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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
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COMPUTER SCIENCES DIVISION
ENVIRONMENTAL SCIENCES DIVISION

QUANTITATIVE ANALYSIS OF SOIL CHROMATOGRAPHY

I. WATER AND RADIONUCLIDE TRANSPORT

M. Reeves

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, mineral, 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.

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QUANTITATIVE ANALYSIS OF SOIL CHROMATOGRAPHY

I. WATER AND RADIONUCLIDE TRANSPORT

**M. Reeves
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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 ^{86}Sr , ^{109}Cd , ^{93}Nb , and ^{137}Cs . There appeared to be a mobile and non-mobile species 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,

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

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 ^{86}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 , 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.

^{85}Sr Movement in Captina Silt Loam 200-ppm Ca in Eluting Solution.

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

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

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

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

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.

$$0 \leq x < \infty \quad (3)$$

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 column. 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.

$$\frac{\partial x}{\partial t} = \frac{\partial V}{\partial \theta} \quad (4)$$

Here the Darcy velocity

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

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

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

Eqs. (4) and (5) become

$$\frac{\partial x}{\partial t} = \frac{\partial W}{\partial \alpha} \quad (7)$$

and

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

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

$$V = (\theta_1 - \theta_0) W - K_0 \sin \epsilon \quad (9)$$

where $K_0 = K(\theta_0)$. Expressed in terms of variable α , the boundary and initial conditions become

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

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:

$$\int_0^1 d\alpha \frac{\partial x}{\partial t} = W_1 - W \quad (11)$$

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

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

[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

$$\frac{\partial x^{(n)}}{\partial \alpha} = \frac{Q}{\kappa \sin \epsilon + W_1 - \int_0^1 d\alpha \frac{\partial x^{(n-1)}}{\partial t}} \quad (13)$$

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

$$w^{(n)} = w_1 - \int_0^1 d\phi \frac{\partial x^{(n-1)}}{\partial t} \quad (14)$$

The second integral

$$x^{(n)} = \int_0^1 \frac{Q d\gamma}{\kappa \sin \epsilon + w_1 - \int_0^1 d\phi \frac{\partial x^{(n-1)}}{\partial t}} \quad (15)$$

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.,

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

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

$$w^{(1)} = w_1 \quad (17)$$

and

$$x^{(1)} = \int_0^1 d\gamma \frac{Q}{\kappa \sin \epsilon + w_1} \quad (18)$$

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 $\alpha = 0$:

$$\int_0^1 d\alpha \frac{\partial x}{\partial t} = w_1 - w_0 \quad (19)$$

where, from Eq. (8),

$$w_0 = - \frac{Q}{\partial x / \partial \alpha} \bigg|_{\alpha=0} - \kappa \sin \epsilon \bigg|_{\alpha=0} \quad (20)$$

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

$$W_1 = \int_0^1 J_\alpha \frac{\partial x}{\partial t} dt \quad (21)$$

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

$$\frac{\partial x^{(1)}}{\partial t} = - \frac{\partial W_1}{\partial t} \int_0^1 d\gamma \frac{Q}{(\kappa \sin \epsilon + W_1)^2} \quad (22)$$

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

$$t = \int_0^1 d\alpha \int_0^1 d\gamma Q(\gamma) I(\gamma) \quad (23)$$

where

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

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

$$t = \int_0^1 d\gamma \gamma Q(\gamma) I(\gamma) \quad (25)$$

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

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

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

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

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:

$$\begin{aligned} W_1 &= \int_0^1 d\phi \frac{\partial x^{(1)}}{\partial t} = \int_0^\infty d\phi \frac{\partial x^{(1)}}{\partial t} \\ &= W_1 \int_0^\infty d\phi \frac{\partial x^{(1)}}{\partial t} / \int_0^1 d\phi \frac{\partial x^{(1)}}{\partial t} . \end{aligned} \quad (27)$$

Differentiating Eq. (18) with respect to time yields

$$W_1 = \int_0^1 d\phi \frac{\partial x^{(1)}}{\partial t} = W_1 J(\alpha)/J(1) \quad (28)$$

where

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

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:

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

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

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

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

and

$$x^{(2)} = \int_0^1 d\gamma \frac{Q}{\kappa \sin \epsilon + W_1 J(\alpha)/J(1)} . \quad (32)$$

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

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

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 horizontal 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 $\theta_0 = 0.2376 \text{ cm}^3 \text{ cm}^{-3}$ and the end-point moisture content $\theta_1 = 0.4950 \text{ cm}^3 \text{ cm}^{-3}$, respectively.

2. Capillary rise. The case of capillary rise ($\epsilon = 90^\circ$) 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 $\epsilon \neq 90^\circ$, however, although acceptable, are not of the same quality. This may be seen in Fig. 8 for the case of infiltration ($\epsilon = 90^\circ$) and in Fig. 9 for the case of horizontal flow ($\epsilon = 0^\circ$). 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 $Q_1 = Q(\alpha = 1) = 1.85 \times 10^{-2} \text{ cm}^2 \text{ sec}$, 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

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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 $J(a)/J(1)$, the discrepancy would appear to lie in this quantity. However, increases in the order of the Gauss quadrature procedure used to evaluate $J(a)$ at nodal points a , [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]:

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

where $h < 0$ is the pressure head. Parameters K_s , h_0 , 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 $h \rightarrow 0$. Also, it may be seen that at the critical pressure $K(h_0) = K_s/2$. In addition, the slope of the conductivity curve at $h = h_0$ 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:

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

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

$$\delta = \frac{\theta_1 - \theta_r}{\theta_1 + \theta_r} \quad (36)$$

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.

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

This equation may be differentiated

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

and inverted

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

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

$$\delta' = \frac{\theta_1 - \theta}{\theta_1 + \theta} \quad (40)$$

Parameters θ_1 , h_0 , and d' have meanings similar to that of their counterparts K_s , h_s , 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 $\theta(h_c) = \theta_1/5$ provided $\theta_1 \ll \theta_1/5$. At this same pressure the slope is directly proportional to the pore-size distribution parameter d' , i.e. $d\theta/dh(h_c) \sim |d'|$. 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

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

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 non-zero value to the storage function at saturation, i.e. $F(0) = \theta_1\beta'$. Thus the diffusivity

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

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

remains finite at $h = 0$ in accord with the analysis of Philip [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 $t = 10^5$ 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

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

(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' :

$$c_b = \theta c + \rho s' \quad (2)$$

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

$$s' = \frac{\theta}{n} k_d c \quad (3)$$

[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

$$c_b = R_d \theta c \quad (4)$$

where

$$R_d = 1 + \frac{\rho k_d}{n} \quad (5)$$

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

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

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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 Scheidegger [Bear, 1972]

$$\theta D = a_L |V| \quad (7)$$

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:

$$\mathcal{L}(c) = 0 \quad (8)$$

Consider a trial function of the form

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

where the N_i are basis functions spanning the region of interest $0 \leq x \leq L$, 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.

$$\mathcal{L}(c') \neq 0 \quad (10)$$

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

$$\int_0^L dx N_i(x) \mathcal{L}(c') = 0 \quad (11)$$

(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

$$\int_0^L dx N_i(x) \mathcal{L}\left(\sum_j N_j(x) c_j\right) = 0 \quad (12)$$

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 $0 \leq x \leq 1$, 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 sparse 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

$${}_r c(x, t) = \{N(x)\}^T \{{}_r c'\} \quad (13)$$

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

$$\int_0^L dx \{N\} \mathcal{L}(\{N\}^T \{{}_r c'\}) dx = 0 \quad (14)$$

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

$$[{}_r A] \{\dot{c}\} + [{}_r B] \{c\} + [{}_r R'] = 0 \quad (15)$$

where

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

$$[{}_r B] = {}_r J \int_{-1}^1 ds \left(\frac{\partial}{\partial x} \{N\} \theta D \frac{\partial}{\partial x} \{N\}^T \right. \quad (17)$$

$$\left. - \frac{\partial}{\partial x} \{N\} V \{N\}^T + \{N\} R_d \left(\frac{\partial \theta}{\partial t} + \lambda \theta \right) \{N\}^T \right)$$

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

and

$$\{,R'\} = \{N\} X \int_{s=-1}^{s=1} . \quad (18)$$

Quantities $\{,A\}$ and $\{,B\}$ are 2×2 matrices whereas $\{,R'\}$ is a 2×1 column vector. The first term on the left-hand side of Eq. (6) contributes both to $\{,A\}$ through the term R,θ and to $\{,B\}$ through the term $R,(\partial\theta/\partial t)$. The second and third terms on the left-hand side of Eq. (6) contribute, after an integration by parts, both to $\{,B\}$ through the term θD and to $\{,R'\}$. Quantity X in the latter is the mass flux

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

Finally the fourth term in Eq. (6), the radioactive decay, gives rise only to the term in $\{,B\}$ containing $\lambda\theta$.

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

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

Thus the Jacobian is a simple constant:

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

and the vector of basis functions may be written:

$$\{N\} = \frac{1}{2} \{1 + s, s\}, s_j = s(x_j) . \quad (22)$$

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

$$\{,A\} \{,c\}_{t+\omega\Delta t} + \{,B\} \{,c\}_{t+\omega\Delta t} + \{,R'\} = 0 \quad (23)$$

where $0 \leq \omega \leq 1$. 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

$$\{c\}_{t+\omega\Delta t} \approx (\{c\}_{t+\Delta t} - \{c\}_t)/\Delta t \quad (24)$$

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

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

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

$$[C] \{c\}_{t+\Delta t} = \{R\} - \{R'\} \quad (26)$$

where

$$[C] = [A]/\Delta t + \omega [B] \quad (27)$$

and

$$\{R\} = ([A]/\Delta t + (1 - \omega) [B]) \{c\}_t \quad (28)$$

It should be understood that matrices $[A]$, $[B]$, and $\{R\}$, and, hence, $[C]$ and $\{R'\}$, 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 2×2 matrix $[C]$ and the two 2×1 vectors $\{R\}$ and $\{R'\}$. It is now necessary to sum over all m finite elements in order to obtain the corresponding equation for the complete system, namely

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

where

$$\begin{aligned} [C] &= \sum_r [C] \\ \{R\} &= \sum_r \{R\} \\ \{R'\} &= \sum_r \{R'\} \end{aligned} \quad (30)$$

If there are p nodal points in the system, then matrix $[C]$ is $p \times p$ and column vectors $\{R\}$, $\{R^*\}$, and $\{c\}$ are $p \times 1$. 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

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

and

$$\{R\} = \begin{Bmatrix} {}_1R_1 \\ {}_1R_2 + {}_2R_1 \\ {}_2R_2 \end{Bmatrix} \quad (32)$$

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 is imposed at node i , then $R^* = X$ is prescribed. (The appropriate basis function N 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 $R^* = 0$.

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.,

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

Equation (29) then takes the form

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

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

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

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 α_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 α_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 α_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

$$c_b = R_d \theta c \quad (4)$$

where

$$R_d = 1 + \frac{\rho k_d}{n} \quad (5)$$

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 α_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 $1000 \text{ cm}^3/\text{gm}$.

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

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

Here

$$q^2 = a_L V / \theta R_d \quad (37a)$$

and

$$v = V / \theta R_d \quad (37b)$$

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

$$c = e^{\mu x} g \quad \mu = v/2q^2 \quad (38)$$

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

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

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

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

where

$$\omega_m = \frac{m\pi}{L} \quad (41a)$$

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

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 $\theta^e(x,t)$, it is required to find soil parameters for the best-fitting theoretical function $\theta(x,t,K_s,h_w,d,\beta_w,h_w,d')$ so that the corresponding Darcy velocities may be determined. Secondly, given these velocities and the experimentally determined concentrations $c^e(x,t)$, it is required to find mass-transport parameters for the best fitting theoretical function $c(x,t,k_d,a_1,\rho,n)$. It is, of course, desirable independently to measure parameters a_1 , ρ , and n whenever possible in order to reduce numerical error in the determination of k_d .

