

```
      ITMIN=1
      CALL PRTTAB
      IF (KWTR.EQ.0) GO TO 10
      IF (KSTRW.EQ.1) CALL STRWI
      ITMIN=1
      DO 70 ITM=1,NT
         CALL WINTP(T(ITM))
         CALL WTIME(T(ITM))
         TIME=T(ITM)
         CALL WTRN1
         IF (KWTR.EQ.2) CALL WTRN2
         CALL PRTW1(ITM)
         IF (KWTR.EQ.2) CALL PRTW2(ITM)
         IF (KSTRW.EQ.1) CALL STRWT(T(ITM))
   70    CONTINUE
      GO TO 10
C
C  DO COUPLED CALCULATION.
C
   80 CALL DATAM
      CALL DINW
   90 CALL PWCAL
      CALL MINL
      CALL WINL
      CALL PRTTAB
      TIME=0.
      CALL PRINTM(0)
      IF (KSTRM.EQ.1) CALL STRMI
      TIME =DELT
      DO 120 ITM=1,NTI
         V1P=V1
         CALL MTRAN
         CALL PRINTM(ITM)
         IF (KSTRM.EQ.1.AND.KPR(ITM).GT.0) CALL STRMT
         IF (KSS.EQ.0) GO TO 10
         IF (TIME.EQ.TMAX) GO TO 10
         IF (KTSTP.NE.0) GO TO 100
         DELT=DELT*(1.+CHNG)
         GO TO 110
  100    IF (ITM.EQ.1) TCON=DELT*V1**(1.+CHNG)
         DELT=TCON/V1**(1.+CHNG)
  110    DELT=DMIN1(DELT,DELMAX)
         TIME =TIME+DELT
         IF (TIME.LT.TMAX) GO TO 120
         DELT=DELT-(TIME-TMAX)
         TIME=TMAX
  120    CONTINUE
      GO TO 10
C
C  SEARCH FOR MATERIAL-TRANSPORT VARIABLES ONLY, UNCOUPLED CALCULATION.
C
  130 CALL DATAM
      CALL DATAS
      DELT0=DELT
      IF (NSCY.LE.0) GO TO 150
      IF (MXFUN.LE.0) GO TO 150
      DO 140 ISCY=1,NSCY
         CALL SHPREP(ISCY)
         CALL SEARCH(MP,P,CHIS,PH,PL,ACC,RED,TOLSTP,TOLFUN,DELP,KPRS,
     1    MEVAL,MXFUN,ICONV)
  140    CONTINUE
  150 KPGM=1
      KSOUT=0
      CALL MEVAL(P,CHIS)
      GO TO 10
C
C  SEARCH FOR WATER-TRANSPORT VARIABLES ONLY.
C
  160 CALL DINW
      CALL DATAS
      KBUFF=0
      IF (NSCY.LE.0) GO TO 180
      IF (MXFUN.LE.0) GO TO 180
      DO 170 ISCY=1,NSCY
         CALL SHPREP(ISCY)
```

```
            CALL SEARCH(NP,P,CHIS,PH,PL,ACC,RED,TOLSTP,TOLFUN,DELP,KPRS,
     1       WEVAL,MXFUN,ICONV)
  170       CONTINUE
  180 KPGM=2
      KSOUT=0
      CALL WEVAL(P,CHIS)
      GO TO 10
C
C  SEARCH FOR MATERIAL TRANSPORT VARIABLES ONLY, COUPLED CALCULATION.
C
  190 CALL DATAM
      CALL DINW
      CALL PWCAL
      CALL WINL
      CALL PRTTAB
      CALL DATAS
      DELT0=DELT
      IF (MXFUN.LE.0) GO TO 210
      IF (NSCY.LE.0) GO TO 210
      DO 200 ISCY=1,NSCY
         CALL SHPREP(ISCY)
         CALL SEARCH(NP,P,CHIS,PH,PL,ACC,RED,TOLSTP,TOLFUN,DELP,KPRS,
     1       MWEVAL,MXFUN,ICONV)
  200    CONTINUE
  210 KPGM=3
      KSOUT=0
      CALL MWEVAL(P,CHIS)
      GO TO 10
C
C  SEARCH FOR BOTH MATERIAL- AND WATER-TRANSPORT VARIABLES.  COUPLED
C  CALCULATION.
C
  220 CALL DATAM
      CALL DINW
      CALL DATAS
      DELT0=DELT
      KBUFF=1
      IF (NSCY.LE.0) GO TO 240
      IF (MXFUN.LE.0) GO TO 240
      DO 230 ISCY=1,NSCY
         CALL SHPREP(ISCY)
         CALL SEARCH(NP,P,CHIS,PH,PL,ACC,RED,TOLSTP,TOLFUN,DELP,KPRS,
     1       MWVAL2,MXFUN,ICONV)
  230    CONTINUE
  240 KPGM=3
      KSOUT=0
      CALL MWVAL2(P,CHIS)
      GO TO 10
10000 FORMAT(2I5,8A8)
10100 FORMAT(/' CALCULATION..  TYPE',I5,'..  PROBLEM',I5,'.. ' ,8A8/)
      END
      SUBROUTINE MTR
C
C  FUNCTION OF SUBROUTINE--TO CONTROL THE INTEGRATION OF THE
C  MATERIAL-FLOW EQUATION, WHICH CONSISTS OF ASSEMBLY, APPLICATION
C  OF BOUNDARY CONDITIONS, AND MATRIX SOLUTION OF THE RESULTING
C  SET OF EQUATIONS.
C
      IMPLICIT REAL*8 (A-H,O-Z)
      REAL*4 PMAT
      REAL*8 KD,LAMBDA
      COMMON/CTRL/KPGM,KMTR,KWI,KSTRM,KSTRW,ISTOP,KSS,KDIG,KMOUT, KWOUT,
     1 KTSTP,KSOUT,KSRCH,KBUFF,KANL,KIC,KSTRS
      COMMON/CRVAR/TIME,TH(100,2),THK(100,2),THW(100,2),DTH(100,2),
     1 VX(100,2),VXP(100,2),VKW(100,2)
      COMMON/GEOM/X(101),BB(2),DCOSB(2),DCOS(2),DELT,CHNG,DELMAX,TMAX,
     1 IPX(101),IE(100,3),NPN(2),NPST(2),NPTST(2),NBE(2),NTSE(2), ISB(2,
     1 2),IS(2,2),NNP,NEL,NMAT,IBAND,NBC,NST,NTST,NBEL,NTI,NNOR
      COMMON/MPROP/PROP(1,5),NXI
      COMMON/MRVAR/ A(101,2),B(101,3),R(101),RP(101),RI(101),RB(101),
     1 DP(101),R1(101),RT(101),XTMP(101),BFLX(101),BFLXP(101), FX(100,2)
     1 ,FRATE(10),FLOW(10),TFLOW(10),Z,PMAT(3,5)
      COMMON/MIVAR/KPRO,KPR(1000),MAXDIF,MAXEL,MAXNP,MAXMAT,MAXBW,
     1 MAXNTI,MNPPM
      COMMON/BI/ TH1,TH0,THB,SINEPS
```

```
      COMMON/NUMITG/ NORDR1,NORDER,NITP,ITHMIN,IGSS,ITMIN, IGSSV(3)
      DIMENSION ZNOR(5),ZBETA(5,5)
      DATA ZNOR/0.0,7.886751345948136D-1,1.068579021301628D0,0.0,4.7
     1 326839125829540D-1/
      DATA ZBETA/5*0.0,3.660254037844393D-1,-1.366025403784439D0, 3*0.0,
     1 -2.101383127306029D-1,9.523655116991617D-1,-1.742227198968559D0,
     1 2*0.0,5*0.0,1.674662850648816D-1,-1.000068213033804D0,
     1 2.364268696938704D0,-2.454680874324783D0,-7.698589464499790D-2/
C
C ******************************************************************
C
      ENTRY MINL
      IF (NNOR.NE.1) GO TO 10
      ZNOR(1)=W
      ZBETA(1,NNOR)=-1.
   10 NPB1=ISB(1,1)
      NPB2=ISB(2,1)
      KMOUT=0
      KDIG=0
C
C COMPUTE BAND-WIDTH VARIABLES.
C
      IHALFB=MAXDIF
      IBAND=2*IHALFB+1
      IHBP=IHALFB+1
      IF (IBAND.LE.MAXBW) GO TO 20
      PRINT 10100,IBAND,MAXBW
C
C PREPARE INITIAL VARIABLES.
C
   20 IF (KIC.NE.0) GO TO 40
      DO 30 NP=1,NNP
   30    R(NP)=RI(NP)
      GO TO 80
   40 DO 50 NP=1,NNP
         R(NP)=0.
   50    RP(NP)=0.
      DO 70 M=1,NEL
         MTYP=IE(M,3)
         KD=PROP(MTYP,1)
         RHOB=PROP(MTYP,2)
         THETAR=PROP(MTYP,4)
         POR=PROP(MTYP,5)
         IF (THETAR.EQ.0) THETAR=POR/10.
         RD=1.+KD*RHOB/POR
         ANORM=1./(THETAR*RD)
         DO 60 IQ=1,2
            NP=IE(M,IQ)
            WT=0.5
            IF (NP.EQ.NPB1) WT=1.
            IF (NP.EQ.NPB2) WT=1.
            R(NP)=R(NP)+ANORM*RI(NP)*WT
   60       CONTINUE
   70    CONTINUE
   80 DO 90 NP=1,NNP
   90    RP(NP)=R(NP)
C
C READ INITIAL VELOCITIES, PRESSURES, AND WATER CONTENTS, IF NECESSARY.
C
      IF (KPGM.EQ.3) GO TO 140
      IF (KPGM.EQ.6) GO TO 140
      IF (KPGM.EQ.7) GO TO 140
      DO 100 M=1,NEL
         MTYP=IE(M,3)
         POR=PROP(MTYP,5)
         DO 100 IQ=1,2
            TH(M,IQ)=POR
  100       VX(M,IQ)=VXI
  110 IF (KVI.EQ.0) GO TO 160
      IF (KSRCH.GT.1) GO TO 160
      DO 120 MI=1,NEL,4
         MK=MIN0(MI+3,NEL)
         READ 10000,((VX(MJ,JQ),JQ=1,2),MJ=MI,MK)
  120    CONTINUE
      DO 130 MI=1,NEL,4
```

```
          MK=MINO(MI+3,NEL)
          READ 10000,((TH(MJ,JQ),JQ=1,2),MJ=MI,MK)
  130     CONTINUE
       IF (KSRCH.GT.0) KSRCH=KSRCH+1
       GO TO 160
C
C  PREPARE TIME-VELOCITY TABLE IF NECESSARY.
C
C
  140 DO 150 M=1,NEL
          DO 150 IQ=1,2
             NP=IE(M,IQ)
             TH(M,IQ)=THO
             VX(M,IQ)=0.
  150        CONTINUE
       ITMIN=1
C
C  CALCULATE MATERIAL FLUX FX(M,IQ).
C
  160 CALL FLUX(FX,VX,RP,TH,MAXEL,MAXNP)
C
C  DETERMINE BOUNDARY FLOWS.
C
      DO 170 I=1,8
  170     TFLOW(I)=0.
      DO 180 NP=1,NNP
  180     BFLX(NP)=0.
      CALL SFLOW(FX,RP,BFLX,BFLXP,FRATE,FLOW,TFLOW,TH,MAXEL,MAXNP)
      DO 190 I=1,8
          FLOW(I)=0.
  190     TFLOW(I)=0.
      FRATE(6)=0.
      FRATE(7)=0.
      FRATE(8)=0.
C
C  CALCULATE BULK CONCENTRATIONS.
C
      DO 200 NP=1,NNP
  200     RB(NP)=0.
      DO 220 M=1,NEL
          MTYP=IE(M,3)
          KD=PROP(MTYP,1)
          RHOB=PROP(MTYP,2)
          POR=PROP(MTYP,5)
          RD=1.+KD*RHOB/POR
          DO 210 IQ=1,2
             NP=IE(M,IQ)
             WT=0.5
             IF (NP.EQ.NPB1) WT=1.
             IF (NP.EQ.NPB2) WT=1.
             RB(NP)=RB(NP)+WT*RD*TH(M,IQ)*R(NP)
  210        CONTINUE
  220     CONTINUE
      RETURN
C
C  ***********************************************************************
C
      ENTRY MTRAN
C
C  PERFORM TRANSIENT-STATE CALCULATION.
C
      W1=W
      W2=1.-W
      DO 240 M=1,NEL
         DO 230 IQ=1,2
            THM(M,IQ)=TH(M,IQ)
  230       VXP(M,IQ)=VX(M,IQ)
  240    CONTINUE
C
C  READ TIME-DEPENDENT VELOCITIES, IF REQUIRED.
C
      IF (KPGM.EQ.3) GO TO 270
      IF (KPGM.EQ.6) GO TO 270
      IF (KPGM.EQ.7) GO TO 270
      IF (KVI.NE.2) GO TO 280
```

```
      IF (KSRCH.GT.0) GO TO 280
      DO 250 M=1,NEL,4
         MK=MINO(MI+3,NEL)
         READ 10000,((VX(MJ,JQ),JQ=1,2),MJ=MI,MK)
  250    CONTINUE
      DO 260 MI=1,NEL,4
         MK=MINO(MI+3,NEL)
         READ 10000,((TH(MJ,JQ),JQ=1,2),MJ=MI,MK)
  260    CONTINUE
      GO TO 280
C
C  CALCULATE TIME-DEPENDENT VELOCITIES AND WATER CONTENTS, IF REQUIRED.
C
  270 CALL WINTP(TIME)
      CALL WTRN2
      CALL MWLINK
C
C  ASSEMBLE COEFFICIENT MATRICES A AND B AND CONSTRUCT
C  THE TIME DERIVATIVE R1 AT THE PREVIOUS TIME NODE.
C
  280 DO 300 M=1,NEL
         DO 290 IQ=1,2
            DTH(M,IQ)=(TH(M,IQ)-THM(M,IQ))/DELT
            THW(M,IQ)=W1*TH(M,IQ)+W2*THM(M,IQ)
  290       VXW(M,IQ)=W1*VX(M,IQ)+W2*VXP(M,IQ)
  300    CONTINUE
      CALL ASEMBL(A,B,R1,RP,VXW,THW,DTH,W,MAXNP,MAXBW,MAXEL,KSS)
C
C  APPLY BOUNDARY CONDITIONS.
C
      DO 310 NP=1,NNP
  310    R(NP)=0.
      CALL BC(A,B,R,RP,DP,VXW,W,MAXNP,MAXEL,MAXBW,KSS)
C
C  FORM THE FIRST-DERIVATIVE TERM R1 = A * DR/DT.
C
      DO 330 NI=1,NNP
         R1(NI)=R(NI)
         JBL=MAX0(1,IHBP-NI+1)
         JBU=MINO(IBAND,IHBP-NI+NNP)
         DO 320 JB=JBL,JBU
            NJ=NI+JB-IHBP
            R1(NI)=R1(NI)-B(NI,JB)*RP(NJ)
  320       CONTINUE
  330    CONTINUE
C
C  FORM MATRIX A + Z*DELT*B.
C
      ZD=ZNOR(NNOR)*DELT
      DO 360 NI=1,NNP
         JBAU=MINO(IHBP,1-NI+NNP)
         DO 340 JBA=1,JBAU
            JB=IHALFB+JBA
            B(NI,JB)=A(NI,JBA)+ZD*B(NI,JB)
  340       CONTINUE
         KBU=MINO(NI-1,IHALFB)
         IF (KBU.LT.1) GO TO 360
         DO 350 KB=1,KBU
            NIA=NI-KB
            JBA=KB+1
            JB=IHBP-KB
            B(NI,JB)=A(NIA,JBA)+ZD*B(NI,JB)
  350       CONTINUE
  360    CONTINUE
C
C  TRIANGULARIZE MATRIX A + Z*DELT*B.
C
      CALL SOLVE(1,B,R,NNP,IHALFB,MAXNP,MAXBW)
      DO 370 NI=1,NNP
  370    R(NI)=0.
      DO 430 INOR=1,NNOR
C
C  DETERMINE A * R, WHERE R CONTAINS THE PREVIOUS ITERATE.
C
         DO 380 NI=1,NNP
```

```
  380          RT(NI)=0.
          DO 410 NI=1,NNP
             JBU=MINO(NNP-NI+1,IHBP)
             DO 390 JB=1,JBU
                NJ=NI+JB-1
                RT(NI)=RT(NI)+A(NI,JB)*R(NJ)
  390           CONTINUE
             KBU=MINO(NI-1,IHALFB)
             IF (KBU.LT.1) GO TO 410
             DO 400 KB=1,KBU
                NJ=NI-KB
                JB=KB+1
                RT(NI)=RT(NI)+A(NJ,JB)*R(NJ)
  400           CONTINUE
  410        CONTINUE
C
C  FORM THE NEW LOAD VECTOR.
C
          ZDB=ZBETA(INOR,NNOR)*DELT
          DO 420 NI=1,NNP
  420        R(NI)=RT(NI)-ZDB*R1(NI)
C
C  BACK SUBSTITUTE.
C
          CALL SOLVE(2,B,R,NNP,IHALFB,MAXNP,MAXBW)
  430     CONTINUE
       DO 440 NI=1,NNP
  440     R(NI)=RP(NI)+R(NI)
C
C  CALCULATE MATERIAL FLUX FX(M,IQ).
C
       CALL FLUX(FX,VX,R,TH,MAXEL,MAXNP)
C
C  DETERMINE BOUNDARY FLOWS.
C
       CALL SFLOW(FX,R,BFLX,BFLXP,FRATE,FLOW,TFLOW,TH,MAXEL,MAXNP)
C
C  CALCULATE BULK CONCENTRATIONS.
C
       DO 450 NP=1,NNP
  450     RB(NP)=0.
       DO 470 M=1,NEL
          MTYP=IE(M,3)
          KD=PROP(MTYP,1)
          RHOB=PROP(MTYP,2)
          POR=PROP(MTYP,5)
          RD=1.+KD*RHOB/POR
          DO 460 IQ=1,2
             NP=IE(M,IQ)
             WT=0.5
             IF (NP.EQ.NPB1) WT=1.
             IF (NP.EQ.NPB2) WT=1.
             RB(NP)=RB(NP)+WT*RD*TH(M,IQ)*R(NP)
  460        CONTINUE
  470     CONTINUE
       DO 480 NP=1,NNP
  480     RP(NP)=R(NP)
       RETURN
10000  FORMAT(8F10.0)
10100  FORMAT(////12H BANDWIDTH =,I4,25H EXCEEDS MAX. ALLOWABLE =,I4///)
       END
       SUBROUTINE DATAS
C
C
C  FUNCTION OF SUBROUTINE--TO READ, PRINT, AND CHECK MATERIAL-TRANSPORT
C  VARIABLES PERTAINING TO SIMULATION TIME, NODE-ELEMENT CONFIGURATION,
C  BOUNDARY INITIAL CONDITIONS, AND PROPERTIES OF BOTH THE MATERIAL
C  BEING TRANSPORTED AND THE POROUS MEDIA.
C
C
       IMPLICIT REAL*8 (A-H,O-Z)
       REAL*4 PMAT
       COMMON/CTRL/KPGM,KWTR,KWI,KSTRM,KSTRW,ISTOP,KSS,KDIG,KMOUT, KWOUT,
     1 KTSTP,KSOUT,KSRCH,KBUFF,KANL,KIC,KSTRS
       COMMON/GEOM/X(101),BB(2),DCOSB(2),DCOS(2),DELT,CHNG,DELMAX,TMAX,
```

```
     1 IPX(101),IE(100,3),NPM(2),NPST(2),NPTST(2),NBE(2),NTSE(2), ISB(2,
     1 2),IS(2,2),NNP,NEL,NMAT,IBAND,NBC,NST,NTST,NBEL,NTI,NNOR
      COMMON/MIVAR/KPRO,KPR(1000),MAXDIF,MAXEL,MAXNP,MAXMAT,MAXBW,
     1 MAXNTI,NMPPM
      COMMON/MPROP/PROP(1,5),VXI
      COMMON/MRVAR/ A(101,2),B(101,3),R(101),RP(101),RI(101),RB(101),
     1 DP(101),R1(101),RT(101),XTMP(101),BFLX(101),BFLXP(101), FX(100,2)
     1 ,FRATE(10),FLOW(10),TFLOW(10),W,PMAT(3,5)
      ISTOP=0
      READ 11000,NNP,NEL,NMAT,NCM,NTI,NBC,NST,KVI,KSTRM,KSS,KTSTP, NELL,
     1 NELU,NNOR,KIC,KMESH
      NTST=0
      IF (KSS.NE.0) KSS=1
      IF (KSTRM.NE.0) KSTRM=1
      IF (NNOR.LT.1) NNOR=1
      IF (NNOR.EQ.4) NNOR=3
      IF (NNOR.GT.5) NNOR=5
      READ 11100, DELT,CHNG,DELMAX,TMAX,W,X0,XMX,DXL1,DXU1,VXI
      IF (KSS.NE.0) GO TO 10
      NNOR=1
      W=1.
   10 IF (KMESH.NE.1) GO TO 20
      NEL=NELL+NELU
      NNP=NEL+1
      IF (NELU.EQ.0) X0=XMX
      IF (NELL.EQ.0) X0=0.
   20 IF (DELMAX.LE.0.D0) DELMAX=1.E50
      IF (TMAX.LE.0.D0) TMAX=1.E50
      PRINT 10000,NNP,NEL,NMAT,NCM,NTI,NBC,NST,KVI,KSTRM,KSS, KTSTP,
     1 NELL,NELU,NNOR,KIC,KMESH
      PRINT 10100,DELT,CHNG,DELMAX,TMAX,W,X0,XMX,DXL1,DXU1,VXI
      READ 11200,KPRO,(KPR(ITM),ITM=1,NTI)
      PRINT 10200
      PRINT 11300,KPRO,(KPR(ITM),ITM=1,NTI)
C
C  CHECK TO BE SURE INPUT DATA DOES NOT EXCEED STORAGE CAPACITY.
C
      IF (NNP.GE.0.AND.NNP.LE.MAXNP) GO TO 30
      ISTOP=ISTOP+1
      PRINT 12400, MAXNP
   30 IF (NEL.GE.0.AND.NEL.LE.MAXEL) GO TO 40
      ISTOP=ISTOP+1
      PRINT 12500, MAXEL
   40 IF (NMAT.GE.0.AND.NMAT.LE.MAXMAT) GO TO 50
      ISTOP=ISTOP+1
      PRINT 12900, MAXMAT
   50 IF (NCM.GE.0.AND.NCM.LE.MAXEL) GO TO 60
      ISTOP=ISTOP+1
      PRINT 12600,MAXEL
   60 IF (NTI.GE.0.AND.NTI.LE.MAXNTI) GO TO 70
      ISTOP=ISTOP+1
      PRINT 12700, MAXNTI
   70 IF (NBC.GE.0.AND.NBC.LE.MAXNP) GO TO 80
      ISTOP=ISTOP+1
      PRINT 13000,MAXNP
   80 IF (NST.GE.0.AND.NST.LE.MAXNP) GO TO 90
      ISTOP=ISTOP+1
      PRINT 13100,MAXNP
   90 IF (NTST.GE.0.AND.NTST.LE.MAXNP) GO TO 100
      ISTOP=ISTOP+1
      PRINT 13200,MAXNP
  100 IF (KVI.GE.0.AND.KVI.LE.3) GO TO 110
      ISTOP=ISTOP+1
      PRINT 12800
  110 IF (ISTOP.EQ.0) GO TO 120
      PRINT 13300, ISTOP
      STOP
C
C  READ AND PRINT MATERIAL PROPERTIES.
C
  120 IF (NMPPM.LE.0) GO TO 140
      PRINT 10300,((PMAT(I,J),I=1,3),J=1,NMPPM)
      DO 130 I=1,NMAT
         READ 11100,(PROP(I,J),J=1,NMPPM)
  130    PRINT 11400,I,(PROP(I,J),J=1,NMPPM)
```

```
C
C  GENERATE NODAL-POINT DATA, IF REQUIRED.
C
  140 IF (KMESH.NE.0) GO TO 220
      NP=1
      X(NP)=X0
      IF (NELL.EQ.0) GO TO 160
      NV=NELL
      NVM=NV-1
      DXAV=X0/DFLOAT(NV)
      SDX=2.*(DXAV-DXL1)/DFLOAT(NVM)
      DXI=DXL1
      DO 150 JV=1,NV
         NP=NP+1
         X(NP)=X(NP-1)-DXI
         DXI=DXI+SDX
  150    CONTINUE
      X(NP)=0.
  160 IF (NELU.EQ.0) GO TO 180
      NP=NP+1
      X(NP)=X0+DXU1
      NV=NELU
      NVM=NV-1
      DXAV=(XMX-X0)/DFLOAT(NV)
      SDX=2.*(DXAV-DXU1)/DFLOAT(NVM)
      DXI=DXU1+SDX
      DO 170 JV=2,NV
         NP=NP+1
         X(NP)=X(NP-1)+DXI
         DXI=DXI+SDX
  170    CONTINUE
      X(NP)=XMX
C
C  PUT GENERATED X-VALUES IN ASCENDING ORDER.
C
  180 CALL DSORT(X,IPX,NNP)
C
C  PRINT GENERATED NODAL-POINT DATA.
C
      PRINT 10400
      DO 190 NP=1,NNP
  190    PRINT 11600,NP,X(NP)
C
C  GENERATE ELEMENT DATA.
C
      MTYP=1
      DO 200 M=1,NEL
         NI=M
         NJ=NI+1
         IE(M,1)=NI
         IE(M,2)=NJ
         IE(M,3)=MTYP
  200    CONTINUE
C
C  PRINT GENERATED ELEMENT DATA.
C
      PRINT 10500
      MND=1
      MAXDIF=1
      DO 210 M=1,NEL
  210    PRINT 11700,M,(IE(M,I),I=1,3),MND
      GO TO 430
C
C  READ NODAL-POINT DATA FROM CARDS AND PRINT, IF REQUIRED.
C
  220 IF (KMESH.NE.0) GO TO 390
      PRINT 10400
      NI=1
  230 READ 11900, NJ,X(NJ)
      IF (NJ-NI) 240,270,250
  240 PRINT 13400, NJ
      PRINT 11600, NJ,X(NJ)
      ISTOP=ISTOP+1
      GO TO 230
  250 DF=NJ+1-NI
```

```
      DX=(X(NJ)-X(NI-1))/DF
  260 CONTINUE
      X(NI)=X(NI-1)+DX
  270 PRINT 11600,NI,X(NI)
      NI=NI+1
      IF (NJ-NI) 280,270,260
  280 IF (NI.LE.NNP) GO TO 230
C
C  READ AND PRINT ELEMENT DATA.
C
C  ALSO COMPUTE MAXIMUM NODAL DIFFERENCE FOR EACH ELEMENT.
C
      PRINT 10500
      MAXDIF=0
      MJ = 0
  290 READ 11000, MI,(IE(MI,I),I=1,3),MODL
      MND = IABS(IE(MI,2)-IE(MI,1))
      MAXDIF = MAX0(MND,MAXDIF)
  300 MJ = MJ + 1
      IF (MI-MJ) 310,340,320
  310 PRINT 13500, MI
      PRINT 11700, MI,(IE(MI,I),I=1,3),MND
      ISTOP = ISTOP + 1
  320 DO 330 IQ=1,2
  330    IE(MJ,IQ) = IE(MJ-1,IQ) + 1
      IE(MJ,3) = IE(MJ-1,3)
  340 PRINT 11700, MJ,(IE(MJ,I),I=1,3),MND
      IF (MJ.LT.MI) GO TO 300
      IF (MJ.EQ.NEL) GO TO 380
      IF (MODL.LE.0) GO TO 290
      LL=2
      DO 370 J=1,MODL
         IF (MJ.EQ.MI) GO TO 360
         DO 350 KQ=1,2
  350       IE(MJ,KQ) = IE(MJ-1,KQ) + LL
         IE(MJ,3) = IE(MJ-1,3)
         PRINT 11700, MJ,(IE(MJ,K),K=1,3),MND
  360    LL = 1
  370    MJ = MJ + 1
      MJ = MJ - 1
      IF (MJ.LT.NEL) GO TO 290
  380 CONTINUE
C
C  READ NODAL-POINT DATA IN COMPRESSED FORM, IF REQUIRED.
C
  390 READ 11100,(X(NP),NP=1,NNP)
      CALL DSORT(X,IPX,NNP)
      PRINT 10400
      DO 400 NP=1,NNP
  400    PRINT 11600,NP,X(NP)
C
C  GENERATE ELEMENT DATA.
C
      MTYP=1
      DO 410 M=1,NEL
         NI=M
         NJ=NI+1
         IE(M,1)=NI
         IE(M,2)=NJ
         IE(M,3)=MTYP
  410    CONTINUE
C
C  PRINT GENERATED ELEMENT DATA.
C
      PRINT 10500
      MND=1
      MAXDIF=1
      DO 420 M=1,NEL
  420    PRINT 11700,M,(IE(M,I),I=1,3),MND
C
C  MODIFY MATERIAL TYPES FOR SELECTED ELEMENTS, IF NECESSARY.
C
  430 IF (NCM.LE.0) GO TO 470
      PRINT 10600
      L=0
```

```
  440 READ 11000, MI,MTYP,MK
      IE(MI,3) = MTYP
      PRINT 11800, MI,IE(MI,3)
      L = L + 1
      IF (MK.LE.MI) GO TO 460
      MI = MI + 1
      DO 450 MJ=MI,MK
         IE(MJ,3) = MTYP
         PRINT 11800, MJ,IE(MJ,3)
  450    L = L + 1
  460 IF (L.LT.NCM) GO TO 440
C
C  CHECK MATERIAL TYPES FOR EACH ELEMENT.
C
  470 DO 480 M=1,NEL
         MTYP=IE(M,3)
         IF (MTYP.GT.0.AND.MTYP.LE.NMAT) GO TO 480
         PRINT 14200,M
         ISTOP=ISTOP+1
  480    CONTINUE
      IF (ISTOP.EQ.0) GO TO 490
      PRINT 13700,ISTOP
  490 IF (KMESH.EQ.2) GO TO 540
C
C  READ INITIAL CONDITIONS IN FREE FORM.
C
      NI=0
      NJ=0
  500 IF (NJ.EQ.NNP) GO TO 560
      READ 11900,NJ,RI(NJ)
  510 NI=NI+1
      IF (NI.GT.1) GO TO 520
      IF (NJ.EQ.1) GO TO 520
      PRINT 13600,NJ
      ISTOP=ISTOP+1
      GO TO 710
  520 IF (NJ.EQ.NI) GO TO 500
      IF (NJ.GT.NI) GO TO 530
      PRINT 13600,NJ
      ISTOP=ISTOP+1
      GO TO 710
  530 RI(NI)=RI(NI-1)
      GO TO 510
C
C  READ INITIAL CONDITIONS IN COMPRESSED FORM.
C
  540 READ 11100, (XTMP(NP),NP=1,NNP)
      DO 550 NI=1,NNP
         NJ=IPX(NI)
  550    RI(NI)=XTMP(NJ)
C
C  IDENTIFY BOUNDARY NODES.
C
  560 CALL SURF
      DO 570 NP=1,NNP
  570    DP(NP)=0.
      IF (NBC.EQ.0) GO TO 640
C
C  READ CONSTANT-CONCENTRATION DIRICHLET CONDITIONS BB(NPP) TO BE
C  APPLIED AT NODES NPN(NPP).
C
      NPP=0
  580 IF (NPP.EQ.NBC) GO TO 610
      IF (NPP.LT.NBC) GO TO 590
      PRINT 13000,NBC
      ISTOP=ISTOP+1
      GO TO 610
  590 READ 11900,NI,BBI
  600 NPP=NPP+1
      NPN(NPP)=NI
      BB(NPP)=BBI
      GO TO 580
  610 PRINT 10700
      DO 620 NPP=1,NBC
  620    PRINT 12100,NPN(NPP),BB(NPP)
```

```
C
C  APPLY DIRICHLET BOUNDARY SPECIFICATIONS TO THE INITIAL CONDITIONS.
C
      DO 630 NPP=1,NBC
         NP=NPN(NPP)
  630    RI(NP)=BB(NPP)
  640 IF (NST.LE.0) GO TO 660
C
C  READ SURFACE-TERM FLUX EI TO BE APPLIED AT BOUNDARY
C  NODE NI.
C
      NPP=0
      PRINT 10800
  650 IF (NPP.EQ.NST) GO TO 660
      READ 11900,NI,EI
      DP(NI)=EI
      NPP=NPP+1
      NPST(NPP)=NI
      PRINT 12100,NI,EI
      GO TO 650
  660 IF (NTST.LE.0) GO TO 710
C
C  READ NUMBERS OF NODES FOR WHICH SEEPAGE
C  CONDITIONS OF THE FORM, FLUX = (DARCY FLUX)*CONCENTRATION,
C  ARE TO BE APPLIED.
C
      MPI=0
      NPP=0
      PRINT 10900
  670 IF (NPP.EQ.NTST) GO TO 710
      READ 12000,NI
      MPI=MPI+1
      NPP=NPP+1
      NPTST(NPP)=NI
      DO 690 MPJ=1,NBEL
         M=NBE(MPJ)
         NJ=ISB(MPJ,1)
         IF (NI.NE.NJ) GO TO 690
         NTSE(MPI)=M
         DCOS(MPI)=DCOSB(MPJ)
         DO 680 J=1,2
  680       IS(MPI,J)=ISB(MPJ,J)
         GO TO 700
  690    CONTINUE
      ISTOP =ISTOP+1
      PRINT 13900,NI
      GO TO 710
  700 PRINT 11700,NI
      GO TO 670
  710 IF (ISTOP.EQ.0) GO TO 720
      PRINT 13700, ISTOP
  720 RETURN
10000 FORMAT(////' MATERIAL-TRANSPORT INPUT TABLE 1.. BASIC PARAMETERS'
     1 //5X,
     1' NUMBER OF NODAL POINTS. . . . . . . . . . . . . . . . . . .',I5/ 5X,
     1' NUMBER OF ELEMENTS. . . . . . . . . . . . . . . . . . . . .',I5/ 5X,
     1' NUMBER OF DIFFERENT MATERIALS . . . . . . . . . . . . . . .',I5/ 5X,
     1' NUMBER OF CORRECTION MATERIALS. . . . . . . . . . . . . . .',I5/ 5X,
     1' NUMBER OF TIME INCREMENTS . . . . . . . . . . . . . . . . .',I5/ 5X,
     1' NUMBER OF BOUNDARY CONDITIONS . . . . . . . . . . . . . . .',I5/ 5X,
     1' NUMBER OF SURFACE TERMS . . . . . . . . . . . . . . . . . .',I5/ 5X,
     1' VELOCITY INPUT CONTROL. . . . . . . . . . . . . . . . . . .',I5/ 5X,
     1' AUXILIARY STORAGE CONTROL . . . . . . . . . . . . . . . . .',I5/ 5X,
     1' STEADY-STATE CONTROL. . . . . . . . . . . . . . . . . . . .',I5/ 5X,
     1' TIME-STEP CONTROL . . . . . . . . . . . . . . . . . . . . .',I5/ 5X,
     1' NUMBER OF LOWER VARIABLY SIZED ELEMENTS . . . . . . . . . .',I5/ 5X,
     1' NUMBER OF UPPER VARIABLY SIZED ELEMENTS . . . . . . . . . .',I5/ 5X,
     1' NORSETT TIME INTEGRATION INDEX. . . . . . . . . . . . . . .',I5/ 5X,
     1' INITIAL-CONDITION CONTROL . . . . . . . . . . . . . . . . .',I5/ 5X,
     1' MESH CONTROL. . . . . . . . . . . . . . . . . . . . . . . .',I5)
10100 FORMAT(5X, ' TIME INCREMENT. . . . . . . . . . . . . . . . . . . ',
     1 E10.4/ 5X, ' MULTIPLIER FOR INCREASING DELT. . . . . . . . . . . ',
     1 F10.6/ 5X, ' MAXIMUM VALUE OF DELT . . . . . . . . . . . . . . . ',
     1 E10.4/ 5X, ' MAXIMUM VALUE OF TIME . . . . . . . . . . . . . . . ',
     1 E10.4/ 5X, ' TIME-INTEGRATION PARAMETER. . . . . . . . . . . . . ',
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     1 F10.6/ 5X, ' ORIGIN OF MESH GENERATION . . . . . . . . . . . . . . ',
     1 F10.4/ 5X, ' MAXIMUM X-VALUE . . . . . . . . . . . . . . . . . . . ',
     1 F10.4/ 5X, ' LOWER FIRST X-INCREMENT . . . . . . . . . . . . . . . ',
     1 F10.4/ 5X, ' UPPER FIRST X-INCREMENT . . . . . . . . . . . . . . . ',
     1 F10.4/ 5X, ' CONSTANT DARCY VELOCITY . . . . . . . . . . . . . . . ',
     1 E10.4)
10200 FORMAT(//6X,'OUTPUT CONTROL')
10300 FORMAT(////' MATERIAL-TRANSPORT INPUT TABLE 2.. ',
     1 'MATERIAL PROPERTIES'// ' MAT. NO.', 9(3A4))
10400 FORMAT(////' MATERIAL-TRANSPORT TABLE 3.. NODAL-POINT DATA', //
     1 7X,'NODE', 8X,'X')
10500 FORMAT(////' MATERIAL-TRANSPORT TABLE 4.. ELEMENT DATA' //11X,
     1 'GLOBAL INDICES OF ELEMENT NODES'/7X,'ELEMENT', 3X,'1',7X,'2',
     1 6X,'MATERIAL',6X, 'NODE DIFF.' )
10600 FORMAT(////' CORRECTIONS TO MATERIAL TYPES FOR SELECTED ELEMENTS'/
     1 )
10700 FORMAT(////' MATERIAL-TRANSPORT INPUT TABLE 5.. BOUNDARY ',
     1 'CONDITIONS OF FORM R=BB' //' NODE',7X,'BB')
10800 FORMAT(////' MATERIAL-TRANSPORT INPUT TABLE 6.. SURFACE TERMS' ,
     1 ' FLUX=EI AT NODE NI','NODE',7X,'EI'/)
10900 FORMAT(////' MATERIAL-TRANSPORT INPUT TABLE 7.. SEEPAGE-SURFACE',
     1 ' INFORMATION'//5X//'NODE'/)
11000 FORMAT(16I5)
11100 FORMAT(8F10.0)
11200 FORMAT(80I1)
11300 FORMAT(10X,101I1)
11400 FORMAT(I8,9D12.4)
11500 FORMAT(I5,2F10.3)
11600 FORMAT(I10,2D15.4)
11700 FORMAT(I10,2I8,I10,I15)
11800 FORMAT(I10,32X,I10)
11900 FORMAT(I5,5X,F10.0)
12000 FORMAT(2I5,F10.0)
12100 FORMAT(I5,D15.4)
12200 FORMAT(3I5,5X,2F10.0)
12300 FORMAT(2I5,2(1PD15.4))
12400 FORMAT(////33H TOO MANY NODAL POINTS, MAXIMUM =, I5///)
12500 FORMAT(////30H TOO MANY ELEMENTS, MAXIMUM = ,I5///)
12600 FORMAT(////41H TOO MANY CORRECTION MATERIALS, MAXIMUM =,I5///)
12700 FORMAT(////36H TOO MANY TIME INCREMENTS, MAXIMUM =,I5///)
12800 FORMAT(////29H CHECK VELOCITY INPUT CONTROL///)
12900 FORMAT(////30H TOO MANY MATERIALS, MAXIMUM =,I5///)
13000 FORMAT(////36H CHECK BOUNDARY CONDITIONS, MAXIMUM=,I5///)
13100 FORMAT(////30H CHECK SURFACE TERMS, MAXIMUM=,I5///)
13200 FORMAT(////31H CHECK TRANSIENT S.T., MAXIMUM=,I5///)
13300 FORMAT(////28H EXECUTION HALTED BECAUSE OF,I5,13H FATAL ERRORS///)
13400 FORMAT(////30H ERROR IN NODAL-POINT CARD NO.,I5///)
13500 FORMAT(////26H ERROR IN ELEMENT CARD NO.,I5///)
13600 FORMAT(////36H ERROR IN INITIAL-CONDITION CARD NO.,I5///)
13700 FORMAT(////45H ASSEMBLY AND SOLUTION WILL NOT BE PERFORMED,,I5,
     1 19H  FATAL CARD ERRORS///)
13800 FORMAT(////36H ERROR IN FIRST SEEPAGE-SURFACE CARD///)
13900 FORMAT(////41H ERROR IN TRANSIENT-SURFACE CARD FOR NODE,I5///)
14000 FORMAT(////49H ERROR IN FIRST R=BB TYPE BOUNDARY-CONDITION CARD //
     1  /)
14100 FORMAT(////33H ERROR IN FIRST SURFACE-TERM CARD///)
14200 FORMAT(////40H ERROR IN MATERIAL TYPE CODE FOR ELEMENT ,I5///)
      END
      SUBROUTINE FLUX(FX,VX,R,TH,MAXEL,MAXNP)
C
C
C  FUNCTION OF SUBROUTINE--TO DETERMINE MATERIAL FLUX FX(M,KQ).
C
C
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON/GEOM/X(101),BB(2),DCOSB(2),DCOS(2),DELT,CHNG,DELMAX,TMAX,
     1 IPX(101),IE(100,3),NPN(2),NPST(2),NPTST(2),NBB(2),NTSB(2), ISB(2,
     1 2),IS(2,2),NNP,NEL,NMAT,IBAND,NBC,NST,NTST,NBBL,NTI,NNOR
      COMMON/MPROP/PROP(1,5),WXI
      DIMENSION DNX(2,2),XQ(2),VX(MAXEL,2),FX(MAXEL,2),R(MAXNP),
     1 TH(MAXEL,2)
      ISTOP=0
      DO 50 M=1,NEL
C
C  FOR EACH ELEMENT M PREPARE VARIABLES XQ(IQ) FOR Q4D,
```

```
C  WHICH DETERMINES DERIVATIVES DNX(IQ,KQ) OF EACH OF
C  THE TWO BASIS FUNCTIONS N(IQ) AT EACH NODAL POINT KQ.
C
         DO 10 IQ=1,2
            NP=IE(M,IQ)
   10       XQ(IQ)=X(NP)
         CALL Q4D(DNX,XQ)
C
C  FOR EACH NODAL POINT KQ SUM OVER CONTRIBUTIONS FROM EACH BASIS-
C  INTERPOLATION FUNCTION N(IQ) TO OBTAIN DERIVATIVES DRX
C  OF THE CONCENTRATION R(NP).
C
   20    DO 40 KQ=1,2
            DRX=0.
            DO 30 IQ=1,2
               NP=IE(M,IQ)
   30          DRX=DRX+DNX(IQ,KQ)*R(NP)
C
C  FORM THE DISPERSIVE FLUXES IN FX(M,KQ).
C
            MTYP=IE(M,3)
            AL=PROP(MTYP,3)
            AM=0.
            TAU=0.
            DD=AM*TAU
            VXK=VX(M,KQ)
            DXX=AL*VXK+DD
            FX(M,KQ)=-DXX*DRX
C
C  ADD THE ADVECTIVE FLUXES TO FX(M,KQ).
C
            FX(M,KQ)=FX(M,KQ)+VXK*R(NP)
   40       CONTINUE
   50    CONTINUE
      RETURN
      END
      SUBROUTINE Q4D(DNX,XQ)
C
C
C  FUNCTION OF SUBROUTINE--TO COMPUTE X DERIVATIVES DNX(IQ,KQ)
C  OF EACH BASIS FUNCTION N(IQ) AT EACH NODE KQ OF THE
C  ELEMENT.  RESULTS ARE IN THE GLOBAL COORDINATE SYSTEM.
C
C
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION S(2),DNX(2,2),XQ(2)
      DATA S / -1.0D+00, 1.0D+00 /
C
C  EVALUATE QUANTITIES FOR USE IN THE JACOBIAN DJ/8, BELOW, NECESSARY
C  FOR TRANSFORMATION FROM GLOBAL TO LOCAL COORDINATES.
C
      X21 = XQ(2) - XQ(1)
C
C  LOOP OVER EACH NODE
C
      DO 10 KQ=1,2
C
C  LOCAL COORDINATES OF ANY GIVEN NODE ARE (SS,TT).
C
         SS = S(KQ)
C
C  EVALUATE 'JACOBIAN'.
C
         DJ = X21
         DJI = 1.0/DJ
C
C  DETERMINE THE DERIVATIVES OF EACH BASIS FUNCTION AT NODE KQ.
C
         DNX(1,KQ)=-DJI
         DNX(2,KQ)=DJI
   10    CONTINUE
      RETURN
      END
      SUBROUTINE BC(A,B,R,RP,DP,VXN,W,MAXNP,MAXEL,MAXBW,KSS)
C
```

```
C
C     FUNCTION OF SUBROUTINE--TO APPLY CONSTANT-CONCENTRATION
C     DIRICHLET CONDITIONS AND CONSTANT-FLUX NEUMANN SURFACE
C     BOUNDARY CONDITIONS.
C
C
      IMPLICIT REAL*8 (A-H,O-Z)
      REAL*8 KD
      COMMON/GEOM/X(101),BB(2),DCOSB(2),DCOS(2),DELT,CHNG,DELMAX,TMAX,
     1 IPX(101),IE(100,3),NPN(2),NPST(2),NPTST(2),NBE(2),NTSE(2), ISB(2,
     1 2),IS(2,2),NNP,NEL,NMAT,IBAND,NBC,NST,NTST,NBEL,NTI,NNOR
      DIMENSION A(MAXNP,1),B(MAXNP,1),R(MAXNP),DP(MAXNP),VXW(MAXEL,2),
     1 RP(MAXNP)
      IHALFB=(IBAND-1)/2
      IHBP=IHALFB+1
      IF (NBC.EQ.0) GO TO 140
C
C     APPLY CONSTANT-CONCENTRATION DIRICHLET BOUNDARY CONDITIONS.
C
      DO 130 NPP=1,NBC
C
C     MODIFY ROW NPN(NPP) OF MATRIX B(NP,IB).
C
         NI=NPN(NPP)
         DO 10 IB=1,IBAND
   10       B(NI,IB)=0.0
         B(NI,IHBP)=1.0
         R(NI)=BB(NPP)
C
C     MODIFY LOAD VECTOR R(NP) FOR NON-ZERO BB(NPP).
C
         IF (BB(NPP).EQ.0.0) GO TO 50
         DO 20 IB=1,IHALFB
            NJ=NI-IB
            IF (NJ.LT.1) GO TO 30
            JB=IHBP+IB
   20       R(NJ)=R(NJ)-BB(NPP)*B(NJ,JB)
   30    DO 40 IB=1,IHALFB
            NJ=NI+IB
            IF (NJ.GT.NNP) GO TO 50
            JB=IHBP-IB
   40       R(NJ)=R(NJ)-BB(NPP)*B(NJ,JB)
C
C     ZERO COLUMN NPN(NPP) OF MATRIX B(NP,IB).
C
   50    DO 60 IB=1,IHALFB
            NJ=NI-IB
            IF (NJ.LT.1) GO TO 70
            JB=IHBP+IB
   60       B(NJ,JB)=0.0
   70    DO 80 IB=1,IHALFB
            NJ=NI+IB
            IF (NJ.GT.NNP) GO TO 90
            JB=IHBP-IB
   80       B(NJ,JB)=0.0
C
C     ZERO COLUMN NPN(NPP) OF MATRIX A(NP,IB).
C
   90    DO 100 IB=1,IHALFB
            NJ=NI-IB
            IF (NJ.LT.1) GO TO 110
            JB=IB+1
  100       A(NJ,JB)=0.0
C
C     ZERO ROW NPN(NPP) OF MATRIX A(NP,IB).
C
  110    DO 120 KB=1,IHBP
  120       A(NI,KB)=0.0
  130    CONTINUE
C
C     MODIFY LOAD VECTOR FOR SURFACE TERMS OF THE FORM DR/DZ=C.
C
  140 DO 150 NP=1,NNP
  150    R(NP)=R(NP)+DP(NP)
  160 RETURN
```

```
      END
      SUBROUTINE ASEMBL(A,B,R1,RP,VXW,THW,DTH,N,MAXNP,MAXBW,MAXEL,KSS)
C
C
C  FUNCTION OF SUBROUTINE--TO ASSEMBLE THE GLOBAL COEFFICIENT MATRIX
C  C(NP,IB) AND LOAD VECTOR R(NP) FROM THE ELEMENT MATRICES QA(IQ,JQ)
C  AND QB(IQ,JQ).
C
C
      IMPLICIT REAL*8 (A-H,O-Z)
      REAL*8 KD,LAMBDA
      COMMON/GEOM/X(101),BB(2),DCOSB(2),DCOS(2),DELT,CHNG,DELMAX,TMAX,
     1 IPX(101),IE(100,3),NPN(2),NPST(2),NPTST(2),NBE(2),NTSE(2), ISB(2,
     1 2),IS(2,2),NNP,NEL,NMAT,IBAND,NBC,NST,NTST,NBEL,NTI,NNOR
      COMMON/MPROP/PROP(1,5),VXI
      DIMENSION A(MAXNP,1),B(MAXNP,1),R1(MAXNP),RP(MAXNP),QA(2,2), QB(2,
     1 2), VXQ(2),XQ(2),VXW(MAXEL,2),THW(MAXEL,2), DTH(MAXEL,2),DHQ(2),
     1 DTHQ(2),THQ(2)
      IHALFB=(IBAND-1)/2
      IHBP=IHALFB+1
      CSS=1.
      IF (KSS.EQ.0) CSS=0.
C
C  INITIALIZE MATRICES C(NP,IB) AND R(NP).
C
   10 DO 40 NP=1,NNP
         DO 20 IB=1,IBAND
   20       B(NP,IB)=0.0
         DO 30 IB=1,IHBP
   30       A(NP,IB)=0.0
   40    CONTINUE
C
C  COMPUTE MATRICES QA(IQ,JQ) AND QB(IQ,JQ) FOR EACH ELEMENT M.
C
      DO 70 M=1,NEL
         MTYP=IE(M,3)
         KD=PROP(MTYP,1)
         RHOB=PROP(MTYP,2)
         AL=PROP(MTYP,3)
         LAMBDA=0.
         POR=PROP(MTYP,5)
         AM=0.
         TAU=0.
         DO 50 IQ=1,2
            NP=IE(M,IQ)
            THQ(IQ)=THW(M,IQ)
            DTHQ(IQ)=DTH(M,IQ)
            VXQ(IQ)=VXW(M,IQ)
   50       XQ(IQ)=X(NP)
         CALL Q4(VXQ,QA,QB,XQ,KD,RHOB,AL,LAMBDA,POR,THQ, DTHQ,DHQ,AM,
     1    TAU)
C
C  ASSEMBLE THE UPPER HALF BAND OF MATRIX A(NI,NJ) AND THE FULL BAND
C  OF MATRIX B(NI,NJ).  MATRIX B IS ASYMMETRIC DUE TO THE ADVECTION
C  TERM.
C
         DO 60 IQ=1,2
            NI=IE(M,IQ)
            DO 60 JQ=1,2
               NJ=IE(M,JQ)
               IB=NJ-NI+IHBP
               B(NI,IB)=B(NI,IB)+QB(IQ,JQ)
               IF (NJ.LT.NI) GO TO 60
               IB=NJ-NI+1
               A(NI,IB)=A(NI,IB)+QA(IQ,JQ)*CSS
   60          CONTINUE
   70    CONTINUE
      RETURN
      END
      SUBROUTINE Q4(VXQ,QA,QB,XQ,KD,RHOB,AL,LAMBDA,POR, THQ,DTHQ,DHQ,AM,
     1 TAU)
C
C
C  FUNCTION OF SUBROUTINE--TO EVALUATE THE MATRIX QUADRATURES QA(IQ,JQ)
C  AND QB(IQ,JQ) OVER THE AREA OF ONE ELEMENT.
```

```
C
C
      IMPLICIT REAL*8 (A-H,O-Z)
      REAL*8 N(4),NN,KD,LAMBDA
      DIMENSION QA(2,2),QB(2,2),VXQ(2),S(2),V(2),XQ(2), THQ(2),DTHQ(2),
     1 DHQ(2)
      DATA P / 0.577350269189626 /, S / -1.0D+00, 1.0D+00 /
      RD=1.+KD*RHOB/POR
      DD=AM*TAU
C
C  INITIALIZE MATRICES QA(IQ,JQ) AND QB(IQ,JQ).
C
      DO 10 IQ=1,2
         DO 10 JQ=1,2
            QA(IQ,JQ)=0.0
   10       QB(IQ,JQ)=0.0
C
C  EVALUATE QUANTITIES FOR USE IN JACOBIAN DJAC, BELOW, NECESSARY
C  FOR TRANSFORMATION FROM GLOBAL TO LOCAL COORDINATES.
C
      X21 = XQ(2) - XQ(1)
      DO 40 KG=1,2
C
C  DETERMINE THE LOCAL COORDINATE SS AND EVALUATE THE JACOBIAN AT
C  EACH GAUSS-INTEGRATION POINT KG.
C
         SS = P*S(KG)
         DJ = X21
         DJAC = 0.5*DJ
         DJI=1./DJ
         SM = 1.0 - SS
         SP = 1.0 + SS
C
C  CALCULATE VALUES OF THE BASIS FUNCTIONS N(IQ) AND THEIR DERIVATIVES
C  V(IQ) W.R.T. X AT GAUSS POINT KG.
C
         V(1)=-DJI
         V(2)=DJI
         N(1)=0.5*SM
         N(2)=0.5*SP
C
C  INTERPOLATE WITH THE BASIS-INTERPOLATION FUNCTIONS N(IQ) TO OBTAIN
C  THE ADVECTIVE VELOCITY AT EACH GAUSS INTEGRATION POINT.
C
         THK=0.
         DTHK=0.
         VXK=0.
         DO 20 IQ=1,2
            THK=THK+N(IQ)*THQ(IQ)
            DTHK=DTHK+N(IQ)*DTHQ(IQ)
   20       VXK=VXK+N(IQ)*VXQ(IQ)
C
C  ACCUMULATE THE SUMS TO EVALUATE THE MATRIX INTEGRALS QA(IQ,JQ)
C  AND QB(IQ,JQ).
C
         A=DJAC*RD*THK
         DXX=DJAC*(AL*VXK+DD)
         C=DJAC*RD*(DTHK+LAMBDA*THK)
         VXK=VXK*DJAC
         DO 30 IQ=1,2
            DO 30 JQ=1,2
               NN=N(IQ)*N(JQ)
               VV=V(IQ)*V(JQ)
               VN=V(IQ)*N(JQ)
               QA(IQ,JQ)=QA(IQ,JQ)+A*NN
   30          QB(IQ,JQ)=QB(IQ,JQ)+DXX*VV+C*NN-VXK*VN
   40    CONTINUE
      RETURN
      END
      SUBROUTINE PRINTM(ITM)
C
C
C  FUNCTION OF SUBROUTINE--TO OUTPUT FLOWS, CONCENTRATIONS, MATERIAL
C  FLUXES, WATER CONTENTS, DARCY VELOCITIES, PRESSURE HEADS, AND
C  TOTAL HEADS AS SPECIFIED BY THE PARAMETER KPR.
```

```
C
C
      IMPLICIT REAL*8 (A-H,O-Z)
      REAL*4 PMAT
      COMMON/CTRL/KPGM,KWTR,KWI,KSTRM,KSTRW,ISTOP,KSS,KDIG,KMOUT, KWOUT,
     1 KTSTP,KSOUT,KSRCH,KBUFF,KANL,KIC,KSTRS
      COMMON/CRVAR/TIME,TH(100,2),THM(100,2),THW(100,2),DTH(100,2),
     1 VX(100,2),VXP(100,2),VXW(100,2)
      COMMON/GEOM/X(101),BB(2),DCOSB(2),DCOS(2),DELT,CHNG,DELMAX,TMAX,
     1 IPX(101),IE(100,3),NPN(2),NPST(2),NPTST(2),NBE(2),NTSE(2), ISB(2,
     1 2),IS(2,2),NNP,NEL,NMAT,IBAND,NBC,NST,NTST,NBEL,NTI,NNOR
      COMMON/MIVAR/KPRO,KPR(1000),MAXDIF,MAXEL,MAXNP,MAXMAT,MAXBW,
     1 MAXNTI,NMPPM
      COMMON/MRVAR/ A(101,2),B(101,3),R(101),RP(101),RI(101),RB(101),
     1 DP(101),R1(101),RT(101),XTMP(101),BFLX(101),BFLXP(101), FX(100,2)
     1 ,FRATE(10),FLOW(10),TFLOW(10),W,PMAT(3,5)
      KDIG=KDIG+1
      IF (KMOUT.EQ.0) KMOUT=1
      IF (KPR(ITM).EQ.0) RETURN
      IF (ITM.EQ.0) GO TO 10
C
C  PRINT DIAGNOSTIC FLOW INFORMATION.
C
      PRINT 10700,KDIG,TIME,DELT
      PRINT 10600,(FRATE(I),FLOW(I),TFLOW(I),I=1,8)
      KMOUT=KMOUT+1
   10 IF (KPR(ITM).EQ.1) RETURN
C
C  PRINT CONCENTRATIONS.
C
      PRINT 10000,KMOUT,TIME,DELT
      DO 20 NI=1,NNP,8
         NJMN=NI
         NJMX=MINO(NI+7,NNP)
   20    PRINT 10200,NI,(R(NJ),NJ=NJMN,NJMX)
      KMOUT=KMOUT+1
      PRINT 10100,KMOUT,TIME,DELT
      DO 30 NI=1,NNP,8
         NJMN=NI
         NJMX=MINO(NI+7,NNP)
   30    PRINT 10200,NI,(RB(NJ),NJ=NJMN,NJMX)
      IF (KPR(ITM).EQ.2) RETURN
C
C  PRINT MATERIAL FLUX.
C
      KMOUT=KMOUT+1
      PRINT 10300,KMOUT,TIME,DELT
      DO 40 MI=1,NEL,4
         MK=MINO(MI+3,NEL)
   40    PRINT 10200,MI,((FX(MJ,IQ),IQ=1,2),MJ=MI,MK)
      IF (KPR(ITM).EQ.3) RETURN
C
C  PRINT WATER CONTENTS.
C
      KMOUT=KMOUT+1
      PRINT 10400,KMOUT,TIME,DELT
      DO 50 MI=1,NEL,4
         MK=MINO(MI+3,NEL)
   50    PRINT 10200,MI,((TH(MJ,IQ),IQ=1,2),MJ=MI,MK)
C
C  PRINT DARCY VELOCITIES.
C
      KMOUT=KMOUT+1
      PRINT 10500,KMOUT,TIME,DELT
      DO 60 MI=1,NEL,4
         MK=MINO(MI+3,NEL)
   60    PRINT 10200,MI,((VX(MJ,IQ),IQ=1,2),MJ=MI,MK)
      RETURN
10000 FORMAT(////' OUTPUT TABLE',I4,'.. FLUID CONCENTRATIONS AT TIME =',
     1  1PD12.4,' ,(DELT =',1PD12.4,')'//' NODE I',5X,
     1 'FLUID CONCENTRATION AT NODES I,I+1,...,I+7'/)
10100 FORMAT(////' OUTPUT TABLE',I4,'.. BULK CONCENTRATIONS AT TIME =',
     1 1PD12.4,' ,(DELT =',1PD12.4,')'//' NODE I',5X,
     1 'BULK CONCENTRATION AT NODES I,I+1,...,I+7'/)
10200 FORMAT(I7,8(1PD15.4))
```

```
10300 FORMAT(////' OUTPUT TABLE',I4,'.. MATERIAL FLUX AT TIME =',
     1 1PD12.4,' ,(DELT =',1PD12.4,')',// 63X,
     1 'FLUX-X AT NODES'/17X,'1',14X,'2',14X
     1 '1',14X,'2',14X,'1',14X,'2',14X,'1',14X,'2',/3X,'ELEMENT',2X,
     1 '****************************************************',5X,
     1 '****************************************************')
10400 FORMAT(////' OUTPUT TABLE',I4,'.. WATER CONTENTS AT TIME =',
     1 1PD12.4,' ,(DELT =',1PD12.4,')',// 63X,
     1 'THETA AT NODES'/17X,'1',14X,'2',14X,'1',14X,'2',
     1 14X,'1',14X,'2',14X,'1',14X,'2'/3X,'ELEMENT',2X,