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

$$X^2(\bar{p}) = \sum_{i=1}^{N_t} \sum_{j=1}^{N_s(t)} \left(\left(f(x_j, t_i, \bar{p}) - f^e(x_j, t_i) \right) / \sigma^e(x_j, t_i) \right)^2 \quad (1)$$

Symbol f may be identified with either θ or c , and σ^e is the experimental error. The number of position variables N_s will, in general, be a function of the time t , at which the measurements were taken, as indicated by the argument. Integer N_t represents the total number of such time steps. Formally p may be viewed as a vector in an N_p -dimensional parameter space with components $p_1, p_2, \dots, p_{N_p}$, and $X^2(p)$ is a hypersurface in an $(N_p + 1)$ -dimensional space. The problem is to locate the point 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* [Hocke 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* p_0 is chosen arbitrarily. Then *exploration* begins about this point. First the *exploratory trial point* $p_+ = p_0 + e_1 \Delta p_1$ is chosen where e_1 is a unit vector parallel to the p_1 axis. If a *success* is obtained, i.e. $X^2(p_+) < (1 - T_1)X^2(p_0)$, then an *exploratory move* is made to $p' = p_+$, where T_1 is an acceptance factor for function improvement and p' is the current estimate for the next base point p_1 . If a *failure* is obtained, i.e. $X^2(p) > (1 - T_1)X^2(p_0)$, then a new trial point $p_- = p_0 - e_1 \Delta p_1$ is chosen. If success is achieved at p_- then an exploratory move is made to $p' = p_-$. Here and in the case of incrementation, whenever there is a success, the step is accelerated in preparation for the next exploration, i.e. $\Delta p_1 \rightarrow A \Delta p_1$, where $A > 1$ is an acceleration factor. If this possibility is also exhausted, then there is no exploratory move, i.e. $p' = p_0$. The step size is then reduced in preparation for the next exploration, i.e. $\Delta p_1 \rightarrow B \Delta p_1$, 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

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parameter p_1 . After taking each parameter, in turn, a new base point 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 $p' = 2p_1 - p_0$, followed by exploratory trial moves. (Trial moves are indicated as dashed lines in Fig. 17.) If this series of moves is successful, i.e. $X(p') < (1 - T_1)X(p_1)$, then a pattern move is made to $p_2 = p'$. It should be noted here that the sequence of trial moves outlined above continues even if $X(2p_1 - p_0) > (1 - T_1)X(p_1)$. 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 p_1 , 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 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. $\Delta p_i \leq T_i p_i$ where T_i 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 $f(x, t, p)$ 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.

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 procedure 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 $t(W_i)$ for selected values of the reduced end-point Darcy velocity W_i . 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 $W_i(t)$, 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.

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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 [Eq. (IV.22)] and the Jacobian J and, using known (or assumed) soil-solution properties, performs the integrations necessary to obtain element matrices $[A]$ and $[B]$. 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 $[C]$ and $\{R\}$ from $[A]$ and $[B]$ 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 QMR. 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 QMR.

OPTIMIZATION

The optimization 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 p which minimize $X^2(p)$, 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 $\theta(x,t)$ are to be fitted, whereas MWEVAL is used whenever experimental concentrations $c(x,t)$ 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 p and the material-transport parameters k_a , a_1 , ρ , and n . Routine BUFFW performs this same function for the water-transport parameters. Nodal-point linkage is accomplished by YLAG, SWPREP, and DSORT. Computational 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 I. 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 ^3H 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 ^{87}Sr transport in Fuquay sand and Figs. 26 and 27 pertain to ^{239}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. ^1H distribution in Fuquay sand at $t = 1$ min.

Fig. 23. ^{14}C distribution in Poquos sand at $t = 4$ min.

Table 1. Moisture-Transport Parameters for Fuquay Sand

Conductivity Parameters	K_s	7.57×10^{-5} cm/sec
	h_s	-49.9 cm
	d	1.78
Moisture-Content Parameters	β'	3.97×10^{-4}
	h'_s	-23.2 cm
	d'	-0.419
	θ_r, θ_s	0.00625
	θ_1, 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_1 (cm)	0.150*	0.333*	0.446*	0.126*

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

Fig. 24. ^{86}Sr distribution in Fuquay sand after one wetting with water.

Fig. 25. ^{88}Sr distribution in Fuquay sand after two wettings with water.

Fig. 26. ^{239}Pu distribution in Fujiy sand after one wetting with water.

Fig. 27. ^{239}Pu distribution in Fuquay sand after two wettings with water.

Fig. 28. ^{90}Sr distribution in Fuquay sand directly after spotting.

c. RELATIVE ACTIVITY

Fig. 29. ^{239}Pu distribution in Fuquay sand directly after spotting.

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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 -determinations for ^{239}Pu . First, there is excellent agreement between the two wettings. Secondly, the magnitudes of these numbers is rather small compared to the value $k_d \approx 10^3 \text{ cm}^2/\text{gm}$, 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 $k_d = 83 \text{ cm}^2/\text{gm}$ seems to confirm this explanation. However, it does raise another question regarding the difference between our chromatographic measurement of about $43 \text{ cm}^2/\text{gm}$ 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 ^{87}Sr reported in Table 2. The average value of the two distribution coefficients reported there is $k_d = 31 \text{ cm}^2/\text{gm}$, which is substantially lower than our suspension measurement of $k_d = 85 \text{ cm}^2/\text{gm}$. 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 ^{87}Sr . He got $21 \text{ cm}^2/\text{gm}$ for the former and $490 \text{ cm}^2/\text{gm}$ for the latter with the numbers differing by a factor of about 23.

Figure 30 exhibits experimental and theoretical results for a $0.01 \text{ N Ca(NO}_3\text{)}$ 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.

Fig. 30. ^{90}Sr distribution in Fuquay sand after one wetting with 0.01 N $\text{Ca}(\text{NO}_3)_2$.

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 ^{87}Sr and ^{239}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).
$[A]$	(2x2) matrix of integrals for r-th finite element (L).
a_l	Longitudinal dispersivity (L).
B	Reduction parameter (dimensionless).
$[B]$	(2x2) matrix of integrals for r-th finite element (L T).
b	Dirichlet boundary condition for the concentration (M L ⁻³).
$[C]$	(2x2) matrix of integrals for r-th finite element (L T).
$[C]$	Assembly of all $[C]$ (L T).
c	Concentration of the dissolved constituent (M L ⁻³).
c'	Numerical approximation to c (M L ⁻³).
c_s	Bulk concentration including both dissolved and adsorbed constituents (M L ⁻³).
c_i	Concentration at node i (M L ⁻³).
$\{c\}$	(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 ⁻¹ L ⁻¹) or concentration (M L ⁻³).
f'	Experimental data either for water content (L ⁻¹ L ⁻¹) or concentration (M L ⁻³).
g	Transformed concentration (M L ⁻³).
h	Pressure head (L).
h_c	Critical-pressure parameter of the Gardner conductivity relation (L).
h'_c	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).
J	Jacobian for transformation to local coordinates (L).
K	Hydraulic conductivity (L T).
K_s	Saturated conductivity parameter of the Gardner conductivity relation (L T).
K_0	$K(\theta = \theta_s)$ (L T).

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k_s	Saturated distribution coefficient ($L^3 M^{-1}$).
L	Length of chromatographic column (L).
$\mathcal{L}$	Differential operator for mass-transport (dimensionless).
$\{N\}, N$	Basis functions (dimensionless).
N_t	Number of experimental times (dimensionless).
N_x	Number of experimental positions (dimensionless).
n	Porosity ($L^3 L^{-3}$).
p	Theoretical parameter. May represent either moisture-transport or mass-transport parameter with its associated dimension (variable dimension).
p, p, p'	Vector of theoretical parameters (variable dimension).
Q	Diffusivity ($L^2 T^{-1}$).
q^*	$a_1 V \partial R_a$, the effective diffusivity ($L^2 T^{-1}$).
$\{R\}$	Vector obtained in numerical solution of mass-transport equation ($M L^{-1} T$).
$\{R^r\}$	(2x1) vector of values of the mass flux at the boundaries of the r-th element ($M L^{-1} T$).
$\{R^r\}$	Vector of mass-transport boundary flows ($M L^{-1} T$).
R_a	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 ($M M^{-1}$).
T_p	Parameter step-size tolerance factor (dimensionless).
T_x	X^2 acceptance factor (dimensionless).
t	Time (T).
V	Darcy velocity ($L T^{-1}$).
v	$V \partial R_a$, the effective velocity ($L T^{-1}$).
W	Reduced Darcy velocity ($L T^{-1}$).
$W^{(n)}$	The n-th approximation to the velocity solution of the water-transport equation ($L T^{-1}$).
W_1	$W(\alpha = 1)$ ($L T^{-1}$).
W_0	$W(\alpha = 0)$ ($L T^{-1}$).
X	Mass flux ($M L^{-1} T$).
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 ($M \cdot L^{-3} \cdot T$).
α, β, γ	Reduced water content (dimensionless).
β'	Modified coefficient of compressibility (L^{-1}).
Δp	Parameter increment (variable dimension).
Δt	Time increment (T).
δ	$(\theta_i - \theta_i^*) / (\theta_i + \theta_i^*)$ (dimensionless).
ϵ	Angle of inclination of the chromatographic column (°).
θ	Moisture content ($L^3 \cdot L^{-3}$).
θ_r	Residual moisture-content parameter ($L^3 \cdot L^{-3}$).
θ_i	Initial moisture content ($L^3 \cdot L^{-3}$).
θ_b	Boundary moisture content, equal to the porosity n in this document ($L^3 \cdot L^{-3}$).
θ^*	Experimental water content ($L^3 \cdot L^{-3}$).
κ	Reduced hydraulic conductivity ($L \cdot T$).
λ	Decay constant (T^{-1}).
λ_n	Eigenvalues of transformed mass-transport equation (L^{-1}).
μ	Transformation parameter (L^{-1}).
δ'	$(\theta_i - \theta) / (\theta_i + \theta)$ (dimensionless).
ρ	Bulk density of the medium ($M \cdot L^{-3}$).
σ'	Experimental measurement error either in water content ($L^3 \cdot L^{-3}$) or in concentration ($M \cdot L^{-3}$).
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

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	5.408	7.262	8.760	10.234	11.607
9.936	6.613	6.460	6.303	4.329	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
3.438	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				

4.

6.