     1 '****************************************************',5X
     1 '****************************************************')
10500 FORMAT(////' OUTPUT TABLE',I4,'.. DARCY VELOCITIES AT TIME =',
     1 1PD12.4,' ,(DELT =',1PD12.4,')',// 63X,
     1 'VEL-X AT NODES'/17X,'1',14X,'2',14X,'1',
     1  14X,'2',14X,'1',14X,'2',14X,'1',14X,'2',/3X,'ELEMENT',2X,
     1 '****************************************************',5X,
     1 '****************************************************')
10600 FORMAT(//5X,' TYPE OF FLOW',35X,'RATE',8X,'INC. FLOW',7X,
     1 'TOTAL FLOW'/5X,' CONSTANT-CONCENTRATION NODE FLOW. . . .',3(
     1 E12.4,5X)/5X,' CONSTANT-FLUX-NODE FLOW . . . . . . . . .',3(E12.4,
     1 5X)/5X,' SEEPAGE FLUX-NODE FLOW. . . . . . . . . .',3(E12.4,5X)/
     1 5X,' NUMERICAL LOSSES. . . . . . . . . . . . .',3(E12.4,5X)/5X,
     1 ' NET FLOW. . . . . . . . . . . . . . . . .',3(E12.4,5X)/5X,
     1 ' INCREASE IN MATERIAL CONTENT (LIQUID) .',3(E12.4,5X)/5X,
     1 ' INCREASE IN MATERIAL CONTENT (SOLID). .',3(E12.4,5X)/5X,
     1 ' RADIOACTIVE LOSSES (LIQUID AND SOLID) .',3(E12.4,5X))
10700 FORMAT(///' *****************************************************
     1*****************************************************************
     1******'///' SYSTEM-FLOW TABLE',I4,'.. AT TIME =',1PD12.4,
     1 ' ,(DELT =',1PD12.4,')')
      END
      SUBROUTINE STRM
C
C
C  FUNCTION OF SUBROUTINE--TO STORE PERTINENT QUANTITIES ON AN AUXILIARY
C  DEVICE FOR FUTURE USE, E.G. FOR PLOTTING.  WHAT DEVICE IS TO BE
C  USED MUST BE SPECIFIED BY APPROPRIATE JOB-CONTROL CARDS.
C
C
      IMPLICIT REAL*8 (A-H,O-Z)
      REAL*4 PMAT
      COMMON/PROBID/TITLE(8),NPROB
      COMMON/CRVAR/TIME,TH(100,2),THN(100,2),THW(100,2),DTH(100,2),
     1 VX(100,2),VXP(100,2),VXW(100,2)
      COMMON/GEOM/X(101),BB(2),DCOSB(2),DCOS(2),DELT,CHNG,DELMAX,TMAX,
     1 IPX(101),IE(100,3),NPN(2),NPST(2),NPTST(2),NBE(2),NTSE(2), ISB(2,
     1 2),IS(2,2),NNP,NEL,NMAT,IBAND,NBC,NST,NTST,NBEL,NTI,NNOR
      COMMON/MRVAR/ A(101,2),B(101,3),R(101),RP(101),RI(101),RB(101),
     1 DP(101),R1(101),RT(101),XTMP(101),BFLX(101),BFLXP(101), FX(100,2)
     1 ,FRATE(10),FLOW(10),TFLOW(10),W,PMAT(3,5)
C
C  ******************************************************************
C
      ENTRY STRMI
      PUNCH 10000, (TITLE(I),I=1,8)
      PUNCH 10100,NNP
      PUNCH 10200, (X(NP),NP=1,NNP)
      RETURN
C
C  ******************************************************************
C
      ENTRY STRMT
      PUNCH 10200,TIME
      PUNCH 10200,(R(NP),NP=1,NNP)
      RETURN
10000 FORMAT(8A8)
10100 FORMAT(16I5)
10200 FORMAT(8E10.4)
      END
      SUBROUTINE SURF
C
C
C  FUNCTION OF SUBROUTINE--TO IDENTIFY BOUNDING NODES THRU THE ARRAY
C  ISB(NP,2).
```

```
C
C
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON/GEOM/X(101),BB(2),DCOSB(2),DCOS(2),DELT,CHNG,DELMAX,TMAX,
     1 IPX(101),IE(100,3),NPN(2),NPST(2),NPTST(2),NBE(2),NTSE(2), ISB(2,
     1 2),IS(2,2),NNP,NEL,NMAT,IBAND,NBC,NST,NTST,NBEL,NTI,NNOR
C
C  FIND SURFACE NODES BY LOCATING NON-DUPLICATED NODES.
C
      NBEL=0
      DO 40 MI=1,NEL
         DO 30 IQ=1,2
            DO 20 MJ=1,NEL
               IF (MJ.EQ.MI) GO TO 20
               DO 10 JQ=1,2
                  IF (IE(MI,IQ).EQ.IE(MJ,JQ)) GO TO 30
   10             CONTINUE
   20          CONTINUE
            NBEL=NBEL+1
            NBE(NBEL)=MI
            ISB(NBEL,1)=IE(MI,IQ)
            ISB(NBEL,2)=IQ
   30       CONTINUE
   40    CONTINUE
C
C  CALCULATE DIRECTION COSINES.
C
      DO 50 MP=1,NBEL
         M=NBE(MP)
         NI=IE(M,1)
         NJ=IE(M,2)
         X0=0.5*(X(NI)+X(NJ))
         NP=ISB(MP,1)
         DCOSB(MP)=1.
         IF (X0.GT.X(NP)) DCOSB(MP)=-1.
   50    CONTINUE
      RETURN
      END
      SUBROUTINE SFLOW(FX,R,BFLX,BFLXP,FRATE,FLOW,TFLOW,TH,MAXEL,MAXNP)
C
C
C  FUNCTION OF SUBROUTINE--TO COMPUTE BOUNDARY FLUXES, FLOW RATES,
C  INCREMENTAL FLOWS OCCURRING DURING TIME DELT, TOTAL FLOWS SINCE
C  TIME ZERO, AND THE CHANGE IN MOISTURE CONTENT FOR THE ENTIRE
C  SYSTEM DURING TIME DELT.
C
C
      IMPLICIT REAL*8 (A-H,O-Z)
      REAL*8 KD,LAMBDA
      COMMON/GEOM/X(101),BB(2),DCOSB(2),DCOS(2),DELT,CHNG,DELMAX,TMAX,
     1 IPX(101),IE(100,3),NPN(2),NPST(2),NPTST(2),NBE(2),NTSE(2), ISB(2,
     1 2),IS(2,2),NNP,NEL,NMAT,IBAND,NBC,NST,NTST,NBEL,NTI,NNOR
      COMMON/MPROP/PROP(1,5),WXI
      DIMENSION FX(MAXEL,2),BFLX(MAXNP),BFLXP(MAXNP),XQ(2), RQ(2),
     1 FRATE(10),FLOW(10),TFLOW(10),R(MAXNP),TH(MAXEL,2)
      DATA QR,QD,QL/0.D0,0.D0,0.D0/
C
C  CALCULATE NODAL FLOW RATES.
C
      DO 10 NP=1,NNP
         BFLXP(NP)=BFLX(NP)
   10    BFLX(NP)=0.
      DO 20 MP=1,NBEL
         M=NBE(MP)
         NP=ISB(MP,1)
         IQ=ISB(MP,2)
         BFLX(NP)=FX(M,IQ)*DCOSB(MP)
   20    CONTINUE
C
C  DETERMINE FLOWS AND FLOW RATES THRU THE VARIOUS
C  TYPES OF BOUNDARY NODES, STARTING WITH THE
C  NET FLOWS THROUGH ALL BOUNDARY NODES.
C
      S=0.
      SP=0.
```

```
      DO 30 NP=1,NNP
         S=S+BFLX(NP)
   30    SP=SP+BFLXP(NP)
      FRATE(5)=S
      FLOW(5)=.5*(S+SP)*DELT
C
C  CONSTANT DIRICHLET BOUNDARY NODES.
C
      FRATE(1)=0.
      FLOW(1)=0.
      IF (NBC.LE.0) GO TO 50
      S=0.
      SP=0.
      DO 40 NPP=1,NBC
         NP=NPN(NPP)
         S=S+BFLX(NP)
   40    SP=SP+BFLXP(NP)
      FRATE(1)=S
      FLOW(1)=.5*(S+SP)*DELT
C
C  CONSTANT NEUMANN BOUNDARY NODES.
C
   50 FRATE(2)=0.
      FLOW(2)=0.
      IF (NST.LE.0) GO TO 70
      S=0.
      SP=0.
      DO 60 NPP=1,NST
         NP=NPST(NPP)
         S=S+BFLX(NP)
   60    SP=SP+BFLXP(NP)
      FRATE(2)=S
      FLOW(2)=.5*(S+SP)*DELT
C
C  TRANSIENT SEEPAGE BOUNDARY NODES.
C
   70 FRATE(3)=0.
      FLOW(3)=0.
      IF (NTST.LE.0) GO TO 90
      S=0.
      SP=0.
      DO 80 NPP=1,NTST
         NP=NPTST(NPP)
         S=S+BFLX(NP)
   80    SP=SP+BFLXP(NP)
      FRATE(3)=S
      FLOW(3)=.5*(S+SP)*DELT
C
C  NUMERICAL FLOW THROUGH UNSPECIFIED BOUNDARY NODES.
C
   90 S=0.
      SP=0.
      DO 100 I=1,3
         S=S+FRATE(I)
  100    SP=SP+FLOW(I)
      FRATE(4)=FRATE(5)-S
      FLOW(4)=FLOW(5)-SP
C
C  CALCULATE THE INCREASES IN THE INTEGRATED MATERIAL CONTENTS FOR THE
C  FLUID AND THE SOLID PHASES AND DETERMINE LOSSES DUE TO RADIOACTIVE
C  DECAY.
C
      QRP=QR
      QDP=QD
      QLP=QL
      QR=0.
      QD=0.
      QL=0.
      DO 120 M=1,NEL
         MTYP=IE(M,3)
         KD=PROP(MTYP,1)
         RHOB=PROP(MTYP,2)
         LAMBDA=0.
         POR=PROP(MTYP,5)
         DO 110 IQ=1,2
```

```
              NP=IE(M,IQ)
              XQ(IQ)=X(NP)
  110         RQ(IQ)=R(NP)*TH(M,IQ)
           CALL Q4R(RQ,QRM,XQ)
           QR=QR+QRM
           QDM=RHOB*KD*QRM/POR
           QD=QD+QDM
           QLM=QRM+QDM
           QL=QL+LAMBDA*QLM
  120      CONTINUE
        FLOW(6)=QR-QRP
        FRATE(6)=FLOW(6)/DELT
        FLOW(7)=QD-QDP
        FRATE(7)=FLOW(7)/DELT
        FRATE(8)=-.5*(QL+QLP)
        FLOW(8)=DELT*FRATE(8)
        DO 130 I=1,8
  130      TFLOW(I)=TFLOW(I)+FLOW(I)
        RETURN
        END
        SUBROUTINE Q4R(RQ,QRM,XQ)
C
C
C  FUNCTION OF SUBROUTINE--TO EVALUATE THE CONCENTRATION INTEGRAL
C  OVER THE LENGTH OF ONE ELEMENT.
C
C
        IMPLICIT REAL*8 (A-H,O-Z)
        REAL*8 N(2)
        DIMENSION RQ(2),S(2),XQ(2)
        DATA P / 0.577350269189626 /, S / -1.0D+00, 1.0D+00 /
C
C  EVALUATE QUANTITIES FOR USE IN THE JACOBIAN DJAC, BELOW, NECESSARY
C  FOR TRANSFORMATION FROM GLOBAL TO LOCAL COORDINATES.
C
        X21 = XQ(2) - XQ(1)
        QRM=0.
        DO 20 KG=1,2
C
C  DETERMINE LOCAL COORDINATES SS OF GAUSS-INTEGRATION POINT KG.
C
           SS = P*S(KG)
C
C  EVALUATE THE JACOBIAN DJAC
C
           DJ = X21
           DJAC = 0.5*DJ
C
C  CALCULATE VALUES OF THE BASIS-INTERPOLATION FUNCTIONS N(IQ).
C
           SM = 1.0 - SS
           SP = 1.0 + SS
           N(1)=0.5*SM
           N(2)=0.5*SP
C
C  INTERPOLATE TO OBTAIN THE CONCENTRATION RQP AT THE GAUSS POINT KG.
C
           RQP=0.
           DO 10 IQ=1,2
   10         RQP=RQP+RQ(IQ)*N(IQ)
C
C  ACCUMULATE THE SUM TO EVALUATE THE INTEGRAL QRM.
C
           QRM=QRM+RQP*DJAC
   20      CONTINUE
        RETURN
        END
        SUBROUTINE SOLVE(KKK,C,R,NNP,IHALFB,MAXNP,MAXBW)
C
C
C  FUNCTION OF SUBROUTINE--TO SOLVE THE MATRIX EQUATION CX = R,
C  RETURNING THE SOLUTION X IN R.  IT IS ASSUMED THAT THE ARRAY C(NP,IB)
C  CONTAINS THE FULL BAND OF AN ASYMMETRIC MATRIX.
C
C
```

```
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION C(MAXNP,MAXBW),R(MAXNP)
      IHBP=IHALFB+1
C
C  IF KKK = 1, THEN TRIANGULARIZE THE BAND MATRIX C(NP,IB), BUT
C  IF KKK = 2, THEN SIMPLY SOLVE WITH THE RIGHT-HAND SIDE R(NP)
C
      IF (KKK.EQ.2) GO TO 50
C
C  TRIANGULARIZE MATRIX C(NP,IB).
C
      NU=NNP-IHALFB
      DO 20 NI=1,NU
         PIVOTI=1./C(NI,IHBP)
         NJ=NI+1
         IB=IHBP
         NK=NI+IHALFB
         DO 10 NL=NJ,NK
            IB=IB-1
            A=-C(NL,IB)*PIVOTI
            C(NL,IB)=A
            JB=IB+1
            KB=IB+IHALFB
            LB=IHBP-IB
            DO 10 MB=JB,KB
               NB=LB+MB
   10          C(NL,MB)=C(NL,MB)+A*C(NI,NB)
   20    CONTINUE
      NR=NU+1
      NU=NNP-1
      NK=NNP
      DO 40 NI=NR,NU
         PIVOTI=1./C(NI,IHBP)
         NJ=NI+1
         IB=IHBP
         DO 30 NL=NJ,NK
            IB=IB-1
            A=-C(NL,IB)*PIVOTI
            C(NL,IB)=A
            JB=IB+1
            KB=IB+IHALFB
            LB=IHBP-IB
            DO 30 MB=JB,KB
               NB=LB+MB
   30          C(NL,MB)=C(NL,MB)+A*C(NI,NB)
   40    CONTINUE
      RETURN
C
C  MODIFY LOAD VECTOR R(NP).
C
   50 NU=NNP+1
      IBAND=2*IHALFB+1
      DO 70 NI=2,IHBP
         IB=IHBP-NI+1
         NJ=1
         SUM=0.0
         DO 60 JB=IB,IHALFB
            SUM=SUM+C(NI,JB)*R(NJ)
   60       NJ=NJ+1
   70    R(NI)=R(NI)+SUM
      IB=1
      NL=IHBP+1
      DO 90 NI=NL,NNP
         NJ=NI-IHBP+1
         SUM=0.0
         DO 80 JB=IB,IHALFB
            SUM=SUM+C(NI,JB)*R(NJ)
   80       NJ=NJ+1
   90    R(NI)=R(NI)+SUM
C
C  BACK SOLVE.
C
      R(NNP)=R(NNP)/C(NNP,IHBP)
      DO 110 IB=2,IHBP
         NI=NU-IB
```

```
      NJ=NI
      MB=IHALFB+IB
      SUM=0.0
      DO 100 JB=NL,MB
         NJ=NJ+1
  100    SUM=SUM+C(NI,JB)*R(NJ)
  110 R(NI)=(R(NI)-SUM)/C(NI,IHBP)
      MB=IBAND
      DO 130 IB=NL,NNP
         NI=NU-IB
         NJ=NI
         SUM=0.0
         DO 120 JB=NL,MB
            NJ=NJ+1
  120       SUM=SUM+C(NI,JB)*R(NJ)
  130    R(NI)=(R(NI)-SUM)/C(NI,IHBP)
      RETURN
      END
      SUBROUTINE WTR
C
C
C  FUNCTION OF SUBROUTINE--TO DETERMINE ONE-DIMENSIONAL MOISTURE TRANSPO
C  USING THE ANALYTIC METHOD OF PARLANGE.
C
C
      IMPLICIT REAL*8(A-H,O-Z)
      REAL*4 PMAT
      COMMON/CTRL/KPGM,KWTR,KWI,KSTRM,KSTRW,ISTOP,KSS,KDIG,KMOUT, KWOUT,
     1 KTSTP,KSOUT,KSRCH,KBUFF,KANL,KIC,KSTRS
      COMMON/CRVAR/TIME,TH(100,2),THM(100,2),THW(100,2),DTH(100,2),
     1 VX(100,2),VXP(100,2),VXW(100,2)
      COMMON/GEOM/X(101),BB(2),DCOSB(2),DCOS(2),DELT,CHNG,DELMAX,TMAX,
     1 IPX(101),IE(100,3),NPN(2),NPST(2),NPTST(2),NBE(2),NTSE(2), ISB(2,
     1 2),IS(2,2),NNP,NEL,NMAT,IBAND,NBC,NST,NTST,NBEL,NTI,NNOR
      COMMON/MIVAR/KPRQ,KPR(1000),MAXDIF,MAXEL,MAXNP,MAXMAT,MAXBW,
     1 MAXNTI,NMPPM
      COMMON/MRVAR/ A(101,2),B(101,3),R(101),RP(101),RI(101),RB(101),
     1 DP(101),R1(101),RT(101),XTMP(101),BFLX(101),BFLXP(101), FX(100,2)
     1 ,PRATE(10),FLOW(10),TFLOW(10),W,PMAT(3,5)
      COMMON/BI/ TH1,TH0,THB,SINEPS
      COMMON/CW1/ W1,V1
      COMMON/NUMITG/ NORDR1,NORDER,NITP,ITHMIN,IGSS,ITMIN, IGSSV(3)
      COMMON/TFLX/TTAB(50),V1N(50),V1TAB(50),W1TAB(50),UTAB(50),
     1 TTABL(50),W1TABL(50),TEMP(50),IPTTAB(50),NTTAB
      COMMON/WPROP/AKPAR(50),CDPAR(50),AKSN(25),ALPK(25),D(25), ALPD(25)
     1 ,AKSAT,AKSN0,NKPAR,NKSP,NCDPAR,NDSP
      COMMON/XVAR/XSUP1(50),XSUP2(50),THP(50),ALP(50),VSUP1(50),
     1 VSUP2(50),F(50),QGA(50),QG(50),THTMP(50),AKGSS(212), DGSS(212),
     1 IPTTH(50),NTH,JTH,NGSS
      EXTERNAL TLFUN,TQFUN,TIFUN,TOFUN,GFUN,GAFUN,GSFUN,G2FUN
      DATA IND1/0/,TZMX/0.025/
C
C ********************************************************************
C
      ENTRY WINL
      KWOUT=0
      NTHP=NTH+1
      NTHM=NTH-1
C
C  CALCULATE TABULAR FUNCTION OF REDUCED VELOCITY W1TAB VS. TIME TTAB.
C
      IFP=1
      DO 70 IT=1,NTTAB
         DO 10 I=1,3
            IGSSV(I)=0
   10       CONTINUE
         W1=W1TAB(IT)
         ZMX=(AKSAT*SINEPS-AKSN0)/(THB*W1)
         IF (ZMX.LT.TZMX) GO TO 40
         IF (SINEPS.EQ.0.D0) GO TO 40
         TL=0.
         TQ=0.
         TI=0.
         NRDRP=NORDER
         DO 20 ITH=1,NTHM
```

```
            JTH=ITH+1
            IF (ITH.EQ.NTHM) NRDRP=NORDR1
            CALL GAUSS(ALP(ITH),ALP(JTH),TLA,TLFUN,NRDRP)
            CALL GAUSS(ALP(ITH),ALP(JTH),TQA,TQFUN,NRDRP)
            CALL GAUSS(ALP(ITH),ALP(JTH),TIA,TIFUN,NRDRP)
            TL=TL+TLA
            TQ=TQ+TQA
            TI=TI+TIA
   20       CONTINUE
         IF (TQ.LT.TL) GO TO 30
         PRINT 10000, V1N(IT)
         GO TO 40
   30    TTAB(IT)=TL-TQ
         UTAB(IT)=TTAB(IT)*V1TAB(IT)-W1TAB(IT)*THB*TL+THB*TI
         GO TO 70
   40    IF (IFP.NE.1) GO TO 60
         IFP=0
         TO=0.
         IGSS=0
         NRDRP=NORDER
         DO 50 ITH=1,NTHM
            JTH=ITH+1
            IF (ITH.EQ.NTHM) NRDRP=NORDR1
            CALL GAUSS(ALP(ITH),ALP(JTH),TOA,TOFUN,NRDRP)
            TO=TO+TOA
   50       CONTINUE
   60    W1I=1./W1
         TTAB(IT)=.5*W1I*W1I*TO
         UTAB(IT)=TTAB(IT)*V1TAB(IT)+.5*THB*W1I*TO
   70    CONTINUE
C
C   PUT TABULAR ARRAYS IN ASCENDING ORDER.
C
      CALL DSORT(TTAB,IPTTAB,NTTAB)
      DO 80 IT=1,NTTAB
         IP=IPTTAB(IT)
         TEMP(IT)=W1TAB(IP)
   80    CONTINUE
      DO 90 IT=1,NTTAB
         W1TAB(IT)=TEMP(IT)
   90    CONTINUE
      DO 100 IT=1,NTTAB
         IP=IPTTAB(IT)
         TEMP(IT)=V1TAB(IP)
  100    CONTINUE
      DO 110 IT=1,NTTAB
         V1TAB(IT)=TEMP(IT)
  110    CONTINUE
      DO 120 IT=1,NTTAB
         IP=IPTTAB(IT)
         TEMP(IT)=V1N(IP)
  120    CONTINUE
      DO 130 IT=1,NTTAB
         V1N(IT)=TEMP(IT)
  130    CONTINUE
      DO 140 IT=1,NTTAB
         IP=IPTTAB(IT)
         TEMP(IT)=UTAB(IP)
  140    CONTINUE
      DO 150 IT=1,NTTAB
         UTAB(IT)=TEMP(IT)
  150    CONTINUE
C
C   PREPARE TABULAR ARRAY FOR LOG-LOG INTERPOLATION.
C
      DO 160 I=1,NTTAB
         TTABL(I)=DLOG(TTAB(I))
         W1TABL(I)=DLOG(W1TAB(I))
  160    CONTINUE
      RETURN
C
C   ***********************************************************************
C
      ENTRY WINTP(T)
C
```

```
C  GIVEN T VALUE, INTERPOLATE TO FIND W1 VALUE.
C
      IF (T.LT.TTAB(1)) PRINT 10100,T,TTAB(1)
      IF (T.GT.TTAB(NTTAB)) PRINT 10200,T,TTAB(NTTAB)
      TP=DLOG(T)
      W1P=YLAG(TP,TTABL,W1TABL,IND1,NITP,ITMIN,NTTAB,IEX)
      W1=DEXP(W1P)
      V1=THB*W1-AKSN0
      RETURN
C
C  ***********************************************************************
C
      ENTRY WTIME(T)
      DO 170 I=1,3
         IGSSV(I)=0
  170    CONTINUE
      NRDRP=NORDER
      IF (SINEPS.EQ.0.D0) GO TO 190
      TL=0.
      TQ=0.
      TI=0.
      DO 180 ITH=1,NTHM
         JTH=ITH+1
         IF (ITH.EQ.NTHM) NRDRP=NORDR1
C
C  RECALCULATE T.
C
         CALL GAUSS(ALP(ITH),ALP(JTH),TLA,TLFUN,NRDRP)
         CALL GAUSS(ALP(ITH),ALP(JTH),TQA,TQFUN,NRDRP)
         CALL GAUSS(ALP(ITH),ALP(JTH),TIA,TIFUN,NRDRP)
         TL=TL+TLA
         TQ=TQ+TQA
         TI=TI+TIA
  180    CONTINUE
      TW=TL-TQ
      T=TW
      RETURN
  190 TO=0.
      IGSS=0
      W1I=1./W1
      DO 200 ITH=1,NTHM
         JTH=ITH+1
         IF (ITH.EQ.NTHM) NRDRP=NORDR1
         CALL GAUSS(ALP(ITH),ALP(JTH),TOA,TOFUN,NRDRP)
         TO=TO+TOA
  200    CONTINUE
      TW=.5*W1I*W1I*TO
      RETURN
C
C  ***********************************************************************
C
      ENTRY WTRN1
C
C  CALCULATE FIRST-ORDER POSITIONS AND VELOCITIES.
C
      IGSS=0
      NRDRP=NORDER
      XSUP1(NTH)=0.0
      VSUP1(NTH)=V1
      DO 210 ITH=1,NTHM
         JTH=ITH+1
         IF (ITH.EQ.NTHM) NRDRP=NORDR1
         CALL GAUSS(ALP(ITH),ALP(JTH),XSUP1(ITH),GFUN,NRDRP)
  210    CONTINUE
      DO 220 ITB=1,NTHM
         ITH=NTH-ITB
         JTH=ITH+1
         XSUP1(ITH)=XSUP1(JTH)+XSUP1(ITH)
         VSUP1(ITH)=V1
  220    CONTINUE
      RETURN
C
C  ***********************************************************************
C
      ENTRY WTRN2
```

```
C
C  DETERMINE CORRECTION FRACTION F.
C
      QGA(1)=0.0
      IGSS=0
      NRDRP=NORDER
      DO 230 ITH=1,NTHM
         JTH=ITH+1
         IF (ITH.EQ.NTHM) NRDRP=NORDR1
         CALL GAUSS(ALP(ITH),ALP(JTH),DQ,GAFUN,NRDRP)
         QGA(JTH)=QGA(ITH)+DQ
  230    CONTINUE
      IGSS=0
      NRDRP=NORDER
      QG(NTH)=0.
      DO 240 ITH=1,NTHM
         JTH=ITH+1
         IF (ITH.EQ.NTHM) NRDRP=NORDR1
         CALL GAUSS(ALP(ITH),ALP(JTH),QG(ITH),GSFUN,NRDRP)
  240    CONTINUE
      DO 250 ITB=1,NTHM
         ITH=NTH-ITB
         JTH=ITH+1
         QG(ITH)=QG(JTH)+QG(ITH)
  250    CONTINUE
      DNI=1./QGA(NTH)
      F(1)=0.
      DO 260 ITH=2,NTH
         F(ITH)=(QGA(ITH)+ALP(ITH)*QG(ITH))*DNI
  260    CONTINUE
C
C  CALCULATE SECOND-ORDER POSITIONS AND VELOCITIES.
C
      IGSS=0
      ITHMIN=1
      NRDRP=NORDER
      XSUP2(NTH)=0.0
      VSUP2(NTH)=V1
      DO 270 ITH=1,NTHM
         JTH=ITH+1
         IF (ITH.EQ.NTHM) NRDRP=NORDR1
         CALL GAUSS(ALP(ITH),ALP(JTH),XSUP2(ITH),G2FUN,NRDRP)
  270    CONTINUE
      DO 280 ITB=1,NTHM
         ITH=NTH-ITB
         JTH=ITH+1
         XSUP2(ITH)=XSUP2(JTH)+XSUP2(ITH)
         VSUP2(ITH)=THB*W1*F(ITH)-AKSNO
  280    CONTINUE
      RETURN
C
C  ******************************************************************************
C
      ENTRY NWLINK
C
C  DETERMINE LINKAGE VARIABLES VX AND TH.
C
      CALL DSORT(XSUP2,IPTTH,NTH)
      DO 290 NP=1,NTH
         NPI=IPTTH(NP)
         THTMP(NPI)=VSUP2(NP)
  290    CONTINUE
      XMX=XSUP2(NTH)
      VMN=THTMP(NTH)
      IXMIN=1
      DO 310 NP=1,NNP
         IF (X(NP).LT.XMX) GO TO 300
         XTMP(NP)=VMN
         GO TO 310
  300    XTMP(NP)=YLAG(X(NP),XSUP2,THTMP,IND1,NITP,IXMIN,NTH,IEX)
  310    CONTINUE
      DO 320 N=1,NEL
         DO 320 IQ=1,2
            NP=IE(N,IQ)
            VX(N,IQ)=XTMP(NP)
```

```
  320         CONTINUE
      DO 330 NP=1,NTH
         NPI=IPTTH(NP)
         THTMP(NPI)=THP(NP)
  330    CONTINUE
      THMN=THTMP(NTH)
      IXMIN=1
      DO 350 NP=1,NNP
         IF (X(NP).LT.XMX) GO TO 340
         XTMP(NP)=THMN
         GO TO 350
  340    XTMP(NP)=YLAG(X(NP),XSUP2,THTMP,IND1,NITP,IXMIN,NTH,IEX)
  350    CONTINUE
      DO 360 M=1,NEL
         DO 360 IQ=1,2
            NP=IE(M,IQ)
            TH(M,IQ)=XTMP(NP)
  360       CONTINUE
      RETURN
10000 FORMAT(' NOTICE: A NUMERICAL ERROR OCCURRED IN THE TABULAR '
     1 'TIME CALCULATION FOR W1N =',E12.4)
10100 FORMAT(' NOTICE: THE TIME'E12.4,
     1 ' IS LESS THAN THE LEAST TABULAR VALUE'E12.4)
10200 FORMAT(' NOTICE: THE TIME'E12.4,
     1 ' IS GREATER THAN THE GREATEST TABULAR VALUE'E12.4)
      END
      SUBROUTINE DATAW
C
C
C  FUNCTION OF SUBROUTINE--TO READ, PRINT, AND CHECK WATER-TRANSPORT
C  VARIABLES PERTAINING TO SOIL PROPERTIES, BOUNDARY-INITIAL CONDITIONS,
C  NODAL POSITONS IN BOTH TIME AND WATER CONTENTS, AND MISCELLANEOUS
C  OTHER INFORMATION.
C
C
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON/CTRL/KPGM,KWTR,KVI,KSTRM,KSTRW,ISTOP,KSS,KDIG,KMOUT, KWOUT,
     1 KTSTP,KSOUT,KSRCH,KBUFF,KANL,KIC,KSTRS
      COMMON/MPROP/PROP(1,5),VXI
      COMMON/BI/ TH1,TH0,THB,SINEPS
      COMMON/NUMITG/ NORDR1,NORDER,NITP,ITHMIN,IGSS,ITMIN, IGSSV(3)
      COMMON/TFLX/TTAB(50),V1N(50),V1TAB(50),W1TAB(50),UTAB(50),
     1 TTABL(50),W1TABL(50),TEMP(50),IPTTAB(50),NTTAB
      COMMON/THTB/T(50),NT
      COMMON/WPROP/AKPAR(50),CDPAR(50),AKSN(25),ALPK(25),D(25), ALPD(25)
     1 ,AKSAT,AKSN0,NKPAR,NKSP,NCDPAR,NDSP
      COMMON/XVAR/XSUP1(50),XSUP2(50),THP(50),ALP(50),VSUP1(50),
     1 VSUP2(50),F(50),QGA(50),QG(50),THTMP(50),AKGSS(212), DGSS(212),
     1 IPTTH(50),NTH,JTH,NGSS
      EXTERNAL DUMFUN
      DIMENSION NORDRA(2)
      DATA PI/3.1415926536D0/
C
C  ************************************************************************
C
      ENTRY DINW
C
C  I/O OF NON-ARRAY INTEGER AND REAL PARAMETERS.
C
      READ 10000,KWTR,NTTAB,NT,NTH,NKPAR,NCDPAR,NORDRA(1),NORDRA(2),
     1 NITP,KSTRW,KMESH,KANL
      IF (KSTRW.NE.0) KSTRW=1
      DO 20 I=1,2
         IF (NORDRA(I).LT.2) GO TO 10
         IF (NORDRA(I).LT.15) GO TO 20
         IF (NORDRA(I).EQ.16) GO TO 20
         NORDRA(I)=16
         GO TO 20
   10    NORDRA(I)=2
   20    CONTINUE
      NORDER=NORDRA(1)
      NORDR1=NORDRA(2)
      IF (KPGM.NE.2) KWTR=2
      PRINT 10300,KWTR,NTTAB,NT,NTH,NKPAR,NCDPAR,NORDER,NORDR1,NITP,
     1 KSTRW ,KMESH,KANL
```

```
      READ 10400, TH0,TH1,EPS,DALP1
      PRINT 10500, TH0,TH1,EPS,DALP1
      THB=TH1-TH0
      DTH1=THB*DALP1
      SINEPS=DSIN(EPS*(PI/180.D0))
      IF (EPS.EQ.0.D0) SINEPS=0.D0
C
C  I/O OF SOIL PROPERTIES.
C
      READ 10400, (AKPAR(I),I=1,NKPAR)
      PRINT 10600, (AKPAR(I),I=1,NKPAR)
      READ 10400, (CDPAR(I),I=1,NCDPAR)
      PRINT 10700, (CDPAR(I),I=1,NCDPAR)
C
C  I/O OF TABULAR END-POINT DARCY VELOCITIES IN UNITS OF SATURATED
C  CONDUCTIVITY.
C
      READ 10400, (V1N(I),I=1,NTTAB)
      PRINT 10800, (V1N(I),I=1,NTTAB)
C
C  CONDITIONAL I/O OF THE TIME VALUES.
C
   30 IF (KPGM.NE.2) GO TO 40
      IF (KWTR.EQ.0) GO TO 40
      READ 10400,(T(I),I=1,NT)
      PRINT 10100,(T(I),I=1,NT)
   40 RETURN
C
C  ***********************************************************************
C
      ENTRY PWCAL
C
C  PRELIMINARY WATER-TRANSPORT CALCULATIONS.
C
C
C  GENERATION OF THE WATER CONTENTS.
C
      NTHM=NTH-1
      THB=TH1-TH0
      DTH1=THB*DALP1
      IF (KANL.EQ.0) DUMMY=SPROPI(DUMMY)
      IF (KANL.NE.0) DUMMY=SPANLI(DUMMY)
      DTH=(TH1-TH0)/DFLOAT(NTHM)
      THP(1)=TH0
      THP(NTH)=TH1
      IF (KMESH.NE.0) GO TO 60
      DO 50 I=2,NTHM
         THP(I)=THP(I-1)+DTH
   50    CONTINUE
      GO TO 80
   60 NV=NTHM
      NVM=NV-1
      DTHAV=DTH
      SDTH=2.*(DTHAV-DTH1)/DFLOAT(NVM)
      DTHI=DTH1
      DO 70 JV=1,NVM
         IV=NTH-JV
         THP(IV)=THP(IV+1)-DTHI
         DTHI=DTHI+SDTH
   70    CONTINUE
      THP(1)=TH0
   80 DO 90 I=1,NTH
         ALP(I)=(THP(I)-TH0)/THB
   90    CONTINUE
C
C  CALCULATION OF TABULAR VELOCITIES.
C
      DO 100 I=1,NTTAB
  100    V1TAB(I)=V1N(I)*AKSAT
      DO 110 I=1,NTTAB
  110    W1TAB(I)=(V1TAB(I)+AKSN0)/THB
C
C  PREPARATION OF THE GAUSS GRID OF SOIL PROPERTIES.
C
      IGSS=0
```

```
      NRDRP=NORDER
      DO 120 ITH=1,NTHM
         JTH=ITH+1
         IF (ITH.EQ.NTHM) NRDRP=NORDR1
         CALL GAUSS(ALP(ITH),ALP(JTH),DUMMY,DUMFUN,NRDRP)
  120    CONTINUE
      NGSS=IGSS
      IF (KPGM.EQ.5) GO TO 130
      IF (KPGM.EQ.7) GO TO 130
      IF (KSRCH.NE.0) PRINT 10200
C
C  OUTPUT OF THE WATER CONTENTS.
C
      PRINT 10900, (THP(I),I=1,NTH)
      PRINT 11000, (ALP(I),I=1,NTH)
  130 RETURN
C
10000 FORMAT(16I5)
10100 FORMAT(/' T:'/(8E15.7))
10200 FORMAT(////' WATER-TRANSPORT INPUT TABLE 8.. BASIC PARAMETERS')
10300 FORMAT(////' WATER-TRANSPORT INPUT TABLE 8.. BASIC PARAMETERS'//
     15X,                                                            '
     1FUNCTION TYPE . . . . . . . . . . . . . . . . . . . . . . .',I5/ 5X,'
     1NUMBER OF TABULAR TIME NODES. . . . . . . . . . . . . . . .',I5/ 5X,'
     1NUMBER OF TIME NODES FOR STAND-ALONE OPERATION. . . . . .',I5/ 5X,'
     1NUMBER OF THETA VALUES. . . . . . . . . . . . . . . . . .',I5/ 5X,'
     1NUMBER OF CONDUCTIVITY SOIL PARAMETERS. . . . . . . . . .',I5/ 5X,'
     1NUMBER OF CAPACITY OR DIFFUSIVITY SOIL PARAMETERS . . . .',I5/ 5X,'
     1ORDER OF LEGENDRE-GAUSS INTEGRATION . . . . . . . . . . .',I5/ 5X,'
     1ORDER NEAR ALPHA = 1. . . . . . . . . . . . . . . . . . .',I5/ 5X,'
     1NUMBER OF POINTS IN INTERPOLATING POLYNOMIAL. . . . . . .',I5/ 5X,'
     1AUXILIARY STORAGE CONTROL . . . . . . . . . . . . . . . .',I5/ 5X,'
     1VARIABLE-MESH CONTROL . . . . . . . . . . . . . . . . . .',I5/ 5X,'
     1ANALYTIC SOIL-PROPERTIES CONTROL. . . . . . . . . . . . .',I5)
10400 FORMAT(8F10.0)
10500 FORMAT(5X ' INITIAL CONDITION ON WATER CONTENT THETA. . . . . ',
     1 E10.4/ 5X, ' BOUNDARY CONDITION ON WATER CONTENT THETA . . . . ',
     1 E10.4/ 5X, ' INCLINATION IN DEGREES. . . . . . . . . . . . . . ',
     1 E10.4/ 5X, ' ALPHA INCREMENT NEAR ALPHA = 1. . . . . . . . . . ',
     1 E10.4)
10600 FORMAT(/' AKPAR:'/( 8E15.7))
10700 FORMAT(/' CDPAR:'/(8E15.7))
10800 FORMAT(/' V1/AKSAT:'/(8E15.7))
10900 FORMAT(/' THP:'/(8E15.7))
11000 FORMAT(/' ALP:'/(8E15.7))
11100 FORMAT(20A4)
11200 FORMAT(1H0,20A4)
      END
      SUBROUTINE DSORT(XPT,IPT,NPT)
C
C
C  FUNCTION OF SUBROUTINE--TO TRANSFORM ARRAY XPT INTO ASCENDING
C  ORDER AND OBTAIN THE PREMUTATIVE TRANSFORMATION IPT.
C
C
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION XPT(1),IPT(1)
      DO 10 I=1,NPT
   10    IPT(I)=I
      L=NPT
   20 L=L/2
      IF (L.EQ.0) RETURN
      K=NPT-L
      J=1
   30 I=J
   40 IL=I+L
      IF (XPT(I).LE.XPT(IL)) GO TO 50
      TEMP=XPT(I)
      ITEMP=IPT(I)
      XPT(I)=XPT(IL)
      IPT(I)=IPT(IL)
      XPT(IL)=TEMP
      IPT(IL)=ITEMP
      I=I-L
      IF (I.GE.1) GO TO 40
```

```
   50 J=J+1
      IF (J.GT.K) GO TO 20
      GO TO 30
      END
      FUNCTION SPROP(DUMMY)
C
C
C  FUNCTION OF ROUTINE--INTERPOLATION TO DETERMINE BOTH
C  CONDUCTIVITY AND DIFFUSIVITY.
C
C
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON/BI/ TH1,TH0,THB,SINEPS
      COMMON/NUMITG/ NORDR1,NORDER,NITP,ITHMIN,IGSS,ITMIN, IGSSV(3)
      COMMON/WPROP/AKPAR(50),CDPAR(50),AKSN(25),ALPK(25),D(25), ALPD(25)
     1 ,AKSAT,AKSN0,NKPAR,NKSP,NCDPAR,NDSP
      COMMON/XVAR/XSUP1(50),XSUP2(50),THP(50),ALP(50),VSUP1(50),
     1 VSUP2(50),F(50),QGA(50),QG(50),THTMP(50),AKGSS(212), DGSS(212),
     1 IPTTH(50),NTH,JTH,NGSS
      DATA ALP0/0.0D0/,ALP1/1.D0/,IND1/0/
C
C  *********************************************************************
C
      ENTRY SPROPI(DUMMY)
C
C  SECTION SPROPI INITIALIZES THE SOIL-PROPERTY ARRAYS.
C
      NKSP=NKPAR/2
      NDSP =NCDPAR/2
C
C  EXTRACT CONDUCTIVITY VARIABLES FROM INPUT ARRAY AKPAR.
C
      J=0
      DO 10 I=1,NKPAR,2
         J=J+1
         THT=AKPAR(I)
         ALPK(J)=(THT-TH0)/THB
         AK=AKPAR(I+1)
         AKSN(J)=DLOG(AK)
   10    CONTINUE
C
C  INTERPOLATE TO FIND AKSN0 AT ALP = 0.
C
      IKMIN=1
      AK=YLAG(ALP0,ALPK,AKSN,IND1,NITP,IKMIN,NKSP,IEX)
      AK0=DEXP(AK)
      AKSN0=AK0*SINEPS
      IKMIN=1
      AK=YLAG(ALP1,ALPK,AKSN,IND1,NITP,IKMIN,NKSP,IEX)
      AKSAT=DEXP(AK)
C
C  EXTRACT DIFFUSIVITY VARIABLES FROM INPUT ARRAY CDPAR.
C
      J=0
      DO 20 I=1,NCDPAR,2
         J=J+1
         THT=CDPAR(I)
         ALPD(J)=(THT-TH0)/THB
         D(J)=DLOG(CDPAR(I+1))
   20    CONTINUE
      RETURN
C
C  ******************************************************************** 
C
      ENTRY AKFUN(ALPG)
C
C  INTERPOLATE TO DETERMINE CONDUCTIVITY AT ARBITRARY ALPG.
C
      IKMIN=1
      AK=YLAG(ALPG,ALPK,AKSN,IND1,NITP,IKMIN,NKSP,IEX)
      AK=DEXP(AK)
C
C  DETERMINE REDUCED CONDUCTIVITY-SINE VARIABLE.
C
      AKFUN=(AK-AK0)*SINEPS/THB
```

```
      RETURN
C
C   ********************************************************************
C
      ENTRY DFUN(ALPG)
C
C   INTERPOLATE TO DETERMINE DIFFUSIVITY AT ARBITRARY ALPG.
C
      IDMIN=1
      DF=YLAG(ALPG,ALPD,D,IND1,NITP,IDMIN,NDSP,IEX)
      DFUN=DEXP(DF)
      RETURN
      END
      FUNCTION SPANL(DUMMY)
C
C
C   FUNCTION OF ROUTINE--ANALYTIC GENERATION OF CONDUCTIVITY
C   FROM A GARDNER FORM FACTOR AND OF WATER CONTENT OR CAPACITY
C   FROM A MODIFIED KING FORM FACTOR. DIFFUSIVITY IS THEN THE
C   RATIO OF CONDUCTIVITY TO CAPACITY.
C
C
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON/BI/ TH1,THO,THB,SINEPS
      COMMON/WPROP/AKPAR(50),CDPAR(50),AKSN(25),ALPK(25),D(25), ALPD(25)
     1 ,AKSAT,AKSNO,NKPAR,NKSP,NCDPAR,NDSP
      COMMON/XVAR/XSUP1(50),XSUP2(50),THP(50),ALP(50),VSUP1(50),
     1 VSUP2(50),F(50),QGA(50),QG(50),THTMP(50),AKGSS(212), DGSS(212),
     1 IPTTH(50),NTH,JTH,NGSS
      THETA(ALP)=THB*ALP+THO
      GPF(TH)=(TH1-TH)/(TH1+TH)
C
C   INVERSE OF KING WATER-CONTENT FORM FACTOR.
C
      HF(GP)=HO*(DLOG((G/GP)+DSQRT((G/GP)**2-1.)))**BI
C
C   GARDNER CONDUCTIVITY FORM FACTOR.
C
      AKF(H)=AKS/((H/HC)**AN+1.)
C
C   ********************************************************************
C
      ENTRY SPANLI(DUMMY)
C
C   SECTION SPROPI INITIALIZES THE SOIL-PROPERTY ARRAYS.
C
C   EXTRACT CONDUCTIVITY PARAMETERS FROM INPUT ARRAY AKPAR.
C
      NKSP=3
      AKS=AKPAR(1)
      HC=AKPAR(2)
      AN=AKPAR(3)
C
C   EXTRACT WATER CONTENT VARIABLES FROM INPUT ARRAY CDPAR.
C
      NDSP=3
      CC=CDPAR(1)
      HO=CDPAR(2)
      B=CDPAR(3)
      BI=1./B
      G=GPF(THO)
      CN=2.*B*G*TH1/HO
C
C   FIND AKSNO AT ALP=0.
C
      AKO=0.
      AKSNO=0
      AKSAT=AKS
      RETURN
C
C   SECTIONS AKFUN, THFUN, AND DFUN DETERMINE THE CONDUCTIVITY, OR
C   WATER CONTENT, OR DIFFUSIVITY FOR A SPECIFIED REDUCED WATER CONTENT
C   ALPG.
C
C   ********************************************************************
```

```
C
      ENTRY AKANL(ALPG)
C
C    DETERMINE CONDUCTIVITY AT ARBITRARY ALPG.
C
      IF (ALPG.NE.1.) GO TO 10
      AK=AKS
      GO TO 20
   10 TH=THETA(ALPG)
      GP=GPF(TH)
      H=HF(GP)
      AK=AKF(H)
C
C   DETERMINE REDUCED CONDUCTIVITY-SINE VARIABLE.
C
   20 AKANL=(AK-AK0)*SINEPS/THB
      RETURN
C
C   ************************************************************************
C
      ENTRY DANL(ALPG)
C
C   CALCULATE DIFFUSIVITY AT ARBITRARY ALPG.
C
      IF (ALPG.NE.1.) GO TO 30
      TH=TH1
      AK=AKS
      C=CC*TH
      GO TO 40
   30 TH=THETA(ALPG)
      GP=GPF(TH)
      H=HF(GP)
      AK=AKF(H)
      X=H/H0
      XB=X**B
      XB1=XB/X
      C=CN*XB1*DSINH(XB)/(DCOSH(XB)+G)**2+CC*TH
   40 DANL=AK/C
      RETURN
C
C   ************************************************************************
C
      ENTRY HANL(ALPG)
C
C   CALCULATE THE PRESSURE HEAD AT ARBITRARY ALPG.
C
      IF (ALPG.NE.1.) GO TO 50
      H=0.
      GO TO 60
   50 TH=THETA(ALPG)
      GP=GPF(TH)
      H=HF(GP)
   60 HANL=H
      RETURN
C
C   ************************************************************************
C
C
C   CALCULATE THE WATER CAPACITY AT ARBITRARY ALPG.
C
      ENTRY CANL(ALPG)
      IF (ALPG.NE.1.) GO TO 70
      TH=TH1
      C=CC*TH
      GO TO 80
   70 TH=THETA(ALPG)
      GP=GPF(TH)
      H=HF(GP)
      X=H/H0
      XB=X**B
      XB1=XB/X
      C=CN*XB1*DSINH(XB)/(DCOSH(XB)+G)**2+CC*TH
   80 CANL=C
      RETURN
      END
```

```
      FUNCTION FUNS(ALPG)
C
C
C  PURPOSE OF ROUTINE--TO PROVIDE A COLLECTION OF FUNCTIONS TO BE USED
C  IN THE PARLANGE-TYPE WATER-TRANSPORT CALCULATION.
C
C
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON/CTRL/KPGM,KWTR,KVI,KSTRM,KSTRW,ISTOP,KSS,KDIG,KMOUT, KWOUT,
     1 KTSTP,KSOUT,KSRCH,KBUFF,KANL,KIC,KSTRS
      COMMON/CW1/ W1,V1
      COMMON/NUMITG/ NORDR1,NORDER,NITP,ITHMIN,IGSS,ITMIN, IGSSV(3)
      COMMON/TFLX/TTAB(50),V1N(50),V1TAB(50),W1TAB(50),UTAB(50),
     1 TTABL(50),W1TABL(50),TEMP(50),IPTTAB(50),NTTAB
      COMMON/XVAR/XSUP1(50),XSUP2(50),THP(50),ALP(50),VSUP1(50),
     1 VSUP2(50),F(50),QGA(50),QG(50),THTMP(50),AKGSS(212), DGSS(212),
     1 IPTTH(50),NTH,JTH,NGSS
      DATA IND1/0/
C
C  ****************************************************************
C
      ENTRY TLFUN(ALPG)
C
C  EVALUATE LOGARITHM-TYPE TIME INTEGRAND.
C
      IGSSV(1)=IGSSV(1)+1
      IGSS=IGSSV(1)
      AKSN=AKGSS(IGSS)
      D=DGSS(IGSS)
      F1=ALPG*D/(AKSN*AKSN)
      F2=DLOG((AKSN+W1)/W1)
      TLFUN=F1*F2
      RETURN
C
C  *****************************************************************
C
      ENTRY TQFUN(ALPG)
C
C  DETERMINE QUOTIENT-TYPE TIME INTEGRAND.
C
      IGSSV(2)=IGSSV(2)+1
      IGSS=IGSSV(2)
      AKSN=AKGSS(IGSS)
      D=DGSS(IGSS)
      F1=ALPG*D/AKSN
      F2=1./(AKSN+W1)
      TQFUN=F1*F2
      RETURN
C
C  *****************************************************************
C
      ENTRY TOFUN(ALPG)
C
C  EVALUATE THE TIME INTEGRAL FOR SINEPS=0.
C
      IGSS=IGSS+1
      D=DGSS(IGSS)
      TOFUN=ALPG*D
      RETURN
C
C  *****************************************************************
C
      ENTRY TIFUN(ALPG)
C
C  DETERMINE INTEGRAND ARISING FROM INFINITE VELOCITY LIMIT.
C
      IGSSV(3)=IGSSV(3)+1
      IGSS=IGSSV(3)
      AKSN=AKGSS(IGSS)
      D=DGSS(IGSS)
      TIFUN=ALPG*D/AKSN
      RETURN
C
C  *****************************************************************
C
```

```
      ENTRY GFUN(ALPG)
C
C  DETERMINE POSITION INTEGRAND FOR FIRST-ORDER CALCULATION.
C
      IGSS=IGSS+1
      AKSN=AKGSS(IGSS)
      D=DGSS(IGSS)
      GFUN=D/(AKSN+W1)
      RETURN
C
C  ********************************************************************
C
      ENTRY GAFUN(ALPG)
C
C  CALCULATE INTEGRAND OF FIRST FUNCTION USED IN CORRECTION FRACTION F.
C
      IGSS=IGSS+1
      AKSN=AKGSS(IGSS)
      D=DGSS(IGSS)
      GAFUN=D*ALPG/(AKSN+W1)**2
      RETURN
C
C  ********************************************************************
C
      ENTRY GSFUN(ALPG)
C
C  CALCULATE INTEGRAND OF SECOND FUNCTION USED IN CORRECTION FRACTION F.
C
      IGSS=IGSS+1
      AKSN=AKGSS(IGSS)
      D=DGSS(IGSS)
      GSFUN=D/(AKSN+W1)**2
      RETURN
C
C  ********************************************************************
C
      ENTRY G2FUN(ALPG)
C
C  EVALUATE POSITION INTEGRAND FOR SECOND-ORDER CALCULATION.
C
      IGSS=IGSS+1
      AKSN=AKGSS(IGSS)
      D=DGSS(IGSS)
      FP=YLAG(ALPG,ALP,F,IND1,NIT2,ITHNIN,NTH,IEX)
      G2FUN=D/(AKSN+W1*FP)
      RETURN
C
C  ********************************************************************
C
      ENTRY DUMFUN(ALPG)
C
C  CONSTRUCT GAUSS GRID OF SOIL PROPERTIES.
C
      IGSS=IGSS+1
      IF (KANL.EQ.0)  AKGSS(IGSS)=AKFUN(ALPG)
      IF (KANL.NE.0)  AKGSS(IGSS)=AKANL(ALPG)
      IF (KANL.EQ.0)  DGSS(IGSS)=DFUN(ALPG)
      IF (KANL.NE.0)  DGSS(IGSS)=DANL(ALPG)
      DUMFUN=1.
      RETURN
      END
      SUBROUTINE PRINTW
C
C
C  FUNCTION OF SUBROUTINE--TO OUTPUT WATER-TRANSPORT VARIABLES, I.E. A
C  TABLE OF THE END-POINT VELOCITY AS A FUNCTION OF TIME AND TABLES OF
C  POSITIONS AND VELOCITIES AS FUNCTIONS OF WATER CONTENT.
C
C
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON/CTRL/KPGM,KWTR,KWI,KSTRM,KSTRW,ISTOP,KSS,KDIG,KMOUT, KWOUT,
     1 KTSTP,KSOUT,KSRCH,KBUFF,KANL,KIC,KSTRS
      COMMON/TFLX/TTAB(50),V1M(50),V1TAB(50),W1TAB(50),UTAB(50),
     1 TTABL(50),W1TABL(50),TEMP(50),IPTTAB(50),NTTAB
      COMMON/TWTR/T(50),NT
```

```
      COMMON/XVAR/XSUP1(50),XSUP2(50),THP(50),ALP(50),VSUP1(50),
     1 VSUP2(50),F(50),QGA(50),QG(50),THTMP(50),AKGSS(212), DGSS(212),
     1 IPTTH(50),NTH,JTH,NGSS
C
C
C  *******************************************************************
C
      ENTRY PRTTAB
C
C  PRINT VELOCITY-TIME INTERPOLATION TABLE.
C
      KWOUT=KWOUT+1
      PRINT 10100,KWOUT
      PRINT 10000
      DO 10 ITM=1,NTTAB
         PRINT 10600,TTAB(ITM),W1TAB(ITM),V1TAB(ITM),V1N(ITM),UTAB(ITM)
   10    CONTINUE
      RETURN
C
C  *******************************************************************
C
      ENTRY PRTW1(ITM)
C
C  PRINT FIRST-ORDER POSITION AND VELOCITY VARIABLES.
C
      KWOUT=KWOUT+1
      TIME=T(ITM)
      PRINT 10200,KWOUT,TIME
      DO 20 ITH=1,NTH,8
         JTHMN=ITH
         JTHMX=MIN0(ITH+7,NTH)
         PRINT 10700,ITH,(XSUP1(JTH),JTH=JTHMN,JTHMX)
   20    CONTINUE
      KWOUT=KWOUT+1
      PRINT 10300,KWOUT,TIME
      DO 30 ITH=1,NTH,8
         JTHMN=ITH
         JTHMX=MIN0(ITH+7,NTH)
         PRINT 10700,ITH,(VSUP1(JTH),JTH=JTHMN,JTHMX)
   30    CONTINUE
      RETURN
      ENTRY PRTW2(ITM)
C
C  PRINT SECOND-ORDER POSITION AND VELOCITY VARIABLES.
C
      KWOUT=KWOUT+1
      TIME=T(ITM)
      PRINT 10400,KWOUT,TIME
      DO 40 ITH=1,NTH,8
         JTHMN=ITH
         JTHMX=MIN0(ITH+7,NTH)
         PRINT 10700,ITH,(XSUP2(JTH),JTH=JTHMN,JTHMX)
   40    CONTINUE
      KWOUT=KWOUT+1
      PRINT 10500,KWOUT,TIME
      DO 50 ITH=1,NTH,8
         JTHMN=ITH
         JTHMX=MIN0(ITH+7,NTH)
         PRINT 10700,ITH,(VSUP2(JTH),JTH=JTHMN,JTHMX)
   50    CONTINUE
      RETURN
10000 FORMAT(/T12,'TTAB',T30,'W1TAB',T49,'V1TAB',T67,'V1/AKSAT', T88,
     1 'UTAB')
10100 FORMAT(////' WATER-TRANSPORT OUTPUT TABLE',I4,'.. END-POINT ',
     1 'QUANTITIES VS. TIME')
10200 FORMAT(////' WATER-TRANSPORT OUTPUT TABLE ',I4,'.. FIRST-',
     1 'ORDER POSITIONS AT TIME =',1PD12.4//' NODE I',5X,'POSITIONS ',
     1 'AT THETA NODES I,I,...,I+7'/)
10300 FORMAT(////' WATER-TRANSPORT OUTPUT TABLE',I4,'.. FIRST-',
     1 'ORDER VELOCITIES AT TIME =',1PD12.4// ' NODE I',5X,
     1 'VELOCITIES AT THETA NODES I,I+1,....,I+7'/)
10400 FORMAT(////' WATER-TRANSPORT OUTPUT TABLE',I4,'.. SECOND-',
     1 'ORDER POSITIONS AT TIME =',1PD12.4//' NODE I',5X,'POSITIONS '
     1 'AT THETA NODES I,I+1,...,I+7'/)
10500 FORMAT(////' WATER-TRANSPORT OUTPUT TABLE',I4,'.. SECOND-',
```

```
     1 'ORDER VELOCITIES AT TIME =',1PD12.4//' NODE I',5X,