OUTPUT

NUMBER OF JOURNAL POINTS.	101
NUMBER OF FIBERS.	102
NUMBER OF DIFFERENT MATERIALS	1
NUMBER OF COLLECTION MATERIALS.	3
NUMBER OF TIME INCREMENTS	153
NUMBER OF AMBIENT CONDITIONS	2
NUMBER OF SURFACE LAM.	2
VELOCITY INPUT CONTROL.	3
AUXILIARY STORAGE CONTROL.	3
READY-STATE CONTROL.	1
TIME-STEP CONTROL.	1
NUMBER OF LOWER VARIABLE SIZED ELEMENTS	2
NUMBER OF UPPER VARIABLE SIZED ELEMENTS	2
DUMSETT TIME INTEGRATION INDEX.	1
INITIAL-CONDITIONS CONTROL	1
RESIN CONTROL.	2
TIME INCREMENT.	0.75000-01
MULTIPLIER FOR INCREASING DELT.	0.500000
ASSIGN VALUE OF DELT	3.00000 01
ASSIGN VALUE OF TIME	3.00000 01
TIME-INTEGRATION PARAMETERS.	0.500000
ORIGIN OF RESIN GENERATION	0.0
ASSIGN X-VALUE	23.0000
LOWER FIRST X-INCREMENT	0.0
UPPER FIRST X-INCREMENT	0.5300
CONSTANT DANCE VELOCITY	3.0

SHIP CONTROL

[illegible]

MATERIAL-TRANSPORT INPUT TABLE 2.- MATERIAL PROPERTIES

WAT. NO.	RD	SNOW	AL	THICKEN	FOR
1 3-3		0-0	0-0	0-0	0-0

MATERIAL-TRANSPORT TABLE 1.- MODAL-POINT DATA

PUDE	X
1	0.0
2	0.11050 01
3	0.13150 01
4	0.15250 01
5	0.17350 01
6	0.19450 01
7	0.21550 01
8	0.23650 01
9	0.25750 01
10	0.27850 01
11	0.29950 01
12	0.32050 01
13	0.34150 01
14	0.36250 01
15	0.38350 01
16	0.40450 01
17	0.42550 01
18	0.44650 01

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19	0.46750 01
20	0.48050 01
21	0.50050 01
22	0.53050 01
23	0.55150 01
24	0.57250 01
25	0.59350 01
26	0.61450 01
27	0.63550 01
28	0.65650 01
29	0.67750 01
30	0.69850 01
31	0.71950 01
32	0.74050 01
33	0.76150 01
34	0.78250 01
35	0.80350 01
36	0.82450 01
37	0.84550 01
38	0.86650 01
39	0.88750 01
40	0.90850 01
41	0.92950 01
42	0.95050 01
43	0.97150 01
44	0.99250 01
45	0.10100 02
46	0.10250 02
47	0.10500 02
48	0.10770 02
49	0.10900 02
50	0.11190 02
51	0.11400 02
52	0.11610 02
53	0.11820 02
54	0.12030 02
55	0.12240 02
56	0.12450 02
57	0.12660 02
58	0.12870 02
59	0.13080 02
60	0.13290 02
61	0.13500 02
62	0.13710 02
63	0.13920 02
64	0.14130 02
65	0.14340 02
66	0.14550 02
67	0.14760 02
68	0.14970 02
69	0.15180 02
70	0.15390 02
71	0.15600 02
72	0.15810 02
73	0.16020 02
74	0.16230 02
75	0.16440 02
76	0.16650 02
77	0.16860 02
78	0.17070 02
79	0.17280 02
80	0.17490 02
81	0.17700 02
82	0.17910 02
83	0.18120 02
84	0.18330 02
85	0.18540 02
86	0.18750 02
87	0.18960 02
88	0.19170 02
89	0.19380 02
90	0.19590 02
91	0.19800 02
92	0.20010 02
93	0.20220 02

96 000000 00
 97 000000 00
 98 000000 00
 99 000000 00
 100 000000 00
 101 000000 00

WATERWAY TRANSPORT TABLE NO. 1000000000

WATERWAY TRANSPORT TABLE NO. 1000000000		WATERWAY TRANSPORT TABLE NO. 1000000000		WATERWAY TRANSPORT TABLE NO. 1000000000	
WATERWAY	WATERWAY	WATERWAY	WATERWAY	WATERWAY	WATERWAY
1	1	1	1	1	1
2	2	2	2	2	2
3	3	3	3	3	3
4	4	4	4	4	4
5	5	5	5	5	5
6	6	6	6	6	6
7	7	7	7	7	7
8	8	8	8	8	8
9	9	9	9	9	9
10	10	10	10	10	10
11	11	11	11	11	11
12	12	12	12	12	12
13	13	13	13	13	13
14	14	14	14	14	14
15	15	15	15	15	15
16	16	16	16	16	16
17	17	17	17	17	17
18	18	18	18	18	18
19	19	19	19	19	19
20	20	20	20	20	20
21	21	21	21	21	21
22	22	22	22	22	22
23	23	23	23	23	23
24	24	24	24	24	24
25	25	25	25	25	25
26	26	26	26	26	26
27	27	27	27	27	27
28	28	28	28	28	28
29	29	29	29	29	29
30	30	30	30	30	30
31	31	31	31	31	31
32	32	32	32	32	32
33	33	33	33	33	33
34	34	34	34	34	34
35	35	35	35	35	35
36	36	36	36	36	36
37	37	37	37	37	37
38	38	38	38	38	38
39	39	39	39	39	39
40	40	40	40	40	40
41	41	41	41	41	41
42	42	42	42	42	42
43	43	43	43	43	43
44	44	44	44	44	44
45	45	45	45	45	45
46	46	46	46	46	46
47	47	47	47	47	47
48	48	48	48	48	48
49	49	49	49	49	49
50	50	50	50	50	50
51	51	51	51	51	51
52	52	52	52	52	52
53	53	53	53	53	53
54	54	54	54	54	54
55	55	55	55	55	55
56	56	56	56	56	56
57	57	57	57	57	57
58	58	58	58	58	58
59	59	59	59	59	59

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

INTEGRAL-TRANSPORT INPUT TABLE 5.- BOUNDARY CONDITIONS OF FORM B-BB

NAME BB
1 0.0
101 0.0

OUTER-TRANSPORT INPUT TABLE 6.- BASIC PARAMETERS

FUNCTION TIME	2
NUMBER OF TABULAR TIME SERIES	17
NUMBER OF TIME SERIES 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 LONGHORN-GAUSS INTEGRATION	6
ORDER READ ALPHA = 1.	0
NUMBER OF POINTS IN INTERPOLATING POLYNOMIAL	2
AUXILIARY STORAGE CONTROL	0
VARIABLE-STEP CONTROL	1
ANALYTIC SOIL-PROPERTIES CONTROL	1
INITIAL CONDITION ON WATER CONTENT THETA	0.42500-02
BOUNDARY CONDITION ON WATER CONTENT THETA	0.67100 00
INCLINATION IN DEGREES	0.68000 02
ALPHA INCREMENT READ ALPHA = 1.	0.10000-01

NAME:
0.10000000-03 -0.49900000 02 0.17000000 01

LDPAR:

0.00000000 0.00000000 0.00000000 0.00000000 0.00000000

VARIABLE:

0.10000000	0.20000000	0.30000000	0.40000000	0.50000000	0.60000000	0.70000000	0.80000000	0.90000000	1.00000000
0.00000000	0.10000000	0.20000000	0.30000000	0.40000000	0.50000000	0.60000000	0.70000000	0.80000000	0.90000000
0.00000000	0.00000000	0.10000000	0.20000000	0.30000000	0.40000000	0.50000000	0.60000000	0.70000000	0.80000000
0.00000000	0.00000000	0.00000000	0.10000000	0.20000000	0.30000000	0.40000000	0.50000000	0.60000000	0.70000000
0.00000000	0.00000000	0.00000000	0.00000000	0.10000000	0.20000000	0.30000000	0.40000000	0.50000000	0.60000000

SEARCH INPUT TABLE 10. BASIC PARAMETERS

NUMBER OF SEARCH PARAMETERS	11
MINIMUMAL SEARCH CONTROL	1
MINIMAL CALCULATED EVALUATIONS	10
DELETED CONTROL SYSTEM	1
NUMBER OF EXPERIMENTAL TIME MODES	1
PARAMETER NUMBER CONTROL	1
NUMBER OF SEARCH CYCLES	1
AUXILIARY STORAGE CONTROL	1
ACCELERATION PARAMETER	0.15000 01
REDUCTION PARAMETER	0.25000 00
STEP-SIZE TOLERANCE	0.10000-09
MIN-SQUARE ACCEPTABLE FACTOR	0.10000-09
PARAMETER STEP-LENGTH FRACTION	0.10000 00
DELETED CONTROL	0.10000 01

SEARCH INPUT TABLE 11. EXPERIMENTAL DATA

TABLE AT TIME 0.000000 00

IX	EX	TX	UX
1	0.100000 01	-0.100760 01	0.0
2	0.110000 01	0.200100 00	0.0
3	0.150000 01	-0.313930 00	0.0
4	0.170000 01	-0.313900 00	0.0
5	0.190000 01	0.200100 00	0.0
6	0.210000 01	-0.313930 00	0.300760 01
7	0.230000 01	0.179910 00	0.261160 01
8	0.250000 01	-0.160000 00	0.301770 01
9	0.270000 01	0.553230 00	0.262210 01
10	0.290000 01	0.200100 00	0.281030 01
11	0.310000 01	0.211010 01	0.160250 01
12	0.330000 01	0.002100 01	0.905620 00
13	0.350000 01	0.731690 01	0.610050 00
14	0.370000 01	0.114790 02	0.633270 00
15	0.400000 01	0.163350 02	0.317050 00
16	0.425000 01	0.215300 02	0.244790 00
17	0.440000 01	0.152950 02	0.336700 00
18	0.467500 01	0.575010 01	0.760270 00
19	0.480000 01	0.500920 01	0.796710 00
20	0.509500 01	0.500230 01	0.836890 00
21	0.530000 01	0.162000 01	0.177530 01
22	0.551500 01	0.190070 01	0.154970 01
23	0.570000 01	0.124090 01	0.167500 01
24	0.593000 01	0.179010 00	0.261160 01
25	0.610000 01	0.000000 00	0.0
26	0.630000 01	0.373010 00	0.0
27	0.650000 01	-0.140000 00	0.0
28	0.677500 01	-0.140000 00	0.0
29	0.690000 01	-0.100760 01	0.0
30	0.719500 01	-0.140000 00	0.0
31	0.740000 01	0.124090 01	0.0
32	0.761500 01	0.200100 00	0.0
33	0.780000 01	-0.140000 00	0.0
34	0.803500 01	0.224090 01	0.0
35	0.820000 01	0.726000 00	0.0
36	0.845500 01	0.102000 01	0.0

37	0.045200 01	0.900070 00	0.0
38	0.045200 01	0.907320 01	0.0
39	0.045200 01	-0.900000 00	0.0
40	0.029500 01	0.907320 01	0.0
41	0.029500 01	0.204300 00	0.0
42	0.029500 01	-0.900000 00	0.0
43	0.025200 01	-0.900000 00	0.0
44	0.045200 02	0.329570 -01	0.0
45	0.045200 02	0.204300 00	0.0
46	0.045200 02	0.204300 00	0.0
47	0.045200 02	-0.900000 00	0.0
48	0.045200 02	0.120470 01	0.0
49	0.110750 02	0.204300 00	0.0
50	0.110750 02	0.720460 00	0.0
51	0.100050 02	-0.007330 00	0.0
52	0.110750 02	0.204300 00	0.0
53	0.120250 02	0.204300 00	0.0
54	0.122350 02	0.204300 00	0.0
55	0.120050 02	-0.007330 00	0.0
56	0.120050 02	0.200000 00	0.0
57	0.120050 02	0.329570 -01	0.0
58	0.120750 02	0.379070 00	0.0
59	0.120050 02	-0.900000 00	0.0
60	0.130050 02	-0.313900 00	0.0
61	0.130050 02	0.379070 00	0.0
62	0.130150 02	-0.313900 00	0.0
63	0.045200 02	-0.900000 00	0.0
64	0.045200 02	-0.007330 00	0.0
65	0.045200 02	0.720460 00	0.0
66	0.045200 02	0.204300 00	0.0
67	0.045200 02	0.379070 00	0.0
68	0.154750 02	-0.007330 00	0.0
69	0.120050 02	0.553330 00	0.0
70	0.045200 02	-0.313900 00	0.0
71	0.045200 02	0.204300 00	0.0
72	0.045200 02	0.204300 00	0.0
73	0.045200 02	0.553330 00	0.0
74	0.045200 02	0.329570 -01	0.0
75	0.045200 02	-0.313900 00	0.0
76	0.045200 02	0.553330 00	0.0
77	0.045200 02	0.329570 -01	0.0
78	0.045200 02	0.553330 00	0.0
79	0.045200 02	0.204300 00	0.0
80	0.045200 02	0.329570 -01	0.0
81	0.045200 02	0.720460 00	0.0
82	0.045200 02	0.204300 00	0.0
83	0.045200 02	0.000070 00	0.0
84	0.045200 02	0.329570 -01	0.0
85	0.045200 02	0.204300 00	0.0
86	0.045200 02	0.720460 00	0.0
87	0.045200 02	-0.000070 00	0.0
88	0.045200 02	-0.000070 00	0.0
89	0.045200 02	0.000070 00	0.0
90	0.045200 02	0.329570 -01	0.0
91	0.045200 02	0.204300 00	0.0
92	0.045200 02	-0.000070 00	0.0

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

IP	P	PS	PL	PP
1	0.430750 02	0.100000 01	0.100000 01	0.430750 01
2	0.175000 01	0.175000 01	0.175000 01	0.175000 00
3	0.040190 00	0.100000 01	0.100000 01	0.040190 01
4	0.625000 02	0.625000 02	0.625000 02	0.625000 03
5	0.625000 00	0.625000 00	0.625000 00	0.625000 01
6	0.757000 04	0.757000 04	0.757000 04	0.757000 05
7	-0.099000 02	-0.099000 02	-0.099000 02	-0.099000 01
8	0.170000 01	0.170000 01	0.170000 01	0.170000 00
9	0.107000 03	0.107000 03	0.107000 03	0.107000 04
10	-0.232000 02	-0.232000 02	-0.232000 02	-0.232000 01
11	-0.019000 00	-0.019000 00	-0.019000 00	-0.019000 01

,

[illegible]

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E 1 0.1501220 02 0.42770120 02 0.17500000 01 0.22095500 00 0.62500000-02 0.62500000 00 0.75700000-00 -0.09900000 02
INCREASING THE I-TU VARIABLE
F 3 0.30550000 02 0.42770120 02 0.17500000 01 0.32030000 00 0.62500000-02 0.62500000 00 0.75700000-00 -0.09900000 02
DECREASING THE I-TU VARIABLE
E 3 0.75091100 02 0.42770120 02 0.17500000 01 0.32525250 00 0.62500000-02 0.62500000 00 0.75700000-00 -0.09900000 02
PATTERN NAME EXPLOSION TEST CASE BASE PT.
NAME
* 0.30900000 02 0.39007500 02 0.17500000 00 0.30701100 00 0.62500000-02 0.62500000 00 0.75700000-00 -0.09900000 02
ONLY
0.17000000 01 0.39700000-03 -0.22000000 02 -0.09900000 00
-0.30700000 01 0.0 0.99029750-01 0.0 0.0 0.0
0.0 0.0 0.0
NAME EXPLOSION LOOP
INCREASING THE I-TU VARIABLE
F 1 0.17570230 02 0.39007500 02 0.17500000 00 0.30701100 00 0.62500000-02 0.62500000 00 0.75700000-00 -0.09900000 02
DECREASING THE I-TU VARIABLE
E 1 0.35010500 02 0.39007500 02 0.17500000 01 0.30701100 00 0.62500000-02 0.62500000 00 0.75700000-00 -0.09900000 02
CHECK STEP SIZE
INCREASING THE I-TU VARIABLE
F 3 0.30020500 02 0.39007500 02 0.17500000 00 0.30720150 00 0.62500000-02 0.62500000 00 0.75700000-00 -0.09900000 02
DECREASING THE I-TU VARIABLE
E 3 0.30050000 02 0.39007500 02 0.17500000 00 0.30720000-01 0.62500000-02 0.62500000 00 0.75700000-00 -0.09900000 02
CHECK STEP SIZE
NAME PL. EXPLOSION CODE NAME
THE NUMBER OF FUNCTION EVALUATIONS INCURRED IS
* 0.30900000 02 0.39007500 02 0.17500000 00 0.30701100 00 0.62500000-02 0.62500000 00 0.75700000-00 -0.09900000 02
0.17000000 01 0.39700000-03 -0.22000000 02 -0.09900000 00

```

WATER-TRANSPORT INPUT TABLE 0.. BASIC PARAMETERS

```

TEMP:
0.62500000-02 0.31000000-01 0.35270000-01 0.70072120-01 0.10239020 00 0.12520000 00 0.10761000 00 0.10950000 00
0.19002310 00 0.21100500 00 0.23233170 00 0.25232110 00 0.27002050 00 0.29007500 00 0.30902750 00 0.32752000 00
0.30513000 00 0.30220020 00 0.37002700 00 0.39511000 00 0.41001730 00 0.42000000 00 0.40000200 00 0.45500170 00
0.40000000 00 0.40221150 00 0.40500250 00 0.50703750 00 0.51923050 00 0.53075000 00 0.50170070 00 0.55217700 00
0.50217310 00 0.57100230 00 0.50073500 00 0.50930270 00 0.59730020 00 0.60500900 00 0.61230000 00 0.61001250 00
0.62500000 00