     1 'VELOCITIES AT THETA NODES I,I+1,...,I+7'/)
10600 FORMAT(5(4X,E15.7))
10700 FORMAT(I7,8(1PD15.4))
      END
      SUBROUTINE STRW
C
C
C  FUNCTION OF SUBROUTINE--TO STORE PERTINENT WATER-TRANSPORT
C  QUANTITIES ON AN AUXILLARY DEVICE.
C
C
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON/PROBID/TITLE(8),NPROB
      COMMON/CRVAR/TIME,TH(100,2),THM(100,2),THW(100,2),DTH(100,2),
     1 VX(100,2),VXP(100,2),VXW(100,2)
      COMMON/TFLX/TTAB(50),V1N(50),V1TAB(50),W1TAB(50),UTAB(50),
     1 TTABL(50),W1TABL(50),TEMP(50),IPTTAB(50),NTTAB
      COMMON/TWTR/T(50),NT
      COMMON/XVAR/XSUP1(50),XSUP2(50),THP(50),ALP(50),VSUP1(50),
     1 VSUP2(50),F(50),QGA(50),QG(50),THTMP(50),AKGSS(212), DGSS(212),
     1 IPTTH(50),NTH,JTH,NGSS
C
C  ***********************************************************************
C
      ENTRY STRWI
      PUNCH 10000,(TITLE(I),I=1,8)
      PUNCH 10100,NT
      PUNCH 10100,NTH
      PUNCH 10200,(ALP(I),I=1,NTH)
      PUNCH 10200,(THP(I),I=1,NTH)
      RETURN
C
C  ***********************************************************************
C
      ENTRY STRWT
      PUNCH 10200,TIME
      PUNCH 10200,(XSUP2(I),I=1,NTH)
      PUNCH 10200,(VSUP2(I),I=1,NTH)
      RETURN
10000 FORMAT(8A8)
10100 FORMAT(16I5)
10200 FORMAT(8E10.4)
      END
      SUBROUTINE DATAS
C
C
C  FUNCTION OF SUBROUTINE--TO READ AND PRINT QUANTITIES PERTAINING TO
C  THE PARAMETER SEARCH.  THESE INCLUDE CONTROL PARAMETERS, INITIAL
C  VALUES OF THE SEARCH PARAMETERS, THEIR ALLOWED RANGES, AND THE
C  EXPERIMENTAL DATA.
C
C
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON/CTRL/KPGM,KWTR,KVI,KSTRM,KSTRW,ISTOP,KSS,KDIG,KMOUT, KWOUT,
     1 KTSTP,KSOUT,KSRCH,KBUFF,KANL,KIC,KSTRS
      COMMON/TWTR/T(50),NT
      COMMON/XIV/MYXL(5),MYXU(5),NYX(5),NTX,NXT
      COMMON/XRV/XX(100,5),WX(100,5),YX(100,5),DYX(100,5), YT(100),TX(5)
     1 ,XWTL(5),XWTU(5)
      COMMON/SIP/NP,KPRS,MXFUN,ICONV,NSCY,IPA(5,20)
      COMMON/SRP/ DELTO,CHIS,ACC,RED,TOLSTP,TOLFUN,P(20), PH(20),PL(20),
     1 DELP(20),PL0(20),PH0(20)
      DATA P0/1.D50/
C
C  INPUT AND OUTPUT NON-ARRAY INTEGER AND REAL PARAMETERS.
C
      READ 10000,NP,KPRS,MXFUN,KWT,NTX,KBND,NSCY,KSTRS
      IF (NSCY.LE.0) NSCY=1
      IF (KSTRS.NE.0) KSTRS=1
      PRINT 10200,NP,KPRS,MXFUN,KWT,NTX,KBND,NSCY,KSTRS
      READ 10100,ACC,RED,TOLSTP,TOLFUN,RDP,CWT
      PRINT 10300,ACC,RED,TOLSTP,TOLFUN,RDP,CWT
C
C  READ AND PRINT INITIAL PARAMETERS P AND THEIR LIMITS PH AND PL.
```

```
C
      READ 10100,(P(IP),IP=1,NP)
      IF (NSCY.LE.0) GO TO 20
      DO 10 ISCY=1,NSCY
         READ 10000,(IPA(ISCY,IP),IP=1,NP)
   10    CONTINUE
   20 IF (KBND.EQ.0) GO TO 30
      READ 10100,(PH(IP),IP=1,NP)
      READ 10100,(PL(IP),IP=1,NP)
      GO TO 50
   30 DO 40 IP=1,NP
         PL(IP)=-P0
         PH(IP)=P0
   40    CONTINUE
   50 DO 60 IP=1,NP
         PLO(IP)=PL(IP)
         PHO(IP)=PH(IP)
         DELP(IP)=RDP*P(IP)
   60    CONTINUE
C
C  INPUT EXPERIMENTAL DATA. NOTE THAT YX = THX
C  IN THE WATER-TRANSPORT CASE AND THAT YX = RX
C  IN THE MATERIAL-TRANSPORT CASE.
C
      READ 10100,(TX(ITM),ITM=1,NTX)
      IF (KPGM.NE.5) GO TO 80
      NT=NTX
      DO 70 ITM=1,NT
   70    T(ITM)=TX(ITM)
   80 READ 10000,(NYX(ITM),ITM=1,NTX)
      DO 90 ITM=1,NTX
         NYXL(ITM)=1
   90    NYXU(ITM)=NYX(ITM)
      PRINT 10600
      NXT=0
      DO 230 ITM=1,NTX
         NX=NYX(ITM)
         NX1=NX+1
         READ 10100,(XX(IX,ITM),IX=1,NX)
         READ 10100,(YX(IX,ITM),IX=1,NX)
         IF (KWT.GE.2) READ 10100,(DYX(IX,ITM),IX=1,NX)
         IF (KWT.GE.3) READ 10100,XWTL(ITM),XWTU(ITM)
         IF (XWTU(ITM).LE.XWTL(ITM)) XWTU(ITM)=XX(NX,ITM)
C
C  CALCULATE STATISTICAL WEIGHTS.
C
         IF (KWT.GT.0) GO TO 110
         DO 100 IX=1,NX
            DYX(IX,ITM)=0.
            IF(YX(IX,ITM).GT.0.D0) DYX(IX,ITM)=DSQRT(YX(IX,ITM))
            WT=0.
            IF(DYX(IX,ITM).NE.0.D0) WT=1./DYX(IX,ITM)**2
  100       WX(IX,ITM)=WT
         GO TO 190
  110    IF (KWT.GT.1) GO TO 130
         DO 120 IX=1,NX
            DYX(IX,ITM)=CWT*YX(IX,ITM)
            WT=0.
            IF(DYX(IX,ITM).NE.0.D0) WT=1./DYX(IX,ITM)**2
  120       WX(IX,ITM)=WT
         GO TO 190
  130    DO 140 IX=1,NX
            WT=0.
            IF(DYX(IX,ITM).NE.0.D0) WT=1./DYX(IX,ITM)**2
  140       WX(IX,ITM)=WT
         IF (KWT.EQ.2) GO TO 190
         MX=0
         DO 150 IX=1,NX
            MX=MX+1
            IF (XX(IX,ITM).GE.XWTL(ITM)) GO TO 160
            WX(IX,ITM)=0.
  150       CONTINUE
  160    NYXL(ITM)=MX
         MX=NX1
         DO 170 JX=1,NX
```

```
            IX=NX1-JX
            MX=MX-1
            IF (XX(IX,ITM).LE.XWTU(ITM)) GO TO 180
            WX(IX,ITM)=0.
  170       CONTINUE
  180     MYXU(ITM)=MX
          NXT=NXT+MYXU(ITM)-MYXL(ITM)+1
  190     PRINT 10700,TX(ITM)
C
C  NORMALIZE EXPERIMENTAL POINTS.
C
          MXL=MYXL(ITM)
          MXU=MYXU(ITM)
          SUM=0.
          DO 200 IX=MXL,MXU
  200       SUM=SUM+YX(IX,ITM)
          AN=100./SUM
          ANS=AN*AN
          DO 210 IX=1,NX
            YX(IX,ITM)=AN*YX(IX,ITM)
            DYX(IX,ITM)=AN*DYX(IX,ITM)
  210       WX(IX,ITM)=WX(IX,ITM)/ANS
C
C  OUTPUT EXPERIMENTAL DATA, INCLUDING WEIGHTS.
C
          DO 220 IX=1,NX
            WX(IX,ITM)=DABS(WX(IX,ITM))
  220       PRINT 10500,IX,XX(IX,ITM),YX(IX,ITM),WX(IX,ITM)
  230     CONTINUE
        IF (KWT.EQ.3) GO TO 250
        NXT=0
        DO 240 ITM=1,NTX
  240     NXT=NXT+NYX(ITM)
  250 RETURN
C
C  ************************************************************************
C
        ENTRY SHPREP(ISCY)
C
C  PREPARE AND PRINT STEP SIZES DELP AND PARAMETER BOUNDS PH AND PL.
C
        DO 260 IP=1,NP
  260     DELP(IP)=RDP*P(IP)
        DO 270 IP=1,NP
          PH(IP)=PH0(IP)
          PL(IP)=PL0(IP)
          IF (IPA(ISCY,IP).NE.0) GO TO 270
          PH(IP)=P(IP)
          PL(IP)=P(IP)
  270     CONTINUE
        DO 280 IP=1,NP
          IF (PL(IP).LE.PH(IP)) GO TO 280
          TMP=PH(IP)
          PH(IP)=PL(IP)
          PL(IP)=TMP
  280     CONTINUE
        PRINT 10400
        DO 290 IP=1,NP
  290     PRINT 10500,IP,P(IP),PH(IP),PL(IP),DELP(IP)
        RETURN
10000 FORMAT(16I5)
10100 FORMAT(8F10.0)
10200 FORMAT(////' SEARCH INPUT TABLE 1.. BASIC PARAMETERS'//5X,
     1' NUMBER OF SEARCH PARAMETERS . . . . . . . . . . . . . . .',I5/5X
     1' DIAGNOSTIC PRINTER CONTROL. . . . . . . . . . . . . . . .',I5/5X
     1' MAXIMUM CHI-SQUARED EVALUATIONS . . . . . . . . . . . . .',I5/5X
     1' WEIGHT-CONTROL INTEGER. . . . . . . . . . . . . . . . . .',I5/5X
     1' NUMBER OF EXPERIMENTAL TIME NODES . . . . . . . . . . . .',I5/5X
     1' PARAMETER BOUNDS CONTROL. . . . . . . . . . . . . . . . .',I5/5X
     1' NUMBER OF SEARCH CYCLES . . . . . . . . . . . . . . . . .',I5/5X
     1' AUXILIARY STORAGE CONTROL . . . . . . . . . . . . . . . .',I5)
10300 FORMAT(5X, ' ACCELERATION PARAMETER. . . . . . . . . . . . . . .',
     1 E10.4/5X ' REDUCTION PARAMETER . . . . . . . . . . . . . . . .',
     1 E10.4/5X ' STEP-SIZE TOLERANCE . . . . . . . . . . . . . . . .',
     1 E10.4/5X ' CHI-SQUARE ACCEPTANCE FACTOR. . . . . . . . . . . .',
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     1 E10.4/5X ' PARAMETER STEP-LENGTH FRACTION. . . . . . . . . . ',
     1 E10.4/5X ' WEIGHTING CONSTANT. . . . . . . . . . . . . . . . ',
     1 E10.4)
10400 FORMAT(////' SEARCH INPUT TABLE 2.. ',
     1 'INITIAL VALUES OF PARAMETERS, LIMITS, AND INCREMENTS'//T9,'IP',
     1 T25,'P',T45,'PH',T65,'PL',T85,'DP')
10500 FORMAT(I10,4E20.5)
10600 FORMAT(////' SEARCH INPUT TABLE 3.. EXPERIMENTAL DATA')
10700 FORMAT(/5X' TABLE AT TIME =',E10.4//T9,'IX', T25,'XX',T45,'YX',
     1 T64,'WX')
      END
      SUBROUTINE PRINTS(ITM)
C
C
C  FUNCTION OF SUBROUTINE--TO OUTPUT RESULTS OF PARAMETER SEARCH
C  INCLUDING PARAMETER VALUES AND A TABLE OF CORRESPONDING EXPERIMENTAL
C  AND THEORETICAL VARIABLES.
C
C
      IMPLICIT REAL*8(A-H,O-Z)
      REAL*4 PMAT
      COMMON/CTRL/KPGM,KWTR,KVI,KSTRM,KSTRW,ISTOP,KSS,KDIG,KMOUT, KWOUT,
     1 KTSTP,KSOUT,KSRCH,KBUFF,KANL,KIC,KSTRS
      COMMON/GEOM/X(101),BB(2),DCOSB(2),DCOS(2),DELT,CHNG,DELMAX,TMAX,
     1 IPX(101),IE(100,3),NPN(2),NPST(2),NPTST(2),NBE(2),NTSE(2), ISB(2,
     1 2),IS(2,2),NNP,NEL,NMAT,IBAND,NBC,NST,NTST,NBEL,NTI,NNOR
      COMMON/MRVAR/ A(101,2),B(101,3),R(101),RP(101),RI(101),RB(101),
     1 DP(101),R1(101),RT(101),XTMP(101),BFLX(101),BFLXP(101), FX(100,2)
     1 ,FRATE(10),FLOW(10),TFLOW(10),W,PMAT(3,5)
      COMMON/XIV/MYXL(5),MYXU(5),NYX(5),NTX,NXT
      COMMON/XRV/XX(100,5),WX(100,5),YX(100,5),DYX(100,5), YT(100),TX(5)
     1 ,XWTL(5),XWTU(5)
      COMMON/SIP/NP,KPRS,MXFUN,ICONV,NSCY,IPA(5,20)
      COMMON/SRP/ DELTO,CHIS,ACC,RED,TOLSTP,TOLFUN,P(20), PH(20),PL(20),
     1 DELP(20),PLO(20),PHO(20)
      KSOUT=KSOUT+1
      PRINT 10100,KSOUT
C
C  PRINT FINAL PARAMETER VALUES.
C
      DO 10 IP=1,NP
   10    PRINT 10200,IP,P(IP),PH(IP),PL(IP),DELP(IP)
C
C  OUTPUT EXPERIMENTAL AND THEORETICAL PROFILES.
C
      KSOUT=KSOUT+1
      PRINT 10300,KSOUT
      NX=NYX(ITM)
      PRINT 10400,TX(ITM)
      DO 20 IX=1,NX
   20    PRINT 10200,IX,XX(IX,ITM),YX(IX,ITM),YT(IX),DYX(IX,ITM)
      IF (ITM.NE.NTX) GO TO 30
C
C  OUTPUT CHI/(NODAL POINT).
C
      RES=CHIS/DFLOAT(NXT)
      RES=DSQRT(RES)
      PRINT 10500,RES
   30 RETURN
10000 FORMAT(I5,5X,E10.4)
10100 FORMAT(////' SEARCH OUTPUT TABLE ',I4,
     1 '.. FINAL VALUE OF PARAMETERS, BOUNDS, AND INCREMENTS'//T9,'IP',
     1 T25,'P',T45,'PH',T65,'PL',T85,'DP')
10200 FORMAT(I10,4E20.5)
10300 FORMAT(////' SEARCH OUTPUT TABLE',I4,
     1 '.. EXPERIMENTAL DATA AND THEORETICAL FIT')
10400 FORMAT(/5X' TABLE AT TIME =',E10.4//T9,'IX', T25,'XX',T45,'YX',
     1 T65,'YT',T84,'DYX')
10500 FORMAT(/5X' AVERAGE POINT RESIDUAL =',E12.4)
      END
      SUBROUTINE STRS(ITM)
C
C
C  FUNCTION OF SUBROUTINE--TO STORE NORMALIZED EXPERIMENTAL
C  AND THEORETICAL PROFILES AS OBTAINED FOR THE EXPERIMENTAL
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C   SPACE GRID SO THAT SUCH QUANTITIES MAY BE PLOTTED.
C
C
      IMPLICIT REAL*8 (A-H,O-Z)
      REAL*4 PMAT
      COMMON/PROBID/TITLE(8),NPROB
      COMMON/CTRL/KPGM,KWTR,KVI,KSTRM,KSTRW,ISTOP,KSS,KDIG,KMOUT, KWOUT,
     1 KTSTP,KSOUT,KSRCH,KBUFF,KANL,KIC,KSTRS
      COMMON/GEOM/X(101),BB(2),DCOSB(2),DCOS(2),DELT,CHNG,DELMAX,TMAX,
     1 IPX(101),IE(100,3),NPN(2),NPST(2),NPTST(2),NBE(2),NTSE(2), ISB(2,
     1 2),IS(2,2),NNP,NEL,NMAT,IBAND,NBC,NST,NTST,NBEL,NTI,NNOR
      COMMON/MRVAR/ A(101,2),B(101,3),R(101),RP(101),RI(101),RB(101),
     1 DP(101),R1(101),RT(101),XTMP(101),BFLX(101),BFLXP(101), FX(100,2)
     1 ,FRATE(10),FLOW(10),TFLOW(10),W,PMAT(3,5)
      COMMON/XIV/MYXL(5),MYXU(5),NYX(5),NTX,NXT
      COMMON/XRV/XX(100,5),WX(100,5),YX(100,5),DYX(100,5), YT(100),TX(5)
     1 ,XWTL(5),XWTU(5)
      IF (ITM.GT.1) GO TO 10
      PUNCH 10000,(TITLE(I),I=1,8)
      PUNCH 10100, NTX
      IF (KPGM.EQ.2) NNP=0
      PUNCH 10100,(NYX(I),I=1,NTX),NNP
   10 PUNCH 10200,TX(ITM)
      NX=NYX(ITM)
      PUNCH 10200,(XX(IX,ITM),IX=1,NX)
      PUNCH 10200,(YT(IX),IX=1,NX)
      PUNCH 10200,(YX(IX,ITM),IX=1,NX)
      PUNCH 10200,(DYX(IX,ITM),IX=1,NX)
      IF (KPGM.NE.2) PUNCH 10200,(X(NP),NP=1,NNP)
      IF (KPGM.NE.2) PUNCH 10200,(RB(NP),NP=1,NNP)
      RETURN
10000 FORMAT(8A8)
10100 FORMAT(16I5)
10200 FORMAT(8E10.4)
      END
      SUBROUTINE MEVAL(P,CHIS)
C
C   FUNCTION OF SUBROUTINE--TO EVALUATE CHI-SQUARED FOR THE
C   MATERIAL-TRANSPORT CASE.
C
C
      IMPLICIT REAL*8 (A-H,O-Z)
      REAL*4 PMAT
      COMMON/CTRL/KPGM,KWTR,KVI,KSTRM,KSTRW,ISTOP,KSS,KDIG,KMOUT, KWOUT,
     1 KTSTP,KSOUT,KSRCH,KBUFF,KANL,KIC,KSTRS
      COMMON/CRVAR/TIME,TH(100,2),THM(100,2),THW(100,2),DTH(100,2),
     1 VX(100,2),VXP(100,2),VXW(100,2)
      COMMON/GEOM/X(101),BB(2),DCOSB(2),DCOS(2),DELT,CHNG,DELMAX,TMAX,
     1 IPX(101),IE(100,3),NPN(2),NPST(2),NPTST(2),NBE(2),NTSE(2), ISB(2,
     1 2),IS(2,2),NNP,NEL,NMAT,IBAND,NBC,NST,NTST,NBEL,NTI,NNOR
      COMMON/MPROP/PROP(1,5),WXI
      COMMON/MRVAR/ A(101,2),B(101,3),R(101),RP(101),RI(101),RB(101),
     1 DP(101),R1(101),RT(101),XTMP(101),BFLX(101),BFLXP(101), FX(100,2)
     1 ,FRATE(10),FLOW(10),TFLOW(10),W,PMAT(3,5)
      COMMON/XIV/MYXL(5),MYXU(5),NYX(5),NTX,NXT
      COMMON/XRV/XX(100,5),WX(100,5),YX(100,5),DYX(100,5), YT(100),TX(5)
     1 ,XWTL(5),XWTU(5)
      COMMON/SRP/ DELTO,CHISO,ACC,RED,TOLSTP,TOLFUN,PO(20), PH(20),
     1 PL(20),DELP(20),PLO(20),PHO(20)
      DIMENSION P(1)
      DATA IND1/0/
C
C   CORRELATE SEARCH PARAMETERS WITH PHYSICAL PARAMETERS.
C
      CALL BUFFM(P)
      CHIS=0.
C
C   TIME SEQUENCE CALCULATION.
C
      TIME=0.
      CALL MINL
      IF (KPGM.LE.3) CALL PRINTM(0)
      DELT=DELTO
      TIME=DELTO
      ITM=1
```

```
      ITX=1
   10 IF (TIME.GE.TX(ITX)) GO TO 20
C
C  GENERATE RESULTS FOR INTERMEDIATE STEPS.
C
      CALL MTRAN
      IF (KPGM.LE.3) CALL PRINTM(ITM)
      DELT=DELT*(1.+CHNG)
      DELT=DMIN1(DELT,DELMAX)
      TIME=TIME+DELT
      ITM=ITM+1
      GO TO 10
C
C  CALCULATE CONCENTRAITON PROFILE AT TIME STEP FOR WHICH EXPERIMENTAL
C  DATA IS GIVEN.
C
   20 DELTP=DELT
      DELT=DELT-(TIME-TX(ITX))
      TIME=TX(ITX)
      CALL MTRAN
      IF (KPGM.LE.3) CALL PRINTM(ITM)
      NX=NYX(ITX)
      IXMIN=1
      SUM=0.
      MXL=MYXL(ITX)
      MXU=MYXU(ITX)
      DO 30 IX=1,NX
         YT(IX)=YLAG(XX(IX,ITX),X,RB,IND1,2,IXMIN,NX,IEX)
         IF (IX.LT.MXL) GO TO 30
         IF (IX.GT.MXU) GO TO 30
         SUM=SUM+YT(IX)
   30    CONTINUE
C
C  NORMALIZE THEORETICAL POINTS.
C
      AN=100./SUM
      DO 40 IX=1,NX
         YT(IX)=AN*YT(IX)
C
C  COLLECT CHI-SQUARED.
C
         CHIS=CHIS+WX(IX,ITX)*(YT(IX)-YX(IX,ITX))**2
   40    CONTINUE
      CHIS0=CHIS
      IF (KPGM.GT.3) GO TO 50
      CALL PRINTS(ITX)
      IF (KSTRS.EQ.1) CALL STRS(ITX)
   50 IF (ITX.GE.NTX) GO TO 60
      ITX=ITX+1
      DELT=DELTP
      TIME=TIME+DELT
      ITM=ITM+1
      GO TO 10
   60 RETURN
      END
      SUBROUTINE MWEVAL(P,CHIS)
C
C
C  FUNCTION OF SUBROUTINE--TO GENERATE MATERIAL TRANSPORT PROFILES
C  SUBJECT TO COUPLED MOISTURE MOVEMENT AND TO CALCULATE CHI-
C  SQUARED FOR THE PARAMETER SEARCH.
C
C
      IMPLICIT REAL*8 (A-H,O-Z)
      REAL*4 PMAT
      COMMON/CTRL/KPGM,KWTR,KWI,KSTRM,KSTRW,ISTOP,KSS,KDIG,KMOUT, KWOUT,
     1 KTSTP,KSOUT,KSRCH,KBUFF,KANL,KIC,KSTRS
      COMMON/CRVAR/TIME,TH(100,2),THM(100,2),THW(100,2),DTH(100,2),
     1 VX(100,2),VXP(100,2),VXW(100,2)
      COMMON/GEOM/X(101),BB(2),DCOSB(2),DCOS(2),DELT,CHNG,DELMAX,TMAX,
     1 IPX(101),IE(100,3),NPM(2),NPST(2),NPTST(2),NBE(2),NTSE(2), ISB(2,
     1 2),IS(2,2),NNP,NEL,NMAT,IBAND,NBC,NST,NTST,NBEL,NTI,NNOR
      COMMON/MPROP/PROP(1,5),WXI
      COMMON/MRVAR/ A(101,2),B(101,3),R(101),RP(101),RI(101),RB(101),
     1 DP(101),R1(101),RT(101),XTMP(101),BFLX(101),BFLXP(101), FX(100,2)
```

```
     1 ,FRATE(10),FLOW(10),TFLOW(10),W,PMAT(3,5)
      COMMON/CW1/ W1,V1
      COMMON/XIV/MYXL(5),MYXU(5),NYX(5),NTX,NXT
      COMMON/XRV/XX(100,5),WX(100,5),YX(100,5),DYX(100,5), YT(100),TX(5)
     1 ,XWTL(5),XWTU(5)
      COMMON/SRP/ DELT0,CHIS0,ACC,RED,TOLSTP,TOLFUN,P0(20), PH(20),
     1 PL(20),DELP(20),PL0(20),PH0(20)
      DIMENSION P(1)
      DATA IND1/0/
C
C  CORRELATE SEARCH PARAMETERS WITH PHYSICAL PARAMETERS.
C
      CALL BUFFM(P)
      CHIS=0.
C
C  TIME SEQUENCE CALCULATION.
C
      TIME=0.
      CALL MINL
      IF (KPGM.LE.3) CALL PRINTM(0)
      DELT=DELT0
      TIME=DELT0
      ITM=1
      ITX=1
   10 V1P=V1
      IF (TIME.GE.TX(ITX)) GO TO 40
      IF (TIME.GT.TMAX) GO TO 80
C
C  GENERATE RESULTS FOR INTERMEDIATE STEPS.
C
      CALL MTRAN
      IF (KPGM.LE.3) CALL PRINTM(ITM)
      IF (KTSTP.NE.0) GO TO 20
      DELT=DELT*(1.+CHNG)
      GO TO 30
   20 IF (ITM.EQ.1) TCON=DELT*V1**(1.+CHNG)
      DELT=TCON/V1**(1.+CHNG)
   30 DELT=DMIN1(DELT,DELMAX)
      TIME=TIME+DELT
      ITM=ITM+1
      GO TO 10
C
C  CALCULATE CONCENTRATIION PROFILE AT TIME STEP FOR WHICH EXPERIMENTAL
C  DATA IS GIVEN.
C
   40 DELTP=DELT
      DELT=DELT-(TIME-TX(ITX))
      TIME=TX(ITX)
      CALL MTRAN
      IF (KPGM.LE.3) CALL PRINTM(ITM)
      NX=NYX(ITX)
      IXMIN=1
      SUM=0.
      MXL=MYXL(ITX)
      MXU=MYXU(ITX)
      DO 50 IX=1,NX
         YT(IX)=YLAG(XX(IX,ITX),X,RB,IND1,2,IXMIN,NX,IEX)
         IF (IX.LT.MXL) GO TO 50
         IF (IX.GT.MXU) GO TO 50
         SUM=SUM+YT(IX)
   50    CONTINUE
C
C  NORMALIZE THEORETICAL POINTS.
C
      AN=100./SUM
      DO 60 IX=1,NX
         YT(IX)=AN*YT(IX)
C
C  COLLECT CHI-SQUARED.
C
         CHIS=CHIS+WX(IX,ITX)*(YT(IX)-YX(IX,ITX))**2
   60    CONTINUE
      CHIS0=CHIS
      IF (KPGM.GT.3) GO TO 70
      CALL PRINTS(ITX)
```

```
      IF (KSTRS.EQ.1) CALL STRS(ITX)
   70 IF (ITX.GE.NTX) GO TO 90
      ITX=ITX+1
      DELT=DELTP
      TIME=TIME+DELT
      ITM=ITM+1
      GO TO 10
   80 PRINT 10000
   90 RETURN
10000 FORMAT(////' MAXIMUM TIME EXCEEDED')
      END
      SUBROUTINE MWVAL2(P,CHIS)
C
C
C   FUNCTION OF SUBROUTINE--TO GENERATE MATERIAL TRANSPORT PROFILES
C   SUBJECT TO COUPLED MOISTURE MOVEMENT AND TO CALCULATE CHI-
C   SQUARED FOR THE PARAMETER SEARCH, WHICH INCLUDES BOTH MATERIAL-
C   AND WATER-TRANSPORT PARAMETERS.
C
C
C
C
      IMPLICIT REAL*8 (A-H,O-Z)
      REAL*4 PMAT
      COMMON/CTRL/KPGM,KWTR,KVI,KSTRM,KSTRW,ISTOP,KSS,KDIG,KMOUT, KWOUT,
     1 KTSTP,KSOUT,KSRCH,KBUFF,KANL,KIC,KSTRS
      COMMON/CRVAR/TIME,TH(100,2),THM(100,2),THW(100,2),DTH(100,2),
     1 VX(100,2),VXP(100,2),VXW(100,2)
      COMMON/GEOM/X(101),BB(2),DCOSB(2),DCOS(2),DELT,CHNG,DELMAX,TMAX,
     1 IPX(101),IE(100,3),NPN(2),NPST(2),NPTST(2),NBE(2),NTSE(2), ISB(2,
     1 2),IS(2,2),NNP,NEL,NMAT,IBAND,NBC,NST,NTST,NBEL,NTI,NNOR
      COMMON/MPROP/PROP(1,5),WXI
      COMMON/MRVAR/ A(101,2),B(101,3),R(101),RP(101),RI(101),RB(101),
     1 DP(101),R1(101),RT(101),XTMP(101),BFLX(101),BFLXP(101), FX(100,2)
     1 ,FRATE(10),FLOW(10),TFLOW(10),W,PMAT(3,5)
      COMMON/CW1/ W1,V1
      COMMON/XIV/MYXL(5),MYXU(5),NYX(5),NTX,NXT
      COMMON/XRV/XX(100,5),WX(100,5),YX(100,5),DYX(100,5), YT(100),TX(5)
     1 ,XWTL(5),XWTU(5)
      COMMON/SRP/ DELT0,CHIS0,ACC,RED,TOLSTP,TOLFUN,P0(20), PH(20),
     1 PL(20),DELP(20),PL0(20),PH0(20)
      DIMENSION P(1)
      DATA IND1/0/
C
C   CORRELATE SEARCH PARAMETERS WITH PHYSICAL PARAMETERS.
C
      CALL BUFFM(P)
      CALL BUFFW(P)
C
C   SET UP SOIL PROPERTIES.
C
      CALL PWCAL
      CALL WINL
      CHIS=0.
C
C   TIME SEQUENCE CALCULATION.
C
      TIME=0.
      CALL MINL
      IF (KPGM.LE.3) CALL PRINTM(0)
      DELT=DELT0
      TIME=DELT0