ALP:
0.0 0.00000000-01 0.75230770-01 0.11700230 00 0.15530000 00 0.75230770 00 0.22000150 00 0.26300020 00
0.19002310 00 0.23230770 00 0.30530000 00 0.30700230 00 0.42000000 00 0.40000000 00 0.59000000 00 0.59023000 00
0.50700230 00 0.57530000 00 0.60230770 00 0.62000150 00 0.65300020 00 0.67000150 00 0.70230770 00 0.72530000 00
0.70700230 00 0.70230000 00 0.79000000 00 0.81000000 00 0.82923000 00 0.80700230 00 0.80530000 00 0.80230770 00
0.89000150 00 0.91300020 00 0.92000750 00 0.90230770 00 0.95530000 00 0.90700230 00 0.97923000 00 0.99000000 00
0.10000000 01

```

SYSTEM-FLOW TABLE 11.. AT TIME = 0.12030 00 , (DELTA = 1.00000 00)

TYPE OF FLOW	RATE	INC. FLOW	TOTAL FLOW
CONSTANT-CONCENTRATION MODE FLOW	0.57200-02	0.65750-02	0.07200-01
CONSTANT-FLUX-MODE FLOW	0.0	0.0	0.0
SEEPAGE FLUX-MODE FLOW	0.0	0.0	0.0
UNUSUAL LOSSES	0.0	0.0	0.0
NET FLOW	0.57200-02	0.65750-02	0.07200-01
INCREASE IN MATERIAL CONTENT (LITERS)	-0.19000-02	-0.20070-02	0.15720-01
INCREASE IN MATERIAL CONTENT (GALLONS)	-0.21770 00	-0.22050 00	0.17300 01
WATER-REACTIVE LOSSES (LIQUID AND SOLID)	0.0	0.0	0.0

SYSTEM-FLOW TABLE 21.. AT TIME = 3.51770 01, (DELT = 5.00760 00)

TYPE OF FLOW	RATE	ISC. FLOW	TOTAL FLOW
CONSTANT-CONCENTRATION BORE FLOW. . . .	0.15150-02	0.07070-02	0.12600 00
CONSTANT-FLOW-BORE FLOW.	0.0	0.0	0.0
SEEPAGE FLOW-BORE FLOW.	0.0	0.0	0.0
NUMERICAL LOSSES.	0.0	0.0	0.0
NET FLOW.	0.15150-02	0.07070-02	0.12600 00
INCREASE IN SATURATED CONTENT (LIQUID). .	-0.30000-03	-0.10000-02	0.09620-02
INCREASE IN SATURATED CONTENT (SOLID). .	-0.30000-01	-0.20070 00	0.99090 00
IMPERMEABLE LOSSES (LIQUID AND SOLID). .	0.0	0.0	0.0

SYSTEM-FLOW TABLE 31.. AT TIME = 1.00020 02, (DELT = 1.66220 01)

TYPE OF FLOW	RATE	ISC. FLOW	TOTAL FLOW
CONSTANT-CONCENTRATION BORE FLOW. . . .	0.50360-03	0.10200-01	0.22260 00
CONSTANT-FLOW-BORE FLOW.	0.0	0.0	0.0
SEEPAGE FLOW-BORE FLOW.	0.0	0.0	0.0
NUMERICAL LOSSES.	0.0	0.0	0.0
NET FLOW.	0.50360-03	0.10200-01	0.22260 00
INCREASE IN SATURATED CONTENT (LIQUID). .	-0.51700-00	-0.07700-03	-0.50070-02
INCREASE IN SATURATED CONTENT (SOLID). .	-0.50360-02	-0.97010-01	-0.10050 00
IMPERMEABLE LOSSES (LIQUID AND SOLID). .	0.0	0.0	0.0

SYSTEM-FLOW TABLE 41.. AT TIME = 0.19260 02, (DELT = 1.02030 01)

TYPE OF FLOW	RATE	ISC. FLOW	TOTAL FLOW
CONSTANT-CONCENTRATION BORE FLOW. . . .	0.99730-03	0.95060-02	0.32950 00
CONSTANT-FLOW-BORE FLOW.	0.0	0.0	0.0
SEEPAGE FLOW-BORE FLOW.	0.0	0.0	0.0
NUMERICAL LOSSES.	0.0	0.0	0.0
NET FLOW.	0.99730-03	0.95060-02	0.32950 00
INCREASE IN SATURATED CONTENT (LIQUID). .	-0.90200-00	-0.62330-03	-0.09000-02
INCREASE IN SATURATED CONTENT (SOLID). .	-0.17990-02	-0.60090-01	-0.99300 00
IMPERMEABLE LOSSES (LIQUID AND SOLID). .	0.0	0.0	0.0

SYSTEM-FLOW TABLE 51.. AT TIME = 9.91230 02, (DELT = 7.55760 01)

TYPE OF FLOW	RATE	ISC. FLOW	TOTAL FLOW
CONSTANT-CONCENTRATION BORE FLOW. . . .	-0.30710-05	-0.10070-03	0.35060 00
CONSTANT-FLOW-BORE FLOW.	0.0	0.0	0.0
SEEPAGE FLOW-BORE FLOW.	0.0	0.0	0.0
NUMERICAL LOSSES.	0.0	0.0	0.0
NET FLOW.	-0.30710-05	-0.10070-03	0.35060 00
INCREASE IN SATURATED CONTENT (LIQUID). .	-0.37990-05	-0.20710-03	-0.12960-01
INCREASE IN SATURATED CONTENT (SOLID). .	-0.40000-03	-0.31700-01	-0.10320 01
IMPERMEABLE LOSSES (LIQUID AND SOLID). .	0.0	0.0	0.0

SYSTEM-FLUX TABLE 69.. AT TIME = 2.40000 03 (MULT = 0.05000 01)

TYPE OF FLOW	DATE	INC. FLOW	TOTAL FLOW
CONSTANT-CONCENTRATION MOSE FLOW	-0.20100-04	-0.09520-03	0.33010 00
CONSTANT-FLUX-MOSE FLOW	0.0	0.0	0.0
SEEPAGE FLOW-MOSE FLOW	0.0	0.0	0.0
NUMERICAL LOSSES	0.0	0.0	0.0
NET FLOW	-0.20100-04	-0.09520-03	0.33010 00
INCREASE IN MATERIAL CONTENT (LIQUID)	-0.01950-04	-0.10070-04	-0.10000-01
INCREASE IN MATERIAL CONTENT (SOLID)	-0.06300-04	-0.20600-02	-0.16520 03
REACTIVE LOSSES (LIQUID AND SOLID)	0.0	0.0	0.0

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

IP	P	PI	PL	BP
1	0.39070 02	0.100000 51	0.100000 01	-0.206000 01
2	0.175000 01	0.175000 01	0.175000 01	0.0
3	0.102010 00	0.100000 51	0.100000-01	0.200570-01
4	0.625000-02	0.625000-02	0.625000-02	0.0
5	0.625000 00	0.625000 00	0.625000 00	0.0
6	0.757000-04	0.757000-04	0.757000-04	0.0
7	-0.095000 02	-0.095000 02	-0.095000 02	0.0
8	0.170000 01	0.170000 01	0.170000 01	0.0
9	0.397000-03	0.397000-03	0.397000-03	0.0
10	-0.112000 02	-0.112000 02	-0.112000 02	0.0
11	-0.019000 00	-0.019000 00	-0.019000 00	0.0

SEARCH OUTPUT TABLE 2.. EXPERIMENTAL DATA AND THEORETICAL FIT

TABLE AT TIME =0.24000 04

IX	IX	IX	IX	OUT
1	0.130500 01	-0.100700 01	-0.102300 01	1.377270 00
2	0.131500 01	0.200300 00	-0.090050 00	0.393990 00
3	0.152500 01	-0.313900 00	0.100000 00	0.512000 00
4	0.173500 01	-0.313900 00	0.100700 00	0.512000 00
5	0.190500 01	0.200300 00	0.097010-01	0.393990 00
6	0.215500 01	-0.313900 00	0.005790-01	0.512000 00
7	0.230500 01	0.370010 00	0.271100 00	0.610700 00
8	0.257500 01	-0.100000 00	0.612600 00	0.500020 00
9	0.270500 01	0.553230 00	0.076210 00	0.602550 00
10	0.299500 01	0.200300 00	0.591300 00	0.393990 00
11	0.320500 01	0.2110 00 01	0.195300 01	0.620900 00
12	0.301500 01	0.002100 01	0.030000 01	0.100730 01
13	0.302500 01	0.731600 01	0.775300 01	0.125000 01
14	0.303500 01	0.110700 02	0.120020 02	0.151900 01
15	0.000500 01	0.163350 02	0.100030 02	0.177490 01
16	0.025500 01	0.215300 02	0.170000 02	0.201300 01
17	0.006500 01	0.152950 02	0.100050 02	0.172320 01
18	0.007500 01	0.575010 01	0.102000 02	0.110000 01
19	0.000500 01	0.500920 01	0.090130 01	0.112030 01
20	0.500500 01	0.500230 01	0.300950 01	0.109310 01
21	0.330500 01	0.102000 01	0.101200 01	0.750590 00
22	0.551500 01	0.190070 01	0.315050 00	0.000520 00
23	0.374500 01	0.120070 01	0.135000 00	0.730300 00
24	0.503500 01	0.370010 00	0.272500 00	0.610700 00
25	0.010500 01	0.900090 00	0.200020 00	0.607010 00
26	0.035500 01	0.370010 00	0.233300 00	0.610700 00
27	0.050500 01	-0.100000 00	0.320350 00	0.500920 00
28	0.077500 01	-0.100000 00	0.509590 00	0.500920 00
29	0.090500 01	-0.100700 01	0.003000 00	0.377200 00
30	0.719500 01	-0.100000 00	0.050010 00	0.500920 00
31	0.700500 01	0.200300 00	0.930500-01	0.730300 00
32	0.701500 01	0.200300 00	-0.139050 00	0.500920 00
33	0.702500 01	-0.100000 00	-0.215300 00	0.730300 00
34	0.003500 01	0.120070 01	-0.100150 00	0.730300 00
35	0.030500 01	0.720000 00	-0.120270 00	0.005010 00
36	0.005500 01	0.102000 01	-0.211500 00	0.750590 00

37	0.046500 01	0.100000 00	-0.215000 00	0.607010 00
38	0.007500 01	0.107350 01	0.000730-01	0.709320 00
39	0.000500 01	-0.100000 00	0.277000 00	0.500520 00
40	0.029500 01	0.107350 01	0.570000-01	0.709320 00
41	0.050500 01	0.200300 00	-0.173000 00	0.503990 00
42	0.071500 01	-0.100000 00	-0.730000-01	0.500520 00
43	0.092500 01	-0.100000 00	0.112070 00	0.500520 00
44	0.100350 02	0.329510-01	0.112020 00	0.560150 00
45	0.103050 02	0.200300 00	0.000110-01	0.503990 00
46	0.105550 02	0.200300 00	0.000030-01	0.503990 00
47	0.107050 02	-0.100000 00	-0.752500-01	0.500520 00
48	0.108550 02	0.120400 01	-0.300020-01	0.720300 00
49	0.110050 02	0.200300 00	0.315270 00	0.503990 00
50	0.111950 02	0.720400 00	0.077500 00	0.665610 00
51	0.116050 02	-0.007330 00	0.200020 00	0.002130 00
52	0.118150 02	0.200300 00	-0.090020 00	0.503990 00
53	0.120250 02	0.200300 00	-0.200700 00	0.503990 00
54	0.122350 02	0.000000 00	-0.091200-01	0.607010 00
55	0.120050 02	-0.007330 00	0.002520 00	0.002130 00
56	0.120550 02	0.000000 00	0.330000 00	0.607010 00
57	0.120050 02	0.329510-01	0.205700 00	0.560150 00
58	0.130750 02	0.379010 00	0.533100-01	0.610790 00
59	0.132050 02	-0.100000 00	0.099700-11	0.500520 00
60	0.130950 02	-0.313900 00	0.127000 00	0.512000 00
61	0.127050 02	0.379010 00	-0.005270-01	0.610790 00
62	0.130150 02	-0.313900 00	-0.230020 00	0.512000 00
63	0.004150 02	-0.100000 00	-0.100100 00	0.500520 00
64	0.005350 02	-0.007330 00	0.001000-01	0.002130 00
65	0.006050 02	0.720400 00	0.200710-01	0.665610 00
66	0.007550 02	0.200300 00	0.017200-02	0.503990 00
67	0.000050 02	0.379010 00	0.200000 00	0.610790 00
68	0.151750 02	-0.007330 00	0.290570 00	0.002130 00
69	0.152050 02	0.553230 00	0.510950-01	0.002500 00
70	0.150950 02	-0.313900 00	-0.110000 00	0.512000 00
71	0.150050 02	0.200300 00	-0.122020 00	0.503990 00
72	0.100150 02	0.200300 00	-0.150200 00	0.503990 00
73	0.002250 02	0.553230 00	-0.200020 00	0.602500 00
74	0.000350 02	0.329510-01	-0.000900-00	0.560150 00
75	0.000050 02	-0.313900 00	0.000000 00	0.512000 00
76	0.000550 02	0.553230 00	0.079100-01	0.602500 00
77	0.170050 02	0.329510-01	0.132000 00	0.560150 00
78	0.172750 02	0.553230 00	0.177000 00	0.602500 00
79	0.170050 02	0.200300 00	0.101000 00	0.503990 00
80	0.170950 02	0.329510-01	0.770000-01	0.560150 00
81	0.170050 02	0.720400 00	0.790300-01	0.665610 00
82	0.101150 02	0.200300 00	0.700370-01	0.503990 00
83	0.100250 02	0.000000 00	0.300700-01	0.607010 00
84	0.100350 02	0.329510-01	-0.009110-01	0.560150 00
85	0.100750 02	0.200300 00	-0.503990-01	0.503990 00
86	0.100550 02	0.720400 00	-0.230900 00	0.665610 00
87	0.090050 02	-0.000100 00	-0.391270 00	0.015790 00
88	0.093750 02	-0.660700 00	-0.292030 00	0.009070 00
89	0.095050 02	0.000000 00	-0.100000 00	0.607010 00
90	0.097950 02	0.329510-01	-0.270230-01	0.560150 00
91	0.200050 02	0.200300 00	-0.217900 00	0.503990 00
92	0.202150 02	-0.660700 00	-0.321010 00	0.009070 00

AVERAGE POINT RESIDUAL = 0.13500 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 PHAT
      COMMON/BIVAR/KPRO, KPR (1000), MAXDIP, MAXEL, MAXNP, MAXMAT, MAXBW,
1 MAXNTI, NHPPH
      COMMON/BRVAR/ A(101,2), B(101,3), R(101), R2(101), RI(101), RB(101),
1 DP(101), B1(101), BT(101), XTHP(101), BFLX(101), BFLIP(101), FX(100,2)
1 , PRATE(10), FLOW(10), TFLOW(10), W, PHAT(3,5)
      DATA MAXEL, MAXNP, MAXMAT, MAXBW, MAXNTI, NHPPH/100, 101, 1, 3, 1000, 5/
      DATA PHAT/4H ,4H K0,4H ,4H ,4H H00,4H ,4H ,
1 4H AL,4H ,4H T,4H HETA,4H ,4H ,4H POR,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 PERTURBATIVE METHOD IS USED FOR
C THE MOISTURE TRANSPORT.
C
C DIMENSIONING FORMAT--
C
      COMMON/PROBID/TITLE(8), #PROB
C
      COMMON/CRVAR/TIME, TH (MAXEL, 2), THH (MAXEL, 2), THV (MAXEL, 2),
1 DTH (MAXEL, 2), VI (MAXEL, 2), VIP (MAXEL, 2), VIV (MAXEL, 2)
C
      COMMON/GLOB/I (MAXNP), BB(2), DCOSB(2), DELT, CHNG,
1 DELHAI, TAI, IPI (MAXNP), IE (MAXEL, 3), NPB(2), NPST(2), NPTST(2),
1 NBE(2), BTSE(2), XSB(2,2), IS(2,2), NBP, BEL, WHAT, IBAND, NBC,
1 NST, NTST, NBEL, NTI, NHOB
C
      COMMON/BIVAR/KPRO, KPR (MAXNTI), MAXDIP, MAXEL, MAXNP, MAXMAT,
1 MAXBW, MAXNTI, NHPPH
C
      COMMON/NPROP/PROP (MAXMAT, NHPPH), VII
C
      COMMON/BRVAR/ C (MAXNP, MAXBW), B (MAXNP), BP (MAXNP), RI (MAXNP),
1 BB (MAXNP), DP (MAXNP), XTHP (MAXNP), BFLX (MAXNP), BFLIP (MAXNP),
1 FX (MAXEL, 2), PRATE(10), FLOW(10), TFLOW(10), W, PHAT(3, NHPPH)
C
      COMMON/NUNITG/ BORDER1, BORDER, NIFP, ITHIN, IGSS, ITHIN,
1 IGSSV(3)
C
      COMMON/TPLX/TTAB (NITTAB), V1N (NITTAB), V1TAB (NITTAB),
1 N1TAB (NITTAB), UTAB (NITTAB), TABL (NITTAB), N1TABL (NITTAB),
1 TEMP (NITTAB), IPTTAB (NITTAB), NITAB
C
      COMMON/TUTH/I (MAXNP), NT
C
      COMMON/WPROP/AKPAR (N1SLP), CDPAR (N1SLP), AKSH (N1SLP2),
1 ALPK (N1SLP2), D (N1SLP2), LPPD (N1SLP2), AKSAT, AKSHO, N1PAR,
1 NKSP, NCDPAR, NDSP
C
      COMMON/IVAR/ISUP1 (MAXTHP), ISUP2 (MAXTHP), THP (MAXTHP),
1 ALP (MAXTHP), VSUP1 (MAXTHP), VSUP2 (MAXTHP), P (MAXTHP), QGA (MAXTHP),
1 QG (MAXTHP), THTHP (MAXTHP), AKGSS ( (MAXTHP-1) * XGSS + N1GSS1),
1 DGSS ( (MAXTHP-1) * N1GSS + N1GSS1), IPTTH (MAXTHP), NTH, JTH, NGSS
C
      COMMON/SIP/NP, KPRS, NIFOB, ICONV, NSCY, IPA (MAXCY, MAXSHP)
C
      COMMON/SRP/ DELTO, CHISO, ACC, RED, TOLSTP, TOLFUN, PO (MAXSHP),
1 PH (MAXSHP), PL (MAXSHP), DELP (MAXSHP), PLO (MAXSHP), PMO (MAXSHP)
C
      COMMON/XIV/N1X1 (N1THEX), N1XU (N1THEX), N1X (N1THEX), N1Y, N1T
C
      COMMON/IBV/XI (N1NPEX, N1THEX), XI (N1NPEX, N1THEX), YX (N1NPEX,
1 N1THEX), DYI (N1NPEX, N1THEX), YI (N1NPEX), TX (N1THEX), XUTL (N1THEX),
1 XUTU (N1THEX)
C
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 NHPPH IS THE MAXIMUM NUMBER OF MATERIAL PROPERTIES PER
C MATERIAL,
C
C MAXTHN IS THE MAXIMUM NUMBER OF TIME VALUES USED IN THE
C UNCOUPLED WATER TRANSPORT CALCULATION,
C
C MAXTHP IS THE MAXIMUM NUMBER OF THETA POINTS,

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C	295
C	300
C	305
C	310
C	315
C	320
C	325
C	330
C	335
C	340
C	345
C	350
C	355
C	360
	365
	370
	375
	380
	385
	390
	395
	400
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	410
	415
	420
	425
	430
	435
	440
	445
	450
	455
	460
	465
	470
	475
	480
C	485
C	490
	495
	500
	505
	510
	515
	520
C	525
C	530
C	535
	540
	545
	550
	555
	560
	565
	570
	575
	580
	585
	590
	595
	600
	605
	610
	615
	620
	625
	630
	635
C	640
C	645
C	650
	655
	660
	665

ITHIN=1	570
CALL PRTTAB	575
IF (KUTR.EQ.0) GO TO 10	580
IF (KSTRV.EQ.1) CALL STRV1	585
ITHIN=1	590
DO 70 ITH=1,NT	595
CALL WINTP(T(ITH))	700
CALL WTIME(T(ITH))	705
TIME=T(ITH)	710
CALL WTRN1	715
IF (KUTR.EQ.2) CALL WTRN2	720
CALL PRTW1(ITH)	725
IF (KUTR.EQ.2) CALL PRTW2(ITH)	730
IF (KSTRV.EQ.1) CALL STRV1(T(ITH))	735
70 CONTINUE	740
GO TO 10	745
C	750
C DO COUPLED CALCULATION.	755
C	760
80 CALL DATAN	765
CALL DINN	770
90 CALL PWCAL	775
CALL MINL	780
CALL MINL	785
CALL PRTTAB	790
TIME=0.	795
CALL PRINTB(0)	800
IF (KSTRV.EQ.1) CALL STRV1	805
TIME =DELT	810
DO 120 ITH=1,NTI	815
VIP=V1	820
CALL STRAN	825
CALL PRINTB(ITH)	830
IF (KSTRV.EQ.1.AND.KPR(ITH).GT.0) CALL STRV1	835
IF (KSS.EQ.0) GO TO 10	840
IF (TIME.EQ.TMAX) GO TO 10	845
IF (KTSTP.NE.0) GO TO 100	850
DELT=DELT*(1.+CHNG)	855
GO TO 110	860
100 IF (ITH.EQ.1) TCON=DELT*V1*(1.+CHNG)	865
DELT=TCON/V1*(1.+CHNG)	870
110 DELT=DMIN1(DELT,DELMAX)	875
TIME =TIME+DELT	880
IF (TIME.LT.TMAX) GO TO 120	885
DELT=DELT-(TIME-TMAX)	890
TIME=TMAX	895
120 CONTINUE	900
GO TO 10	905
C	910
C SEARCH FOR MATERIAL-TRANSPORT VARIABLES ONLY, UNCOUPLED CALCULATION.	915
C	920
130 CALL DATAN	925
CALL DATAS	930
DELTO=DELT	935
IF (NSCY.LE.0) GO TO 150	940
IF (NXPUN.LE.0) GO TO 160	945
DO 140 ISCY=1,NSCY	950
CALL SUPREP(ISCY)	955
CALL SEARCH(MP,P,CHIS,PH,PL,ACC,BED,TOLSTP,TOLPUN,DELP,KPRS,	960
1 NEVAL,NXPUN,ICONV)	965
140 CONTINUE	970
150 KPGH=1	975
KSOOT=0	980
CALL NEVAL(P,CHIS)	985
GO TO 10	990
C	995
C SEARCH FOR WATER-TRANSPORT VARIABLES ONLY.	1000
C	1005
160 CALL DINN	1010
CALL DATAS	1015
KRUFF=0	1020
IF (NSCY.LE.0) GO TO 180	1025
IF (NXPUN.LE.0) GO TO 180	1030
DO 170 ISCY=1,NSCY	1035
CALL SUPREP(ISCY)	1040

	CALL SEARCH(MP,P,CHIS,PH,PL,ACC,RED,TOLSTP,TOLFUM,DELP,KPRS,	1045	
1	NEVAL,HXPUN,ICONV)	1050	
170	CONTINUE	1055	
180	KPGH=2	1060	
	KSOUT=0	1065	
	CALL NEVAL(P,CHIS)	1070	
	GO TO 10	1075	
C		1080	
C	SEARCH FOR MATERIAL TRANSPORT VARIABLES ONLY, COUPLED CALCULATION.	1085	
C		1090	
190	CALL DATAN	1095	
	CALL DIMW	1100	
	CALL PUCAL	1105	
	CALL WIND	1110	
	CALL PRTTAB	1115	
	CALL DATAS	1120	
	DELTO=DELT	1125	
	IF (HXPUN.LE.0) GO TO 210	1130	
	IF (MSCY.LE.0) GO TO 210	1135	
	DO 200 ISCY=1, MSCY	1140	
	CALL SHPREP (ISCY)	1145	
	CALL SEARCH(MP,P,CHIS,PH,PL,ACC,RED,TOLSTP,TOLFUM,DELP,KPRS,	1150	
1	HNEVAL,HXPUN,ICONV)	1155	
200	CONTINUE	1160	
210	KPGH=3	1165	
	KSOUT=0	1170	
	CALL HNEVAL(P,CHIS)	1175	
	GO TO 10	1180	
C		1185	
C	SEARCH FOR BOTH MATERIAL- AND WATER-TRANSPORT VARIABLES. COUPLED	1190	
C	CALCULATION.	1195	
C		1200	
220	CALL DATAN	1205	
	CALL DIMW	1210	
	CALL DATAS	1215	
	DELTO=DELT	1220	
	KBUFP=1	1225	
	IF (MSCY.LE.0) GO TO 240	1230	
	IF (HXPUN.LE.0) GO TO 240	1235	
	DO 230 ISCY=1, MSCY	1240	
	CALL SHPREP (ISCY)	1245	
	CALL SEARCH(MP,P,CHIS,PH,PL,ACC,RED,TOLSTP,TOLFUM,DELP,KPRS,	1250	
1	HNEVAL2,HXPUN,ICONV)	1255	
230	CONTINUE	1260	
240	KPGH=3	1265	
	KSOUT=0	1270	
	CALL HNEVAL2(P,CHIS)	1275	
	GO TO 10	1280	
10000	FORMAT(2I5,8A8)	1285	
10100	FORMAT(/' CALCULATION.. TYPE',I5,'.. PROBLEM',I5,'.. ',8A8/)	1290	
	END	1295	
	SUBROUTINE HTR	HTR	0
C		HTR	5
C	FUNCTION OF SUBROUTINE--TO CONTROL THE INTEGRATION OF THE	HTR	10
C	MATERIAL-FLOW EQUATION, WHICH CONSISTS OF ASSEMBLY, APPLICATION	HTR	15
C	OF BOUNDARY CONDITIONS, AND MATRIX SOLUTION OF THE RESULTING	HTR	20
C	SET OF EQUATIONS.	HTR	25
C		HTR	30
	IMPLICIT REAL*8 (A-H,O-Z)	HTR	35
	REAL*8 PHAT	HTR	40
	REAL*8 KD,LAMBDA	HTR	45
	COMMON/CTRL/KPGH,KWTR,KVI,KSTRN,KSTW,ISTOP,KSS,KDIG,KHOUT, KHOUT,	HTR	50
1	KTSTP,KSOUT,KSMCH,KBUFP,KDEL,KIC,KSTRS	HTR	55
	COMMON/CHVAR/TIME,TH(100,2),TNS(100,2),TNW(100,2),DTH(100,2),	HTR	60
1	VI(100,2),VXP(100,2),VNB(100,2)	HTR	65
	COMMON/GEOM/X(101),BB(2),DCOSB(2),DCOS(2),DELT,CHNG,DELHAX,TNAX,	HTR	70
1	IPX(101),IE(100,3),HFN(2),HPSY(2),HPTST(2),HBE(2),HTSE(2),ISB(2,	HTR	75
1	2),IS(2,2),HNP,HBL,HMAE,IBAND,FBC,HST,HTST,HDEL,HTI,HHOR	HTR	80
	COMMON/HPROP/PROP(1,5),HII	HTR	85
	COMMON/HFVAR/ A(101,2),B(101,3),R(101),RP(101),RI(101),RB(101),	HTR	90
1	DP(101),R1(101),RT(101),ITNP(101),BPLX(101),BPLXP(101),FX(100,2)	HTR	95
1	,PRATE(10),FLOW(10),TFLOW(10),H,PHAT(3,5)	HTR	100
	COMMON/HIVAR/KPRO,KPR(1000),RAIDIP,HAIHL,HAXNP,HAXNAT,HAXBW,	HTR	105
1	HAXTYI,HNPPE	HTR	110
	COMMON/BI/ TH1,THO,TN2,SINRPS	HTR	115

COMMON/NUMITG/ NORDR1,NORDER,NITP,ITMIN,IGSS,ITMIN, IGSS7(3)	STR	120
DIMENSION ZNOR(5),ZBETA(5,5)	STR	125
DATA ZNOR/0.0,7.886751345948136D-1,1.068579021301628D0,0.0,0.7	STR	130
1 32083912582954D-1/	STR	135
DATA ZBETA/5*0.0,3.560254037844393D-1,-1.36025403784439D0, 3*0.0,	STR	140
1 -2.101381127306029D-1,9.523655116991617D-1,-1.742227198968559D0,	STR	145
1 2*0.0,5*0.0,1.674662850648816D-1,-1.00006821303384D0,	STR	150
1 2.364268696938704D0,-2.454680874324783D0,-7.69858946449979D0-2/	STR	155
C	STR	160
C *****	STR	165
C	STR	170
ENTRY B1L	STR	175
IF (NNOR.NE.1) GO TO 10	STR	180
ZNOR(1)=W	STR	185
ZBETA(1,NNOR)=-1.	STR	190
10 NPB1=ISB(1,1)	STR	195
NPB2=ISB(2,1)	STR	200
KHOUT=0	STR	205
KDIG=0	STR	210
C	STR	215
C COMPUTE BAND-WIDTH VARIABLES.	STR	220
C	STR	225
IMALPB=MAXDIF	STR	230
IBAND=2*IMALPB+1	STR	235
IMBP=IMALPB+1	STR	240
IF (IBAND.LE.MAXBW) GO TO 20	STR	245
PRINT 10100,IBAND,MAXBW	STR	250
C	STR	255
C PREPARE INITIAL VARIABLES.	STR	260
C	STR	265
20 IF (KIC.NE.0) GO TO 40	STR	270
DO 30 NP=1,NBP	STR	275
30 R(NP)=RI(NP)	STR	280
GO TO 80	STR	285
40 DO 50 NP=1,NBP	STR	290
R(NP)=0.	STR	295
50 NP(NP)=0.	STR	300
DO 70 N=1,NEL	STR	305
NTYP=IE(N,3)	STR	310
KD=PROP(NTYP,1)	STR	315
RHOB=PROP(NTYP,2)	STR	320
THETAR=PROP(NTYP,4)	STR	325
POR=PROP(NTYP,5)	STR	330
IF (THETAR.EQ.0) THETAR=POR/10.	STR	335
KD=1.+KD*RHOB/POR	STR	340
ANORM=1./(THETAR*KD)	STR	345
DO 60 IQ=1,2	STR	350
NP=IE(N,IQ)	STR	355
WT=0.5	STR	360
IF (NP.EQ.NPB1) WT=1.	STR	365
IF (NP.EQ.NPB2) WT=1.	STR	370
R(NP)=R(NP)+ANORM*RI(NP)*WT	STR	375
60 CONTINUE	STR	380
70 CONTINUE	STR	385
80 DO 90 NP=1,NBP	STR	390
90 R(NP)=R(NP)	STR	395
C	STR	400
C READ INITIAL VELOCITIES, PRESSURES, AND WATER CONTENTS, IF NECESSARY.	STR	405
C	STR	410
IF (KPGH.EQ.3) GO TO 140	STR	415
IF (KPGH.EQ.6) GO TO 140	STR	420
IF (KPGH.EQ.7) GO TO 140	STR	425
DO 100 N=1,NEL	STR	430
NTYP=IE(N,3)	STR	435
POR=PROP(NTYP,5)	STR	440
DO 100 IQ=1,2	STR	445
TH(N,IQ)=PQ2	STR	450
100 VI(N,IQ)=VXI	STR	455
110 IF (KVI.EQ.0) GO TO 160	STR	460
IF (KSRCH.GT.1) GO TO 160	STR	465
DO 120 NI=1,NEL,4	STR	470
NK=MIN0(NI+3,NEL)	STR	475
READ 10000,((VI(NJ,JQ),JQ=1,2),NJ=NI,NK)	STR	480
120 CONTINUE	STR	485
DO 130 NI=1,NEL,4	STR	490

NK=MIN0(NI+3,NEL)	STR	495
READ 10000, ((TH(NJ,JQ),JQ=1,2),NJ=NI,NK)	STR	500
130 CONTINUE	STR	505
IF (KSRCH.GT.0) KSRCH=KSRCH+1	STR	510
GO TO 160	STR	515
C	STR	520
C PREPARE TIME-VELOCITY TABLE IF NECESSARY.	STR	525
C	STR	530
C	STR	535
140 DO 150 N=1,NEL	STR	540
DO 150 IQ=1,2	STR	545
NP=IR(N,IQ)	STR	550
TH(N,IQ)=TH0	STR	555
VX(N,IQ)=0.	STR	560
150 CONTINUE	STR	565
ITIM=1	STR	570
C	STR	575
C CALCULATE MATERIAL FLUX PX(N,IQ).	STR	580
C	STR	585
160 CALL FLUX(PX,VX,NP,TH,MAXEL,MAXNP)	STR	590
C	STR	595
C DETERMINE BOUNDARY FLOWS.	STR	600
C	STR	605
DO 170 I=1,8	STR	610
170 TFLOW(I)=0.	STR	615
DO 180 NP=1,NP	STR	620
180 BFLX(NP)=0.	STR	625
CALL SFLOW(PX,NP,BFLX,BFLIP,PRATE,FLOW,TFLOW,TH,MAXEL,MAXNP)	STR	630
DO 190 I=1,8	STR	635
FLOW(I)=0.	STR	640
190 TFLOW(I)=0.	STR	645
PRATE(6)=0.	STR	650
PRATE(7)=0.	STR	655
PRATE(8)=0.	STR	660
C	STR	665
C CALCULATE BULK CONCENTRATIONS.	STR	670
C	STR	675
DO 200 NP=1,NP	STR	680
200 RB(NP)=0.	STR	685
DO 220 N=1,NEL	STR	690
NTYP=IR(N,3)	STR	695
KD=PROP(NTYP,1)	STR	700
RHOB=PROP(NTYP,2)	STR	705
POR=PROP(NTYP,5)	STR	710
RD=1.+KD*RHOB/POR	STR	715
DO 210 IQ=1,2	STR	720
NP=IR(N,IQ)	STR	725
WT=0.5	STR	730
IF (NP.EQ.NPB1) WT=1.	STR	735
IF (NP.EQ.NPB2) WT=1.	STR	740
RB(NP)=RB(NP)+WT*RD*TH(N,IQ)*R(NP)	STR	745
210 CCYTIME	STR	750
220 CONTINUE	STR	755
RETURN	STR	760
C	STR	765
C *****	STR	770
C	STR	775
ENTRY STRAN	STR	780
C	STR	785
C PERFORM TRANSIENT-STATE CALCULATION.	STR	790
C	STR	795
U1=U	STR	800
U2=1.-U	STR	805
DO 240 N=1,NEL	STR	810
DO 230 IQ=1,2	STR	815
TH(N,IQ)=TH(N,IQ)	STR	820
230 VXP(N,IQ)=VX(N,IQ)	STR	825
240 CONTINUE	STR	830
C	STR	835
C READ TIME-DEPENDENT VELOCITIES, IF REQUIRED.	STR	840