      ITM=1
      ITX=1
   10 V1P=V1
      IF (TIME.GE.TX(ITX)) GO TO 40
      IF (TIME.GT.TMAX) GO TO 80
C
C   GENERATE RESULTS FOR INTERMEDIATE STEPS.
C
      CALL MTRAN
      IF (KPGM.LE.3) CALL PRINTM(ITM)
      IF (KTSTP.NE.0) GO TO 20
      DELT=DELT*(1.+CHNG)
      GO TO 30
```

```
   20 IF (ITM.EQ.1) V1P=V1
      DELT=(1.+(1.+CHNG)*(V1P/V1-1.))*DELT
   30 DELT=DMIN1(DELT,DELMAX)
      TIME=TIME+DELT
      ITM=ITM+1
      GO TO 10
C
C  CALCULATE CONCENTRATION PROFILE AT TIME STEP FOR WHICH EXPERIMENTAL
C  DATA IS GIVEN.
C
   40 DELTP=DELT
      DELT=DELT-(TIME-TX(ITX))
      TIME=TX(ITX)
      CALL MTRAN
      IF (KPGM.LE.3) CALL PRINTM(ITM)
      NX=NYX(ITX)
      IXMIN=1
      SUM=0.
      MXL=MYXL(ITX)
      MXU=MYXU(ITX)
      DO 50 IX=1,NX
         YT(IX)=YLAG(XX(IX,ITX),X,RR,IND1,2,IXMIN,NX,IEX)
         IF (IX.LT.MXL) GO TO 50
         IF (IX.GT.MXU) GO TO 50
         SUM=SUM+YT(IX)
   50    CONTINUE
C
C  NORMALIZE THEORETICAL POINTS.
C
      AN=100./SUM
      DO 60 IX=1,NX
         YT(IX)=AN*YT(IX)
C
C  COLLECT CHI-SQUARED.
C
         CHIS=CHIS+WX(IX,ITX)*(YT(IX)-YX(IX,ITX))**2
   60    CONTINUE
      CHISO=CHIS
      IF (KPGM.GT.3) GO TO 70
      CALL PRINTS(ITX)
      IF (KSTRS.EQ.1) CALL STRS(ITX)
   70 IF (ITX.GE.NTX) GO TO 90
      ITX=ITX+1
      DELT=DELTP
      TIME=TIME+DELT
      ITM=ITM+1
      GO TO 10
   80 PRINT 10000
   90 RETURN
10000 FORMAT(////' MAXIMUM TIME EXCEEDED')
      END
      SUBROUTINE BUFFM(P)
C
C
C  FUNCTION OF SUBROUTINE--TO MAKE THE CORRESPONDENCE
C  BETWEEN THE ARBITRARY PARAMETERS OF ARRAY P
C  AND THE PHYSICAL MATERIAL-TRANSPORT PARAMETERS.
C  THIS ROUTINE MAY BE MODIFIED BY THE USER.
C
C
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION P(1)
      COMMON/MIVAR/KPRO,KPR(1000),MAXDIF,MAXEL,MAXNP,MAXMAT,MAXBW,
     1 MAXNTI,NMPPM
      COMMON/BI/ TH1,THO,THB,SINEPS
      COMMON/MPROP/PROP(1,5),WXI
      REAL*8 KD,LAMBDA
      MTYP=1
C
C  PROPERTIES ARE P(I), PROP(I) = KD, RHOB, AL,
C  THETAB, AND POR.
C
      DO 10 IP=1,NMPPM
         PROP(MTYP,IP)=P(IP)
   10    CONTINUE
```

```
      RETURN
      END
      SUBROUTINE WEVAL(P,CHIS)
C
C
C  FUNCTION OF SUBROUTINE--TO EVALUATE CHI-SQUARED FOR THE
C  WATER-TRANSPORT CASE.
C
C
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON/CTRL/KPGM,KWTR,KVI,KSTRM,KSTRW,ISTOP,KSS,KDIG,KMOUT, KWOUT,
     1 KTSTP,KSOUT,KSRCH,KBUFF,KANL,KIC,KSTRS
      COMMON/NUMITG/ NORDR1,NORDER,NITP,ITHMIN,IGSS,ITMIN, IGSSV(3)
      COMMON/TWTR/T(50),NT
      COMMON/XIV/NYXL(5),NYXU(5),NYX(5),NTX,NXT
      COMMON/XRV/XX(100,5),WX(100,5),YX(100,5),DYX(100,5), YT(100),TX(5)
     1 ,XWTL(5),XWTU(5)
      COMMON/XVAR/XSUP1(50),XSUP2(50),THP(50),ALP(50),VSUP1(50),
     1 VSUP2(50),F(50),QGA(50),QG(50),THTMP(50),AKGSS(212), DGSS(212),
     1 IPTTH(50),NTH,JTH,NGSS
      COMMON/SRP/ DELTO,CHIS0,ACC,RED,TOLSTP,TOLFUN,P0(20), PH(20),
     1 PL(20),DELP(20),PL0(20),PH0(20)
      DIMENSION P(1)
C
C  CORRELATE SEARCH PARAMETERS WITH PHYSICAL PARAMETERS.
C
      CALL BUFFW(P)
C
C  SET UP SOIL PROPERTIES.
C
      CALL PWCAL
C
C  TIME SEQUENCE CALCULATION, AND COLLECT CHI-SQUARED.
C
      CHIS=0.
      CALL WINL
      ITMIN=1
      DO 20 ITM=1,NTX
         NX=NYX(ITM)
         TIME=TX(ITM)
         CALL WINTP(TIME)
         CALL WTIME(TCAL)
         CALL WTRN2
         CALL SWPREP(ITM)
         DO 10 IX=1,NX
            CHIS=CHIS+WX(IX,ITM)*(YT(IX)-YX(IX,ITM))**2
   10       CONTINUE
         CHIS0=CHIS
         IF (KPGM.GT.3) GO TO 20
         CALL PRINTS(ITM)
         IF (KSTRS.EQ.1) CALL STRS(ITM)
   20    CONTINUE
      RETURN
      END
      SUBROUTINE SWPREP(ITM)
C
C
C  FUNCTION OF SUBROUTINE--TO PREPARE THE WATER CONTENT FOR COMPARISON
C  WITH EXPERIMENTAL DATA.
C
C
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON/BI/ TH1,THO,THB,SINEPS
      COMMON/NUMITG/ NORDR1,NORDER,NITP,ITHMIN,IGSS,ITMIN, IGSSV(3)
      COMMON/WPROP/AKPAR(50),CDPAR(50),AKSN(25),ALPK(25),D(25), ALPD(25)
     1 ,AKSAT,AKSN0,NKPAR,NKSP,NCDPAR,NDSP
      COMMON/XIV/NYXL(5),NYXU(5),NYX(5),NTX,NXT
      COMMON/XRV/XX(100,5),WX(100,5),YX(100,5),DYX(100,5), YT(100),TX(5)
     1 ,XWTL(5),XWTU(5)
      COMMON/XVAR/XSUP1(50),XSUP2(50),THP(50),ALP(50),VSUP1(50),
     1 VSUP2(50),F(50),QGA(50),QG(50),THTMP(50),AKGSS(212), DGSS(212),
     1 IPTTH(50),NTH,JTH,NGSS
      DATA IND1/0/
C
C  SORT THE THEORETICAL POSITION-GRID VALUES INTO ASCENDING ORDERS.
```

```
C
      NX=NYX(ITM)
      CALL DSORT(XSUP2,IPTTH,NTH)
C
C  ORDER WATER-CONTENT VALUES CORRESPONDINGLY.
C
      DO 10 ITH=1,NTH
         JTH=IPTTH(ITH)
         THTMP(JTH)=THP(ITH)
   10    CONTINUE
C
C  INTERPOLATE ON THE EXPERIMENTAL POSITION GRID.
C
      SUM=0.
      MXL=MYXL(ITM)
      MXU=MYXU(ITM)
      XMX=XSUP2(NTH)
      THMN=THTMP(NTH)
      IXMIN=1
      DO 40 IX=1,NX
         X=XX(IX,ITM)
         IF (X.LT.XMX) GO TO 20
         THT=THMN
         GO TO 30
   20    THT=YLAG(X,XSUP2,THTMP,IND1,NITP,IXMIN,NTH,IEX)
   30    YT(IX)=THT-THO
         IF (IX.LT.MXL) GO TO 40
         IF (IX.GT.MXU) GO TO 40
         SUM=SUM+YT(IX)
   40    CONTINUE
C
C  NORMALIZE THEORETICAL POINTS.
C
      AN=100./SUM
      DO 50 IX=1,NX
   50    YT(IX)=AN*YT(IX)
      RETURN
      END
      SUBROUTINE BUFFW(P)
C
C
C  FUNCTION OF SUBROUTINE--TO MAKE THE CORRESPONDENCE
C  BETWEEN THE ARBITRARY PARAMETERS OF ARRAY P AND
C  THE PHYSICAL WATER-TRANSPORT PARAMETERS. THIS ROUTINE
C  MUST BE MODIFIED BY THE USER SO AS TO MATCH HIS
C  SPECIFICATION OF THE PHYSICAL PARAMETERS IN SPROP.
C
C
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION P(1)
      COMMON/CTRL/KPGM,KWTR,KWI,KSTRM,KSTRW,ISTOP,KSS,KDIG,KMOUT, KWOUT,
     1 KTSTP,KSOUT,KSRCH,KBUFF,KAML,KIC,KSTRS
      COMMON/MIVAR/KPRO,KPR(1000),MAXDIF,MAXEL,MAXNP,MAXMAT,MAXBW,
     1 MAXNTI,NMPPM
      COMMON/MPROP/PROP(1,5),WXI
      COMMON/BI/ TH1,THO,THB,SINEPS
      COMMON/WPROP/AKPAR(50),CDPAR(50),AKSW(25),ALPK(25),D(25), ALPD(25)
     1 ,AKSAT,AKSWO,NKPAR,NKSP,NCDPAR,NDSP
      IPP=0
C
C  IF KBUFF IS NON-ZERO, THEN THE WATER-TRANSPORT PARAMETERS FOLLOW THE
C  NMPPM MATERIAL-TRANSPORT QUANTITIES.
C
      IF (KBUFF.NE.0) IPP=NMPPM
      DO 10 IP=1,3
         IPP=IPP+1
         AKPAR(IP)=P(IPP)
         IP3=IPP+3
         CDPAR(IP)=P(IP3)
   10    CONTINUE
      IF (KBUFF.NE.0) GO TO 20
      IP=IP3+1
      THO=P(IP)
      IP=IP+1
      TH1=P(IP)
```

```
      RETURN
   20 MTYP=1
      TH0=PROP(MTYP,4)
      TH1=PROP(MTYP,5)
      RETURN
      END
      DOUBLE PRECISION FUNCTION YLAG(XI,X,Y,IND1,N1,IMIN,IMAX,IEX)
C  PROGRAM AUTHORS  A. A. BROOKS AND E.C. LONG,
C  COMPUTING TECHNOLOGY CENTER, UNION CARBIDE CORP., NUCLEAR DIV.,
C  OAK RIDGE, TENN.
C
C     LAGRANGIAN INTERPOLATION
C     XI IS INTEPOLATED ENTRY INTO X-ARRAY
C     N IS THE ORDER OF LAGRANGRAN INTERPOLATION
C     Y IS ARRAY FROM WHICH YLAG IS OBTAINED BY INTERPOLATION
C     IND IS THE MIN-I FOR X(I).GT.XI
C     IF IND=0,X-ARRAY WILL BE SEARCHED
C     IMIN IS MIN INDEX FOR SEARCH OF X-ARRAY
C     IMAX IS MAX INDEX OF X-AND Y-ARRAYS
C     EXTRAPOLATION CAN OCCUR,IEX=-1 OR +1
C
C
      DIMENSION X(1),Y(1)
      DOUBLE PRECISION P,D,S,XD,XI,X,Y,YLAG
      IND=IND1
      N=N1
      IEX=0
      IF (N.LE.IMAX) GO TO 10
      N=IMAX
      IEX=N
   10 IF (IND.GT.0) GO TO 40
      DO 20 J = IMIN,IMAX
         IF (XI-X(J)) 30,130,20
   20    CONTINUE
      IEX=1
      GO TO 70
   30 IND=J
      IMIN = J
   40 IF (IND.GT.1) GO TO 50
      IEX=-1
   50 INL=IND-(N+1)/2
      IF (INL.GT.0) GO TO 60
      INL=1
   60 INU=INL+N-1
      IF (INU.LE.IMAX) GO TO 80
   70 INL=IMAX-N+1
      INU=IMAX
   80 S=0.
      P=1.
      DO 110 J=INL,INU
         P=P*(XI-X(J))
         D=1.
         DO 100 I=INL,INU
            IF (I.NE.J) GO TO 90
            XD=XI
            GO TO 100
   90       XD=X(J)
  100       D=D*(XD-X(I))
  110    S=S+Y(J)/D
      YLAG=S*P
  120 RETURN
  130 YLAG=Y(J)
      IMIN = J+1
      GO TO 120
      END
      SUBROUTINE SEARCH(NP,P,FB,PH,PL,ACC,RED,TOLSTP,TOLFUN,DELP,XPRS,
     1 EVAL,MXFUN,ICONV)
C
C
C  FUNCTION OF SUBROUTINE--TO MINIMIZE THE FUNCTION HEREIN DENOTED AS F
C  BY VARYING THE PARAMETERS P WITHIN THE ALLOWED RANGE (PL,PH).  THE
C  OPTIMAL-SEARCH METHOD OF WEISSMAN AND WOOD (1966) IS USED.
C
C  PROGRAM AUTHOR G. W. WESTLEY
C  COMPUTING TECHNOLOGY CENTER, UNION CARBIDE CORP., NUCLEAR DIV.,
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C  OAK RIDGE, TENN.
C
C
      REAL*8 P(1),PL(1),PH(1),DELP(1),BP(20),ACC,RED,TOLSTP, TOLFUN,FB,
     1 FP,FBP,STOR,TEMP,PAT,EVAL
      INTEGER*4 RVS(20)
      IF (KPRS.GT.0) PRINT 10600, NP,MXFUN, ACC,RED,TOLSTP,TOLFUN,
     1 (PH(I),P(I),PL(I),I=1,NP)
      ICONV = 0
      IEXP=0
      DO 10 I=1,NP
         IF (P(I).GT.PH(I)) P(I) = PH(I)
         IF (P(I).LT.PL(I)) P(I) = PL(I)
         IF (PH(I).EQ.PL(I)) DELP(I) = 0.D0
   10    BP(I)=P(I)
      NFUN=1
      CALL EVAL(P,FB)
      FP=FB
      FBP=FB
   20 MNFAL=0
      IF (NFUN.GE.MXFUN) GO TO 220
      IF (KPRS.GT.0) PRINT 11000, NFUN
      IF (KPRS.GT.0) PRINT 10700,FBP,(BP(I),I=1,NP)
      IF (KPRS.GT.0) PRINT 11700, (DELP(I),I=1,NP)
C
C  START THE EXPLORATORY LOOP.  IF IEXP = 1, THEN IT FOLLOWS A
C  PATTERN MOVE.  IF IT IS 0, THEN IT FOLLOWS A BASE POINT.
C
      IF (KPRS.GT.1) PRINT 10000
      DO 120 I=1,NP
         RVS(I) = 0
         IF (DELP(I).EQ.0.0D0) GO TO 110
         STOR = P(I)
C
C  INCREMENT THE I-TH VARIBLE BY ITS CURRENT STEP AND CHECK FOR
C  ANY RANGE LIMITATIONS.  CHECK THE FUNCTION VALUE AT THIS
C  NEW POINT AGAINST FP FOR IMPROVEMENT.
C
         P(I)=P(I) + DELP(I)
         IF (P(I).GT.PH(I).OR.P(I).LT.PL(I)) GO TO 40
         IF (KPRS.GT.1) PRINT 10100
         NFUN=NFUN + 1
         CALL EVAL(P,FB)
         IF (KPRS.GT.1) PRINT 10800, I, FB,(P(J),J=1,NP)
         IF (FB.GE.FP-TOLFUN*DABS(FP)) GO TO 40
         IF (IEXP.NE.0) GO TO 30
         IF (KPRS.GT.1) PRINT 10200
         DELP(I)=DELP(I)*ACC
   30    FP=FB
         GO TO 120
   40    P(I) = STOR - DELP(I)
C
C  DECREMENT THE I-TH VARIBLE AFTER A FAILURE OF THE INCREMENT
C  PROCEDURE TO GIVE ANY IMPROVEMENT.  PROCEED AS ABOVE.
C
         IF (P(I).GT.PH(I).OR.P(I).LT.PL(I)) GO TO 60
         IF (KPRS.GT.1) PRINT 10300
         NFUN=NFUN + 1
         CALL EVAL(P,FB)
         IF (KPRS.GT.1) PRINT 10900, I, FB,(P(J),J=1,NP)
         IF (FB.GE.FP-TOLFUN*DABS(FP)) GO TO 60
         IF (IEXP.NE.0) GO TO 50
         IF (KPRS.GT.1) PRINT 10300
         DELP(I) = DELP(I) * ACC
   50    RVS(I) = 1
C
C  THE REVERSE STEP YIELDED AN IMPROVEMENT, SO TRY THIS DIRECTION
C  FIRST ON THE NEXT PASS.
C
         GO TO 30
   60    P(I) = STOR
         IF (IEXP.EQ.1) GO TO 120
C
C  VARIBLE INCREMENTING AND DECREMENTING FAILED TO YIELD ANY IM-
C  PROVEMENT.  REDUCE THE STEP SIZE AND TEST AGAINST
```

```
C  ABS(P(I)) • TOLSTP TO SEE IF THE DELP IS AT ITS MINIMUM.
C
         IF (KPRS.GT.1) PRINT 10400
         DELP(I)=DELP(I)*RED
         TEMP=DABS(P(I)/DELP(I))*TOLSTP
         IF (1.D0-TEMP) 70,80,100
   70    DELP(I)=DELP(I)*TEMP
   80    TEMP=1.D-10/DABS(DELP(I))
         IF (1.D0.GE.TEMP) GO TO 110
   90    DELP(I)=DELP(I)*TEMP
         GO TO 110
  100    TEMP=1.D-10/DABS(DELP(I))
         IF (1.D0-TEMP) 90,110,120
  110    MNFAL=MNFAL + 1
  120    CONTINUE
      IF ((FBP-FP).LE.TOLFUN*DABS(FBP)) GO TO 150
C
C  IF THE FUNCTION VALUE AT THE NEW POINT IS LESS THAN THE FUNCTION
C  VALUE AT THE OLD POINT (BASE POINT)  MINUS TOLFUN * ABS(OLD
C  POINT)  ACCEPT AS A BETTER POINT.  IF NOT, GO TO STATEMENT 140
C
      IF (KPRS.GT.0) PRINT 10500
      IF (KPRS.GT.2) PRINT 11200, NFUN
      DO 130 I=1,NP
         IF (RVS(I).EQ.0) GO TO 130
         DELP(I) = -DELP(I)
  130    CONTINUE
      FBP=FP
      DO 140 I=1,NP
         PAT=BP(I)
         BP(I)=P(I)
         P(I) = 2.D0 * BP(I) - PAT
         P(I)=DMAX1(P(I),PL(I))
  140    P(I)=DMIN1(P(I),PH(I))
      NFUN=NFUN + 1
      CALL EVAL(P,FP)
C
C  PERFORM THE PATTERN MOVE AS 2. * NEW POINT  -  OLD POINT AND
C  USE THE FUNCTION VALUE AT THIS POINT AS THE VALUE OF FP.
C
      IF (KPRS.GT.2) PRINT 11300, FP,(P(I),I=1,NP)
      IEXP=1
      GO TO 20
  150 IF (IEXP.EQ.1) GO TO 170
C
C  BASE POINT EXPLORATORY MODE FAILURE .
C
      IF (MNFAL.GE.NP) GO TO 190
      IF (KPRS.GT.2) PRINT 11500
      DO 160 I=1,NP
         IF (RVS(I).EQ.0) GO TO 160
         DELP(I) = -DELP(I)
  160    CONTINUE
      GO TO 20
  170 IEXP = 0
C
C  PATTERN MODE EXPLORATORY FAILURE.  RESTORE OLD BASE POINT AND
C  REVERT TO BASE MODE EXPLORATION.
C
      FP = FBP
      DO 180 I=1,NP
  180    P(I) = BP(I)
      IF (KPRS.GT.2) PRINT 11600
      GO TO 20
  190 IF (FP.LE.FBP) GO TO 210
C
C  THE PROGRAM ASSUMES THAT IT HAS FOUND A LOCAL MINIMUM SINCE
C  EACH VARIBLE HAS REACHED ITS MINIMUM STEP SIZE.
C
      FP=FBP
      DO 200 I=1,NP
  200    P(I)=BP(I)
  210 IF (KPRS.GT.0) PRINT 11400, FP,(P(I),I=1,NP)
      FB = FP
      IF (KPRS.GT.0) PRINT 11000, NFUN
```

```
      GO TO 240
  220 ICONV = 1
      IF (KPRS.GT.0) PRINT 11400, NFUN
      IF (KPRS.GT.0) PRINT 10700,FBP,(BP(I),I=1,NP)
      FB = FBP
      DO 230 I=1,NP
  230    P(I) = BP(I)
C
C  ON RETURN FB HOLDS THE BEST FUNCTION VALUE AND P THE BEST POINT.
C
C  IF THE NUMBER OF FUNCTIONS EVALUATIONS WAS EXCEEDED THEN
C  ONE OF THE BEST POINTS IS RETURNED.
C
  240 RETURN
10000 FORMAT(' BEGIN EXPLORATORY LOOP')
10100 FORMAT(' INCREMENT THE I-TH VARIABLE')
10200 FORMAT(' ACCELERATE THE STEP SIZE')
10300 FORMAT(' DECREMENT THE I-TH VARIABLE')
10400 FORMAT(' REDUCE STEP SIZE')
10500 FORMAT(' ACCEPT NEW POINT')
10600 FORMAT(////,2X,'NP',5X,'NFUN', 16X, 'ACC',8X,'RED',8X,'TOLSTP',
     1 7X,'TOLFUN'/1H ,I3,5X,I4, 13X,F7.4,4X, F7.4,4X,D10.3,3X, D10.3/
     1 11X,'PH',17X, 'P',16X,'PL'/(4X,D15.7,3X,D15.7,3X,D15.7))
10700 FORMAT(' *  'D15.7,2X,7D15.7/ ('     ',17X,7D15.7))
10800 FORMAT(' P', I2,D15.7,2X,7D15.7/ ('     ',18X,7D15.7))
10900 FORMAT(' R', I2,D15.7,2X,7D15.7/ ('     ', 18X,7D15.7))
11000 FORMAT(' NFUN= ',I5)
11100 FORMAT(' THE OPTIMUM VALUE HAS BEEN FOUND '/' *  ' , D15.7,2X,
     1 7D15.7/('     '17X,7D15.7))
11200 FORMAT(' AFTER',I5, ' NFUN A NEW BASE PT. - START PATTERN MOVE')
11300 FORMAT(' RESULT OF PATTERN MOVE'/' P  ',D15.7,2X,7D15.7/ (
     1 '     '17X,7D15.7))
11400 FORMAT(' THE NUMBER OF FUNCTION EVALUATIONS  EXCEEDED ',I5)
11500 FORMAT(' BASE PT. EXPLORATORY MODE FAILURE')
11600 FORMAT(' PATTERN MODE EXPLORATORY FAILURE RESTORE BASE PT.')
11700 FORMAT(' DELP',16X,7D15.7/(1H ,19X,7D15.7))
      END
      SUBROUTINE GAUSS(A,B,RGAUSS,Y,M)
C
C
C  FUNCTION OF SUBROUTINE--TO INTEGRATE FUNCTION Y FROM A TO B USING
C  AN M-TH ORDER GAUSS-LEGENDRE ALGORITHM.
C
C
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION WT(63),ZZ(63),MPT(15)
      DIMENSION WT1(33),WT2(30),ZZ1(33),ZZ2(30)
      EQUIVALENCE (WT(1),WT1(1)),(WT(34),WT2(1))
      EQUIVALENCE (ZZ(1),ZZ1(1)),(ZZ(34),ZZ2(1))
C
C  M SHOULD BE IN (2,16) EXCEPT M=15.
C  Y(Z) IS FUNCTION SUBROUTINE FOR THE INTEGRAND.
C
C  GAUSS-LEGENDRE ABSCISSAS.
C
      DATA ZZ1 / .57735026918963D+00, .77459666924148D+00,
     1 .00000000000000D+00, .86113631159405D+00, .33998104358486D+00,
     1 .90617984593866D+00, .53846931010568D+00, .00000000000000D+00,
     1 .93246951420315D+00, .66120938646626D+00, .23861918608320D+00,
     1 .94910791234276D+00, .74153118559939D+00, .40584515137740D+00,
     1 .00000000000000D+00, .96028985649754D+00, .79666647741363D+00,
     1 .52553240991633D+00, .18343464249565D+00, .96816023950763D+00,
     1 .83603110732664D+00, .61337143270059D+00, .32425342340381D+00,
     1 .00000000000000D+00, .97390652851717D+00, .86506336668898D+00,
     1 .67940956829902D+00, .43339539412925D+00, .14887433898163D+00,
     1 .97822865814606D+00, .88706259976810D+00, .73015200557405D+00,
     1 .51909612920681D+00/
      DATA ZZ2 / .26954315595234D+00, .00000000000000D+00,
     1 .98156063424672D+00, .90411725637047D+00, .76990267419430D+00,
     1 .58731795428662D+00, .36783149899818D+00, .12523340851147D+00,
     1 .98418305471859D+00, .91759839922298D+00, .80157809073331D+00,
     1 .64234933944034D+00, .44849275103645D+00, .23045831595513D+00,
     1 .00000000000000D+00, .98628380869681D+00, .92843488366357D+00,
     1 .82720131506976D+00, .68729290481168D+00, .51524863635815D+00,
     1 .31911236892789D+00, .10805494870734D+00, .98940093499165D+00,
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     1 .94457502307323D+00, .86563120238783D+00, .75540440835500D+00,
     1 .61787624440264D+00, .45801677765723D+00, .28160355077926D+00,
     1 .95012509837637D-01/
C
C  GAUSS-LEGENDRE WEIGHTS.
C
      DATA WT1 / .10000000000000D+01, .55555555555556D+00,
     1 .88888888888889D+00, .34785484513745D+00, .65214515486255D+00,
     1 .23692688505619D+00, .47862867049937D+00, .56888888888889D+00,
     1 .17132449237917D+00, .36076157304814D+00, .46791393457269D+00,
     1 .12948496616887D+00, .27970539148928D+00, .38183005050512D+00,
     1 .41795918367347D+00, .10122853629038D+00, .22238103445337D+00,
     1 .31370664587789D+00, .36268378337836D+00, .81274388361574D-01,
     1 .18064816069486D+00, .26061069640294D+00, .31234707704000D+00,
     1 .33023935500126D+00, .66671344308688D-01, .14945134915058D+00,
     1 .21908636251598D+00, .26926671931000D+00, .29552422471475D+00,
     1 .55668567116174D-01, .12558036946490D+00, .18629021092773D+00,
     1 .23319376459199D+00/
      DATA WT2 / .26280454451025D+00, .27292508677790D+00,
     1 .47175336386512D-01, .10693932599532D+00, .16007832854335D+00,
     1 .20316742672307D+00, .23349253653835D+00, .24914704581340D+00,
     1 .40484004765316D-01, .92121499837728D-01, .13887351021979D+00,
     1 .17814598076194D+00, .20781604753689D+00, .22628318026290D+00,
     1 .23255155323087D+00, .35119460331752D-01, .80158087159760D-01,
     1 .12151857068790D+00, .15720316715819D+00, .18553839747794D+00,
     1 .20519846372130D+00, .21526385346316D+00, .27152459411754D-01,
     1 .62253523938648D-01, .95158511682493D-01, .12462897125553D+00,
     1 .14959598881658D+00, .16915651939500D+00, .18260341504492D+00,
     1 .18945061045507D+00/
C
C  POINTER TABLE.
C
      DATA MPT/ 0, 1, 3, 5, 8, 11, 15, 19, 24, 29, 35, 41, 48, 55, 55 /
      AB=(B-A)*.5
      ABM=(B+A)*.5
      MP=M
      MPT0=MPT(MP-1)
      G=0.
      J=1
   10 NP=J
      D=AB
      IF (NP+NP.LE.MP) GO TO 20
      NP=MP-NP+1
      D=-D
   20 NP=MPT0+NP
      W=WT(NP)*AB
      Z=ZZ(NP)*D+ABM
   30 G=Y(Z)*W+G
      J=J+1
      IF (J.LE.MP) GO TO 10
      RGAUSS=G
      RETURN
      END
```