C	STR	845
IF (KPGM.EQ.3) GO TO 270	STR	850
IF (KPGM.EQ.6) GO TO 270	STR	855
IF (KPGM.EQ.7) GO TO 270	STR	860
IF (KVL.EQ.2) GO TO 280	STR	865

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      IF (KSRCD.GT.0) GO TO 240
      DO 250 N=1,NEL,4
        NK=NIN0(NI+3,NEL)
        READ 10000, ((VX(NJ,JQ),JQ=1,2),NJ=NI,NK)
250    CONTINUE
      DO 260 NI=1,NEL,4
        NK=NIN0(NI+3,NEL)
        READ 10000, ((TH(NJ,JQ),JQ=1,2),NJ=NI,NK)
260    CONTINUE
      GO TO 280

C
C   CALCULATE TIME-DEPENDENT VELOCITIES AND WATER CONTENTS, IF REQUIRED.
C
270  CALL WINTP(TIME)
      CAL' WTRN2
      CALL HULINK

C
C   ASSEMBLE COEFFICIENT MATRICES A AND B AND CONSTRUCT
C   THE TIME DERIVATIVE R1 AT THE PREVIOUS TIME NODE.
C
280  DO 300 N=1,NEL
      DO 290 IQ=1,2
        DTH(N,IQ)=(TH(N,IQ)-THN(N,IQ))/DELT
        THN(N,IQ)=N1*TH(N,IQ)+N2*THN(N,IQ)
290    VXN(N,IQ)=N1*VX(N,IQ)+N2*VXN(N,IQ)
300    CONTINUE
      CALL ASSEMBL(A,B,R1,RP,VXN,THN,DPH,N,NAINP,NAIBN,NAIEL,KSS)

C
C   APPLY BOUNDARY CONDITIONS.
C
      DO 310 NP=1,NNP
310    R(NP)=0.
      CALL BC(A,B,R,RP,DP,VXN,N,NAINP,NAIEL,NAIBN,KSS)

C
C   FORM THE FIRST-DERIVATIVE TERM R1 = A * DB/DT.
C
      DO 330 NI=1,NNP
        R1(NI)=R(NI)
        JBL=NAK0(1,INBP-NI+1)
        JBU=NIN0(1BAND,INBP-NI+NNP)
        DO 320 JB=JBL,JBU
          NJ=NI+JB-INBP
          R1(NI)=R1(NI)-B(NI,NJ)*RP(NJ)
320    CONTINUE
330  CONTINUE

C
C   FORM MATRIX A + Z*DELT*B.
C
      ZD=ZINOR(INOR)*DELT
      DO 360 NI=1,NNP
        JBAU=NIN0(INBP,1-NI+NNP)
        DO 340 JBA=1,JBAU
          JB=INALPB+JBA
          B(NI,JB)=A(NI,JBA)+ZD*B(NI,JB)
340    CONTINUE
        KBU=NIN0(NI-1,INALPB)
        IF (KBU.LT.1) GO TO 360
        DO 350 KB=1,KBU
          NIA=NI-KB
          JBA=KB+1
          JB=INBP-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,B,NNP,INALPB,NAI',NAIBN)
      DO 370 NI=1,NNP
370    R(NI)=0.
      DO 430 INOB=1,NNQB
C
C   DETERMINE A * B, WHERE B CONTAINS THE PREVIOUS ITERATE.
C
      DO 380 NI=1,NNP

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      BTR 870
      BTR 975
      BTR 980
      BTR 985
      BTR 990
      BTR 995
      BTR 900
      BTR 905
      BTR 910
      BTR 915
      BTR 920
      BTR 925
      BTR 930
      BTR 935
      BTR 940
      BTR 945
      BTR 950
      BTR 955
      BTR 960
      BTR 965
      BTR 970
      BTR 975
      BTR 980
      BTR 985
      BTR 990
      BTR 995
      BTR 1000
      BTR 1005
      BTR 1010
      BTR 1015
      BTR 1020
      BTR 1025
      BTR 1030
      BTR 1035
      BTR 1040
      BTR 1045
      BTR 1050
      BTR 1055
      BTR 1060
      BTR 1065
      BTR 1070
      BTR 1075
      BTR 1080
      BTR 1085
      BTR 1090
      BTR 1095
      BTR 1100
      BTR 1105
      BTR 1110
      BTR 1115
      BTR 1120
      BTR 1125
      BTR 1130
      BTR 1135
      BTR 1140
      BTR 1145
      BTR 1150
      BTR 1155
      BTR 1160
      BTR 1165
      BTR 1170
      BTR 1175
      BTR 1180
      BTR 1185
      BTR 1190
      BTR 1195
      BTR 1200
      BTR 1205
      BTR 1210
      BTR 1215
      BTR 1220
      BTR 1225
      BTR 1230
      BTR 1235
      BTR 1240

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380      RT(NI)=0.
      DO 410 NI=1,NMP
        JAU=MIN0(NMP-NI+1,INAP)
        DO 390 JB=1,JBU
          NJ=NI+JB-1
          RT(NI)=RT(NI)+A(NI,JB)*R(NJ)
390      CONTINUE
        KBU=MIN0(NI-1,INALPB)
        IF (KBC.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,NBON)*DELT
      DO 420 NI=1,NMP
420      R(NI)=RT(NI)-ZDB*R1(NI)

C
C   BACK SUBSTITUTE.
C
      CALL SOLVE(2,B,R,NMP,INALPB,MAXNP,BAXBU)
430      CONTINUE
      DO 440 NI=1,NMP
440      R(NI)=RP(NI)+R(NI)

C
C   CALCULATE MATERIAL FLUX FX(M,IQ).
C
      CALL FLUX(FX,VI,R,TH,MAXEL,MAXNP)

C
C   DETERMINE BOUNDARY FLOWS.
C
      CALL SPLOW(FX,R,BFLX,BFLXP,PRATE,FLOW,TFLOW,TH,MAXEL,MAXNP)

C
C   CALCULATE BULK CONCENTRATIONS.
C
      DO 450 NP=1,NMP
450      RB(NP)=0.
      DO 470 N=1,NEL
        NTYP=IE(N,3)
        KD=PROP(NTYP,1)
        RMOB=PROP(NTYP,2)
        POR=PROP(NTYP,5)
        RD=1.+KD*RMOB/POR
        DO 460 IQ=1,2
          BP=IE(N,IQ)
          BT=0.5
          IF (NP.EQ.NPB1) BT=1.
          IF (NP.EQ.NPB2) BT=1.
          RB(NP)=RB(NP)+BT*RD*TH(N,IQ)*R(BP)
460      CONTINUE
470      CONTINUE
      DO 480 NP=1,NMP
480      RP(NP)=R(NP)
      RETURN

10000 FORMAT(8F10.0)
10100 FORMAT(////12H BANDWIDTH =,I4,25H RECEDES MAX. ALLOWABLE =,I4//)
      END
      SUBROUTINE DATAN
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
C   IMPLICIT REAL*8 (A-H,O-Z)
      REAL*8 PRAT
      COMMON/CTRL/KPCN,KSTR,KMI,LSTR,KSTW,ISTOP,KSS,KDIG,KROST,KROUT,
1 KSTP,KROUT,KSDCH,KSTW,KANL,KIC,KSTRS
      COMMON/GEOM/I(101),RB(2),DCOS(2),BCOS(2),DELT,CNCG,DELRAT,THAT,

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NTR 1245
NTR 1250
NTR 1255
NTR 1260
NTR 1265
NTR 1270
NTR 1275
NTR 1280
NTR 1285
NTR 1290
NTR 1295
NTR 1300
NTR 1305
NTR 1310
NTR 1315
NTR 1320
NTR 1325
NTR 1330
NTR 1335
NTR 1340
NTR 1345
NTR 1350
NTR 1355
NTR 1360
NTR 1365
NTR 1370
NTR 1375
NTR 1380
NTR 1385
NTR 1390
NTR 1395
NTR 1400
NTR 1405
NTR 1410
NTR 1415
NTR 1420
NTR 1425
NTR 1430
NTR 1435
NTR 1440
NTR 1445
NTR 1450
NTR 1455
NTR 1460
NTR 1465
NTR 1470
NTR 1475
NTR 1480
NTR 1485
NTR 1490
NTR 1495
NTR 1500
NTR 1505
NTR 1510
NTR 1515
NTR 1520
NTR 1525
NTR 1530
NTR 1535
NTR 1540
NTR 1545
DATA 0
DATA 5
DATA 10
DATA 15
DATA 20
DATA 25
DATA 30
DATA 35
DATA 40
DATA 45
DATA 50
DATA 55
DATA 60
DATA 65

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1 IPX(101),IR(100,3),NPH(2),NPST(2),NPTST(2),NBE(2),NTSE(2),ISB(2,DATA 70
1 2),IS(2,2),NHP,NEL,NHAT,IBAND,NBC,NST,NTST,NBEL,NTI,NHOR DATA 75
COMMON/NHVAR/KPRO,KPR(1000),HANDIF,HAIEL,HAHNP,HAHNTAT,HAHNSW, DATA 80
1 HAHNTI,NHPPH DATA 85
COMMON/NHPROP/PROP(1,5),VII DATA 90
COMMON/NHVAR/ A(101,2),B(101,3),R(101),RP(101),JI(101),RB(101), DATA 95
1 DP(101),R1(101),RT(101),XTHP(101),BPLI(101),BPLIP(101),FX(100,2) DATA 100
1 ,FRATE(10),FLOW(10),TFLOW(10),U,PHAT(3,5) DATA 105
ISTOP=0 DATA 110
READ 11000,NHP,NEL,NHAT,NCH,NTI,NBC,NST,KVI,KSTRN,KSS,KTSTP,NELL,DATA 115
1 NELL,NHOR,KIC,KHESH DATA 120
NTST=0 DATA 125
IF (KSS.NE.0) KSS=1 DATA 130
IF (KSTRN.NE.0) KSTRN=1 DATA 135
IF (NHOR.LT.1) NHOR=1 DATA 140
IF (NHOR.EQ.4) NHOR=3 DATA 145
IF (NHOR.GT.5) NHOR=5 DATA 150
READ 11100,DELT,CHNG,DELMAX,THAI,W,XO,IXI,DXL1,DXU1,VII DATA 155
IF (KSS.NE.0) GO TO 10 DATA 160
NHOR=1 DATA 165
W=1. DATA 170
10 IF (KHESH.NE.1) GO TO 20 DATA 175
NEL=NELL+NELU DATA 180
NHP=NEL+1 DATA 185
IF (NELU.EQ.0) XO=IXI DATA 190
IF (NELL.EQ.0) XO=0. DATA 195
20 IF (DELMAX.LE.0.D0) DELMAX=1.E50 DATA 200
IF (THAI.LE.0.D0) THAI=1.E50 DATA 205
PRINT 10000,NHP,NEL,NHAT,NCH,NTI,NBC,NST,KVI,KSTRN,KSS,KTSTP, DATA 210
1 NELL,NELU,NHOR,KIC,KHESH DATA 215
PRINT 10100,DELT,CHNG,DELMAX,THAI,W,XO,IXI,DXL1,DXU1,VII DATA 220
READ 11200,KPRO,(KPR(ITB),ITB=1,NTI) DATA 225
PRINT 10200 DATA 230
PRINT 11300,KPRO,(KPR(ITB),ITB=1,NTI) DATA 235
C DATA 240
C CHECK TO BE SURE INPUT DATA DOES NOT EXCEED STORAGE CAPACITY. DATA 245
C DATA 250
IF (NHP.GE.0.AND.NHP.LE.NAHNP) GO TO 30 DATA 255
ISTOP=ISTOP+1 DATA 260
PRINT 12400,NAHNP DATA 265
30 IF (NEL.GE.0.AND.NEL.LE.NAIEL) GO TO 40 DATA 270
ISTOP=ISTOP+1 DATA 275
PRINT 12500,NAIEL DATA 280
40 IF (NHAT.GE.0.AND.NHAT.LE.NAHAT) GO TO 50 DATA 285
ISTOP=ISTOP+1 DATA 290
PRINT 12900,NAHAT DATA 295
50 IF (NCH.GE.0.AND.NCH.LE.NACHL) GO TO 60 DATA 300
ISTOP=ISTOP+1 DATA 305
PRINT 12600,NAIEL DATA 310
60 IF (NTI.GE.0.AND.NTI.LE.NAHNTI) GO TO 70 DATA 315
ISTOP=ISTOP+1 DATA 320
PRINT 12700,NAHNTI DATA 325
70 IF (NBC.GE.0.AND.NBC.LE.NAHNP) GO TO 80 DATA 330
ISTOP=ISTOP+1 DATA 335
PRINT 13000,NAHNP DATA 340
80 IF (NST.GE.0.AND.NST.LE.NAHNP) GO TO 90 DATA 345
ISTOP=ISTOP+1 DATA 350
PRINT 13100,NAHNP DATA 355
90 IF (NTST.GE.0.AND.NTST.LE.NAHNP) GO TO 100 DATA 360
ISTOP=ISTOP+1 DATA 365
PRINT 13200,NAHNP DATA 370
100 IF (KVI.GE.0.AND.KVI.LE.3) GO TO 110 DATA 375
ISTOP=ISTOP+1 DATA 380
PRINT 12800 DATA 385
110 IF (ISTOP.EQ.0) GO TO 120 DATA 390
PRINT 13300,ISTOP DATA 395
STOP DATA 400
C DATA 405
C READ AND PRINT MATERIAL PROPERTIES. DATA 410
C DATA 415
120 IF (NHPPH.LE.0) GO TO 100 DATA 420
PRINT 10300,((PHAT(I,J),I=1,3),J=1,NHPPH) DATA 425
DO 130 I=1,NHAT DATA 430
READ 11100,(PROP(I,J),J=1,NHPPH) DATA 435
130 PRINT 11400,I,(PROP(I,J),J=1,NHPPH) DATA 440

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C		DATA 445
C	GENERATE NODAL-POINT DATA, IF REQUIRED.	DATA 450
C		DATA 455
	140 IF (KRESH.NE.0) GO TO 220	DATA 460
	NP=1	DATA 465
	X(NP)=X0	DATA 470
	IF (NELL.EQ.0) GO TO 160	DATA 475
	NV=NELL	DATA 480
	NVM=NV-1	DATA 485
	DXAV=X0/DFLOAT(NV)	DATA 490
	SDX=2.*(DXAV-DX1)/DFLOAT(NVM)	DATA 495
	DXI=DX1	DATA 500
	DO 150 JV=1,NV	DATA 505
	NP=NP+1	DATA 510
	X(NP)=X(NP-1)-DXI	DATA 515
	DXI=DXI+SDX	DATA 520
	150 CONTINUE	DATA 525
	X(NP)=0.	DATA 530
	160 IF (NELLU.EQ.0) GO TO 180	DATA 535
	NP=NP+1	DATA 540
	X(NP)=X0+DXU1	DATA 545
	NV=NELLU	DATA 550
	NVM=NV-1	DATA 555
	DXAV=(XNI-X0)/DFLOAT(NV)	DATA 560
	SDX=2.*(DXAV-DXU1)/DFLOAT(NVM)	DATA 565
	DXI=DXU1+SDX	DATA 570
	DO 170 JV=2,NV	DATA 575
	NP=NP+1	DATA 580
	X(NP)=X(NP-1)+DXI	DATA 585
	DXI=DXI+SDX	DATA 590
	170 CONTINUE	DATA 595
	X(NP)=XNI	DATA 600
C		DATA 605
C	PUT GENERATED X-VALUES IN ASCENDING ORDER.	DATA 610
C		DATA 615
	180 CALL DSORT(X,IRX,NBP)	DATA 620
C		DATA 625
C	PRINT GENERATED NODAL-POINT DATA.	DATA 630
C		DATA 635
	PRINT 10400	DATA 640
	DO 190 NP=1,NBP	DATA 645
	190 PRINT 11600,NP,X(NP)	DATA 650
C		DATA 655
C	GENERATE ELEMENT DATA.	DATA 660
C		DATA 665
	NCTP=1	DATA 670
	DO 200 N=1,NEL	DATA 675
	NI=N	DATA 680
	NJ=NI+1	DATA 685
	IR(N,1)=NI	DATA 690
	IR(N,2)=NJ	DATA 695
	IR(N,3)=NCTP	DATA 700
	200 CONTINUE	DATA 705
C		DATA 710
C	PRINT GENERATED ELEMENT DATA.	DATA 715
C		DATA 720
	PRINT 10500	DATA 725
	NM2=1	DATA 730
	MAXDIP=1	DATA 735
	DO 210 N=1,NEL	DATA 740
	210 PRINT 11700,N,(IR(N,L),L=1,3),END	DATA 745
	GO TO 430	DATA 750
C		DATA 755
C	READ NODAL-POINT DATA FROM CARDS AND PRINT, IF REQUIRED.	DATA 760
C		DATA 765
	220 IF (KRESH.NE.0) GO TO 300	DATA 770
	PRINT 10400	DATA 775
	NI=1	DATA 780
	230 READ 11900, NJ,X(NJ)	DATA 785
	IF (NJ-NI) 240,270,250	DATA 790
	240 PRINT 13400, NJ	DATA 795
	PRINT 11600, NJ,X(NJ)	DATA 800
	ISTOP=ISTOP+1	DATA 805
	GO TO 230	DATA 810
	250 NP=NJ+1-NI	DATA 815