APPENDIX C

DEFINITION OF INPUT PARAMETERS

Parameters are listed below by input data-set numbers in the order of their occurrence in the "Data Input Guide." Such an ordering scheme facilitates easy cross-referencing between Appendices C and D.

1.	KPGM	The program option parameter. If its value is three or less, then a simple one-shot calculation is performed with no optimization. If KPGM = 1, then only the mass transport is determined. If KPGM = 2, then only the water transport is obtained. If, however, KPGM = 3, then a coupled (mass-and-water) transport calculation is performed. For values greater than three, parameter optimization is performed. For KPGM = 4, only the mass transport is considered. For KPGM = 5, only the water transport is considered. For KPGM = 6 coupled transport is considered, but only the mass-transport parameters may be varied in the optimization, or automatic search, process. The option KPGM = 7 is identical to the KPGM = 6 option with only one exception, namely that an automatic search of both mass- and water-transport occurs.
	NPROB	A problem identification number.
	TITLE(I)	An array containing the title of the problem.
2.	NNP	Number of nodal points.
	NEL	Number of elements. This parameter is overridden and set to NELL + NELU if either of the latter is nonzero.
	NMAT	Number of different types of soils comprising system.
	NCM	Number of correction materials.
	NTI	Number of time increments.
	NBC	Number of Dirichlet boundary conditions.
	NST	Number of Neumann boundary conditions (surface terms).
	KVI	Velocity input control parameter.
	KSTRM	Control parameter for storage of mass-transport on auxiliary storage. If KSTRM = 0, there is no storage, but if it does not equal 0, there is storage on logical unit 1 via subroutine STRM. (See Appendix B for a listing of this routine.)
	KSS	Steady-state control. If KSS = 0, the steady-state solution is obtained. If KSS = 1, transient-state solutions are obtained.
	KTSTP	Time-step control. Via this parameter the time step is varied either exponentially, KTSTP = 0, or as a power law of the end-point Darcy velocity V1, KTSTP $\neq$ 0.
	NELL	Number of elements for which $x < X0$.
	NELU	Number of elements for which $x > X0$.

	NNOR	Time integration parameter. If NNOR = 1, then integration proceeds as described in Chapter IV, Section 5. Otherwise Norsett integration O(Δt**(NNOR+1)) is used. Acceptable values are NNOR = 1, 2, 3, and 5.
	KIC	Initial-condition control. If KIC ≠ 0, then the initial conditions are bulk concentrations. Otherwise they are fluid concentrations.
	KMESH	Mesh control parameter. If KMESH = 0, then a free-form input is used with partial automatic generation. If KMESH = 1, then complete automatic generation is specified. If KMESH = 2, then there is no automatic generation, and a compressed-form format is used.
3.	DELT	Initial time increment ... T.
	CHNG	Parameter used for changing the time increment ... (dimensionless).
	DELMAX	Maximum value of DELT ... T.
	TMAX	Maximum value of the time ... T.
	W	Time-integration parameter ... (dimensionless).
	X0	Variable-mesh parameter. Position about which variable mesh is concentrated ... L.
	XMX	Variable-mesh parameter. Length of chromatographic column ... L.
	DXL1	Variable-mesh parameter. X-increment immediately below point X0 ... L.
	DXU1	Variable-mesh parameter. X-increment immediately above point X0 ... L.
	VXI	Space- and time-independent Darcy velocity ... L/T.
4.	KPR0	Printer control for steady-state and initial conditions. If KPR0 = 0, there is no output. If KPR0 = 1, only integrated flow variables pertaining to the material balance are printed. If KPR0 = 2, then both bulk and fluid concentrations are output. If KPR0 = 3, material fluxes and those variables mentioned previously are printed. Finally, if KPR0 ⩾ 4, then water contents and Darcy velocities are also output.
	KPR(ITM)	Printer control similar to KPR0 used to control time-dependent output.
5.	PROP(I,J)	Material property J for soil type I. In terms of the formal names given in the chapter on notation, PROP(I,1) = k_d, PROP(I,2) = ρ, PROP(I,3) = a_L, PROP(I,4) = θ_r, and PROP(I,5) = n ... (variable dimensions).
6.	NJ	Nodal-point number.
	X(NJ)	X-coordinate of node NJ ... L.

7.		See definitions for item 6.
8.	MI	Element number.
	IE(MI,I)	Element definition array. Entries IE(MI,1) and IE(MI,2) are numbers of the two nodes which subtend element MI, whereas IE(MI,3) identifies the material type.
9.	MI,MK	Element numbers.
	MTYP	Material-type index.
10.	NJ	Nodal number.
	R(NJ)	Fluid or bulk concentration c or c_b ... M/L**3.
11.		See definitions for item 10.
12.	NI	Nodal number.
	BBI	Fluid concentration of boundary node NI ... M/L**3.
13.	NI	Nodal number.
	EI	Material flux at boundary node. If the direction is along the positive X axis, then it has a positive value, otherwise it is negative ... M/L**2/T.
14.	VX(MI,IQ)	Darcy velocity at node IQ of element MI ... L/T.
15.	TH(MI,IQ)	Water content at node IQ of element MI ... L**3/L**3.
16.		See item 12.
17.		See item 13.
18.	KWTR	Water-transport control parameter. This parameter is operative only if KPGM = 2. If KWTR = 0, then only the tabular function $t(W_1)$ is obtained. If KWTR = 1, then, additionally, the first-order calculations for $x^{(1)}$ and $V^{(2)}$ are determined.
	NTTAB	Number of evaluations of the tabular function $t(W_1)$.

	NT	The number of simulation times to be considered.
	NTH	The number of values of θ to be used.
	NKPAR	Number of conductivity parameters to be input.
	NCPAR	Number of capacity parameters to be input.
	NORDER	Order parameter for the Gauss quadrature algorithm when applied to the interval (θ_{i-1}, θ_i), $i < NTH$. NORDER is the number of integration points to be inserted into each interval.
	NORDER1	Same as NORDER except that it is applied to the interval (θ_{i-1}, θ_i), $i = NTH$. Typically the diffusivity is a strongly varying function of water content in this region, and a higher-ordered Gauss integration scheme must be used.
	NITP	Number of Lagrange interpolation points to be used in all water-transport calculations requiring interpolation.
	KSTRW	Control parameter for storage of water-transport output on auxiliary storage. If KSTRW = 0, there is no storage, but if it does not equal 0, there is storage on logical unit 2 via subroutine STRW. (See Appendix B for a listing of this routine.)
	KMESH	Mesh control parameter. If KMESH = 0, then a uniformly spaced water-content grid is used. If KMESH $\neq$ 0, then a variable grid is specified. Typically one desires to concentrate the mesh near the largest water content where $\alpha(NTH) = 1$. The next lower value is then $\alpha(NTH-1) = 1 - DALP1$, where the latter is an input quantity.
	KANL	Analytic soil-properties control. If KANL = 0, then tabular soil properties are used. If KANL $\neq$ 0, then Gardner and King analytic properties are used.
19.	TH0	Initial and residual moisture content ... L**3/L**3.
	TH1	Boundary moisture content and porosity ... L**3/L**3.
	EPS	Angle of inclination ϵ ... (degrees).
	DALP1	Variable-mesh increment between $\alpha = 1$ and its nearest neighbor ... (dimensionless).
20.	AKPAR	Conductivity parameters ... (variable dimensions).
21.	CDPAR	Diffusivity parameters ... (variable dimensions).

22. VIN — End-point Darcy velocity V_1 in units of the saturated conductivity ... (dimensionless).

23. T — The simulation time ... T.

24. NP — Number of search parameters.

KPRS — Output flag. If KPRS = 0, there is no intermediate search output. If KPRS = 1, base points and current step sizes are printed. If KPRS = 2, then there is output as for KPRS = 1 plus exploratory search information. If KPRS = 3, then there is output as for KPRS = 2 plus pattern search information.

MXFUN — Maximum number of function evaluations allowed in searching for the maximum of the X^2 surface.

KWT — Control parameters for adjusting statistical weights. If KWT = 0, then the experimental error is taken to be the square root of the experimental value. If KWT = 1, a percentage error (CWT) is taken. For KWT $\geqslant$ 2 experimental errors are input. For KWT = 3, the statistical weights obtained from the experimental errors are set to zero for all XX < XWT.

NTX — Number of times for which experimental data are input.

KBND — If KBND = 0, all parameter ranges are unbounded. If KBND $\neq$ 0, then upper and lower bounds are input for each search parameter.

NSCY — Number of search cycles.

KSTRS — Control parameter for storage of optimized profiles on auxiliary storage (tape or disk). If KSTRS = 0, there is no storage on punched cards via subroutine STRS. (See Appendix B for a listing of this routine.)

25. ACC — Acceleration parameter for the step size, i.e. Δp_i(new) = ACC*Δp_i(old). ACC = 1.2 is typical ... (dimensionless).

RED — Reduction parameter for the step size, i.e. Δp_i(new) = RED*Δp_i(old). RED = 0.1 is typical ... (dimensionless).

TOLSTP — Step-size tolerance. Generally, the search is terminated whenever $|\Delta p_i/p_i|$ < TOLSTP for all parameters i. TOLSTP = 0.001 is typical ... (dimensionless).

TOLFUN — Tolerance in the function X^2. Generally, the search is terminated whenever the $|\Delta X^2/X^2|$ < TOLFUN. TOLFUN = 0.001 is typical ... (dimensionless).

RDP — Step-size parameter. Initially the search step sizes are taken to be Δp_i = RDP*p_i for all parameters i ... (dimensionless).

CWT — Statistical weight parameter ... (dimensionless).

26. P(IP) — Starting values for parameter search. The meaning of this array depends on the program option. If KPGM = 4, then P contains only the mass-transport quantities k_d, ρ, a_L, θ_r, and n, in that order, for IP = 1(1)5.[†] If KPGM = 5, then P contains only the water-transport variables K_s, h_o, d, β' h'_o, d′, $\theta_0 = \theta_r$ and $\theta_1 = \theta_r$ in that order, for IP = 1(1)8. Option KPGM = 6 requires only the mass-transport input just as for KPGM = 4. Option KPGM = 7, however, requires input appropriate for both mass and water transport. Thus P(IP) contains quantities k_d, ρ, a_L, θ_r, and n for IP = 1(1)5 and quantities k_s, h_o, d, β', h'_o, and d′ for IP = 6(1)11 ... (variable dimensions).

27. IPA(ISCY,IP) — Search parameter indices. A search is carried out on parameter IP on search cycle ISCY only if IPA(ISCY,IP) $\neq$ 0.

28. PH(IP) — Upper bounds for parameter P(IP). These parameters are operative only if KBND $\neq$ 0 ... (variable dimensions).

29. PL(IP) — Lower bounds for parameters P(IP). These parameters are operative only if KBND $\neq$ 0 ... (variable dimensions).

30. TX(ITM) — Experimental times ... T.

31. NYX(ITM) — Number of points in experimental water-content/concentration profile at time ITM.

32. XX(IX,ITM) — Experimental X-coordinate of point IX at time ITM ... L.

33. YX(IX,ITM) — Experimental water-content/concentration value at point IX and time ITM ... (variable dimensions).

34. DYX(IX,ITM) — Experimental error in the water-content/concentration measurement at position IX and time ITM ... (variable dimensions).

35. XWTL(ITM) — The statistical weight is set to zero for all XX > XWTL ... L.

XWTU(ITM) — Similarly the statistical weight is set to zero for all XX > XWTU ... L.

[†] The notation IP = 1(1)5 means that IP = 1, 2, ..., 5.

APPENDIX D

DATA INPUT GUIDE

This appendix and Appendix C both pertain to the data input. Here the input data organization and format are prescribed. Appendix C gives a definition of each input parameter.

1. **Problem identification.** One card per problem.

   List: KPGM,NPROB,(TITLE(I),I=1,1,8)
   Format: 2I5,8A8

Mass-transport input. The following set of data should be included only if mass-transport is specified above. Specifically, only if KPGM = 1,3,4,6, or 7 should card sequences 2 – 19 appear.

2. **Mass-transport integer control parameters.** One card per problem.

   List: NNP,NEL,NMAT,NCM,NTI,NBC,NST,KVI,KSTRM,KSS,KTSTP,NELL, NELU,NNOR,KIC,KMESH
   Format: 16I5

Note on Darcy velocities and water contents. Five quantities must be considered whenever an uncoupled calculation (KPGM = 1, or 4) is performed. They are KVI, the control integer listed above, the input velocity parameters VXI and VX(M,IQ), and porosity n = PROP(I,5) and water content TH(M,IQ). If KVI = 0, then the Darcy velocity and water content are taken to be the spatial and temporal constant VXI (card-set 3) and n (card-set 5), respectively. If KVI = 1, then one spatially dependent array VX(M,IQ) (card-set 12) and one spatially dependent array TH((M,IQ) (card-set 13) are used for all time steps. Finally, if KVI = 2, time dependence is allowed, as well as space dependence, so that arrays VX(M,IQ) and TH(M,IQ) are input for each time step (card-sets 14 and 15).

Note on variable time mesh. By appropriately specifying control parameter KTSTP, the time step may be varied either exponentially

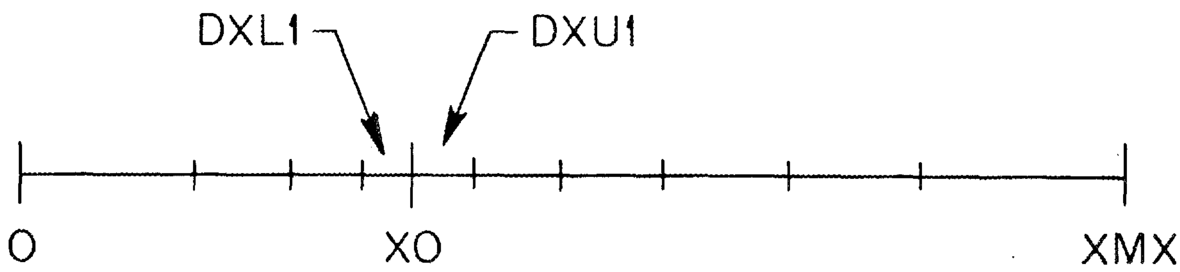
DELT = DELT*(1.+CHNG), KTSTP = 0

or as a power law function of the endpoint Darcy velocity V1

DELT ~ 1./V1**(1.+CHNG), KTSTP ≠ 0

The initial value of time step DELT and the value of parameter CHNG appear in card-set 3. If an uncoupled calculation is called for by the value of KPGM, then only the former equation is used, regardless of the value of KTSTP.

Note on space mesh. Three different options are available here through control parameter KMESH. If KMESH = 0, then nodal positions are input in free form via card-set 6 and elements are defined via card-set 8. If KMESH = 2, then all nodal positions are prescribed by card-set 7. These positions may be in random order since they are subsequently reordered and numbered in terms of ascending values. Element definitions are generated internally and initial conditions are input (card-set 11) in the same order as their corresponding positions. If KMESH = 1, then both nodal positions and elements are generated automatically with the finer mesh concentrated about the point x = XO. Here integers NELL and NELU (above) and real quantities XO, XMX, DXL1, and DXU1 (card-set 3) are operative. Their meanings are apparent from the figure below.



Note on initial conditions. If KIC = 0, then R = c, the fluid concentration, in card-set 9. If, however, KIC ≠ 0, then R = c_b, the bulk concentration in card-set 9.

3. **Mass-transport real control parameters.** Two cards per problem.

 List: DELT,CHNG,DELMAX,TMAX,W,X0,XMX,DXL1,DXU1,VXI
 Format: 8F10.0

Note on time parameter W. If NNOR = 1, then W has a dual role of determining both the accuracy [O(Δt^2), at most] and the intermediate time $t_w = t + \omega\Delta t$ for which time-dependent coefficients are evaluated. If, however, NNOR > 1, then Norsett integration [Norsett, 1974] is used, which is accurate to O(Δt**(NNOR+1)). In the latter case parameter W determines only the intermediate time.

Note on units. The computer code itself functions independently of the chosen system of units. However, consistency of units is required for the input, and dimensions (length, mass, and/or time) are indicated in Appendix C as an aid for the user.

4. **Printer output control.** The number of cards here depends on the number of time increments NTI.

 List: KPR0,(KPR(I),I=1,NTI)
 Format: 80I1

5. **Material properties.** A total of NMAT cards, one for each material.

 List: (PROP(I,J),J=1,5), I=1(1)NMAT
 Format: 8F10.0

6. **Free-form nodal-point positions.** These cards are necessary whenever KMESH = 0. Usually one card per node is needed, a total of NNP cards.

 List: NJ,X(NJ)
 Format: I5,5X,F10.0

However, some automatic generation may be employed in the following manner. If some of the nodes are equidistant, data for only the first and last points of the group are needed. Intermediate nodal positions are generated by linear interpolation.

7. **Compressed-form nodal positions.** These cards are used whenever KMESH = 2. There is no automatic generation of mesh points here. The number of cards depends on the value of NNP.

 List: (X(NJ),NJ=1,NNP)
 Format: 8F10.0

8. Element definitions. These cards are necessary whenever KMESH = 0. Usually one card per element is needed, a total of NEL cards.

List: MI,(IE(MI,I),I=1,3),MODL
Format: 16I5

However, the last parameter of the above list is used to generate element definitions automatically for a group of MODL elements containing sequentially numbered nodes. In such a case MI designates the first number of the group of elements. Field MODL is left blank whenever the automatic generation feature is not used.

9. Material correction. Cards are required here only if NCM > 0. In many cases one card is required per material change, a total of NCM cards.

List: MI,MTYP,MK
Format: 16I5

However, in those cases where numbers of the affected elements range from a lower limit MI to an upper limit MK, automatic correction may be used. Field MK is left blank if the automatic correction facility is not used.

10. Free-form mass-transport initial conditions. Cards are required here whenever KMESH ≠ 2. In the most general case there is one card per node, a total of NNP cards.

List: NJ,R(NJ)
Format: I5,5X,F10.0

Frequently, however, groups of neighboring nodal points NJ have identical values R(NJ). If a gap is recognized in the input sequence of nodal numbers, the initial concentrations are assumed to be identical to the concentration at the lower boundary of the gap.

11. Compressed-form mass-transport initial conditions. Cards are required here only if KMESH = 2. The number of cards depends upon the value of NNP.

List: (R(NJ),NJ=1,NNP)

Here the order is assumed to correspond to that of the mesh points of card-set 7.

12. Dirichlet concentration-type boundary conditions. These cards are necessary only if NBC > 0. Parameter NBC is the number of required cards.

List: NI,BBI
Format: I5,5X,F10.0

13. Neumann flux-type boundary conditions. Cards of this type must be used if and only if NST > 0 The value of parameter NST is the number of required cards.

List: NI,EI
Format: I5,5X,F10.0

14. Darcy velocities at time t = 0. These cards are necessary if and only if the velocity control KVI > 0. The number of cards depends on the number of elements NEL.

List: ((VX(MJ,JQ),JQ=1,2), MJ=MI,MK)
where MK=min(MI+3,NEL) and MI=1(4)NEL
Format: 8F10.0

It should be noted that the velocity input below, like the water-content input below, is ordered by elements.

15. Water contents at time t = 0. These cards are necessary whenever the Darcy-velocity cards are necessary, namely when KVI > 0. The number of cards depends on the value of NEL.

List: ((TH(MJ,JQ),JQ=1,2),MJ=MI,MK)
where MK = min(MI+3,NEL) and MI = 1(4)NEL
Format: 8F10.0

16. Darcy velocities for times t > 0. Cards of this type must be used only whenever KVI = 2. The number of cards depends on the value of NEL.

List: ((VX(MJ,JQ),JQ=1,2),MJ=MI,MK)
where MK = min(MI+3,NEL) and MI = 1(4)NEL
Format: 8F10.0

Note. Whenever KVI = 2, card sequences of the form of sequences 14 and 15 below must appear for each time to be used in the simulation.

17. Water contents for times t > 0. Cards of this type must be used only whenever KVI = 2. The number of cards depends on the value of NEL.

List: ((TH(MJ,JQ),JQ=1,2),MJ=MI,MK)
where MK = min (MI+3,NEL) and MI = 1(4)NEL
Format: 8F10.0

Moisture-transport input. The following set of data should be included only if a moisture-transport calculation is indicated by card 1. Specifically, only if KPGM = 2,3,5,6, or 7, should card sequences 18 – 23 appear.

18. Moisture-transport integer control parameters. One card per problem.

List: KWTR,NTTAB,NT,NTH,NKPAR,NCDPAR,NORDER,NORDER1,NITP, KSTRW,KMESH,KANL
Format: 16I5

Note on soil properties. Input parameters NKPAR, NCDPAR, and KANL (above), and AKPAR(I) and CDPAR(I) (below) all pertain to soil properties and are interrelated. If, for example, KANL = 0, then array AKPAR contains the NKPAR entries θ_1, K_1, θ_2, K_2, ... and array CDPAR contains the NCDPAR entries θ'_1, Q_1, θ'_2, Q_2, ... Here K is the conductivity, Q is the diffusivity, and θ and θ' are water content values, where θ_i is not necessarily equal to θ'_i. If, on the other hand, KANL $\neq$ 0, then array AKPAR contains the parameters Ks, h_0, and d, in that order, and CDPAR contains the parameters β', h'_0, and d'. Thus, in this case NKPAR = 3 and NCDPAR = 3.

Note on variable water-content mesh. Frequently a uniform distributed set of NTH water contents θ (or α) will be sufficient. Here KMESH = 0. However, whenever computer time is a problem, it is desirable to concentrate the mesh in the most active region near $\alpha = 1$. This may be done by specifying KMESH $\neq$ 0 and supplying the first increment DALP1 (below). The resulting mesh will begin $\alpha_{NTH} = 1$, $\alpha_{NTH-1} = 1 -$ DALP1. The remaining points will then be distributed in accordance with an algebraic progression of increment values.

19. Moisture-transport real control parameters. One card per problem.

List: TH0,TH1,EPS,DALP1
Format: 8F10.0

20. Conductivity parameters. If KANL $\neq$ 0 (see note above), one card is sufficient. Otherwise the number of cards is determined by NKPAR.

List: (AKPAR(I),I=1,NKPAR)
Format: 8F10.0

21. Diffusivity parameters. If KANL $\neq$ 0 (see note above), one card is sufficient. Otherwise the number of cards is determined by NCDPAR.

List: (CDPAR(I),I=1,NCDPAR)
Format: 8F10.0

22. End-point Darcy velocities. The number of cards depends on the value of NTTAB.

List: (V1N(I),I=1,NTTAB)
Format: 8F10.0

23. **Simulation times.** This sequence of cards is used if and only if KPGM = 2. The number of cards is a function of parameter NT.

List: (T(I),I=1,NT)
Format: 8F10.0

Optimization input. The following set of data should be included only if an optimization, or parameter search, is indicated by card 1. Specifically, only if KPGM > 3, should card sequences 24 – 35 appear.

24. **Search integer control variables.** One card per problem.

List: NP,KPRS,MXFUN,KWT,NTX,KBND,NSCY,KSTRS
Format: 16I5

Note on statistical weights. Variables KWT (above) and CWT, YX, DYX, XWTL, and XWTU (below) are interrelated in the following manner: If the control integer KWT = 0, then the experimental error in a given measurement YX is taken to be $\sqrt{YX}$ and the weight, WX = 1/YX [see Eq. (5.1)], is internally generated. If KWT = 1, then CWT is the relative error, the experimental error is CWT*YX, and again the statistical weight, WX = 1/(CWT*YX)**2, is internally generated. If KWT $\geqslant$ 2, then the experimental error is read into array DYX(IX,ITM) as a function of both position index IX and time index ITM. These values are then converted to statistical weights in accordance with the relation WX = 1/DYX**2. If KWT = 3, then WX is set to zero for all XX < WXTL and for all XX > XWTU.

Note on parameter constraints. If KBND ≠ 0, then inequality constraints must be input in the form of an upper bound PH(IP) and a lower bound PL(IP) for each parameter IP.

Note on search cycles. In order to guard against unrealistic parameter values, it is sometimes desirable to search on the parameters sequentially. This may be done by setting NSCY equal to the desired number of search cycles and identifying the parameter groupings through the IPA array below.

25. **Search real control variables.** One card per problem.

List: ACC,RED,TOLSTP,TOLFUN,RDP,CWT
Format: 8F10.0

26. **Initial parameter values.** The number of cards depends on the number of parameters NP.

List: (P(IP),IP=1,NP)
Format: 8F10.0

27. **Search-parameter identifiers.** The number of cards depends on the number of parameters NP.

List: (IPA(ISCY,IP),IP=1,NP), ISCY=1,NSCY
Format: 16I5

28. Upper bounds. If KBND $\neq$ 0, then the following card sequence must be present. The number of cards depends on the number of parameters NP.

List: (PH(IP),IP=1,NP)
Format: 8F10.0

29. Lower bounds. If KBND $\neq$ 0, then the following card sequence must appear. The number of cards depends on the number of parameters NP.

List: (PL(IP),IP=1,NP)
Format: 8F10.0

30. Experimental time measurements. The number of cards depends on variable NTX.

List: (TX(ITM),ITM=1,NTX)
Format: 8F10.0

31. Number of water-content/concentration profiles. The number of cards depends on variable NTX.

List: (NYX(ITM),ITM=1,NTX)

Note on input of experimental profile measurements. The following three card sequences are nested within a loop over the time index ITM=1(1)NTX.

32. Position variables for time ITM. The number of cards depends on the value of the index NX = NYX(ITM).

List: (XX(IX,ITM),IX=1,NX)
Format: 8F10.0

33. Concentration/water-content variables for time ITM. The number of cards depends on the value of the index NX = NYX(ITM).

List: (YX(IX,ITM),IX=1,NX)
Format: 8F10.0

34. Experimental errors for time ITM. This sequence of cards should appear only if KWT $\geq$ 2. The number of cards depends on the value of the index NX = NYX(ITM).

List: (DYX(IX,ITM),IX=1,NX)
Format: 8F10.0

35. Modification of statistical weights for time ITM. This sequence of cards should appear only if KWT = 3. One card per value of ITM.

List: XWTL(ITM),XWTU(ITM)
Format: 8F10.0

75. G. H. Daly, Chief, ERDA Waste Management Branch, Division of Waste Management, Production and Reprocessing, U.S. Energy Research and Development Administration, Washington, D.C. 20545

76. G. D. DeBuchananne, U.S. Geological Survey, Mail Stop 410, Reston, VA 22092

77. R. A. Deju, Atlanta Richfield Hanford Company, P.O. Box 250, Richland, WA 99352

78. J. Diechoner, ERDA Waste Management Branch, Division of Waste Management, Production and Reprocessing, U.S. Energy Research and Development Administration, Washington, D.C. 20545

79-83. Division of Waste Management, ERDA-ORO, Oak Ridge, TN 37830

84. A. M. Friedman, Argonne National Laboratory, 9700 South Cass Avenue, Argonne, IL 60439

85. E. O. Frind, Department of Earth Sciences, University of Waterloo, Waterloo, Ontario, CANADA

86. W. C. Luth, U.S. Energy Research and Development Administration, Washington, D.C. 20545

87. G. L. Meyer, U.S. EPA, 9520 Beach Mill Road, Great Falls, VA 22066

88. I. W. Marine, E. I. duPont de Nemours & Company, Savannah River Laboratory, Aiken, SC 29801

89. O. I. Oztunali, Dames and Moore, 20 Haarlem Avenue, White Plains, NY 10603

90. J. Y. Parlange, The Connecticut Agricultural Experiment Station, New Haven, CT 06504

91. G. F. Pinder, Princeton University, Civil Engineering Department, Princeton, NJ 08540

92. Research and Technical Support Division, Oak Ridge Operations, Oak Ridge, TN 37830

93. J. N. Rogers, Division 8321, Sandia Laboratories, P.O. Box 969, Livermore, CA 94550

94. D. M. Roy, Pennsylvania State University, Materials Research Laboratory, University Park, PA 16802

95. D. L. Schreiber, U.S. Nuclear Regulatory Commission, Hydrologic Engineering Section, DSE, NRR (P-328), Washington, D.C. 20555

96. R. J. Serne, Battelle Pacific Northwest Laboratory, P.O. Box 999, Richland, WA 99352

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