```

      DX=(X(NJ)-X(NI-1))/DP
260  CONTINUE
      X(NI)=X(NI-1)+DX
270  PRINT 11600,N1,X(NI)
      N1=N1+1
      IF (NJ-N1) 280,270,260
280  IF (N1.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
      NJ = 0
290  READ 11000, NY, (IE(NI,I),I=1,3),MODL
      NND = IABS(IE(NI,2)-IE(NI,1))
      MAXDIF = MAX0(NND,MAXDIF)
300  NJ = NJ + 1
      IF (NI-NJ) 310,340,320
310  PRINT 13500, NI
      PRINT 11700, NI, (IE(NI,I),I=1,3),NND
      ISTOP = ISTOP + 1
320  DO 330 IQ=1,2
330    IE(NJ,IQ) = IE(NJ-1,IQ) + 1
      IE(NJ,3) = IE(NJ-1,3)
340  PRINT 11700, NJ, (IE(NJ,I),I=1,3),NND
      IF (NJ.LT.NI) GO TO 300
      IF (NJ.EQ.NNI) GO TO 380
      IF (MODL.LE.0) GO TO 290
      LL=2
      DO 370 J=1,MODL
      IF (NJ.EQ.NI) GO TO 360
      DO 350 KQ=1,2
350    IE(NJ,KQ) = IE(NJ-1,KQ) + LL
      IE(NJ,3) = IE(NJ-1,3)
      PRINT 11700, NJ, (IE(NJ,K),K=1,3),NND
360    LL = 1
370    NJ = NJ + 1
      NJ = NJ - 1
      IF (NJ.LT.NNI) 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
      NTYP=1
      DO 410 M=1,NEL
      NI=M
      NJ=NI+1
      IE(M,1)=NI
      IE(M,2)=NJ
      IE(M,3)=NTYP
410  CONTINUE
C
C  PRINT GENERATED ELEMENT DATA.
C
      PRINT 10500
      NND=1
      MAXDIF=1
      DO 420 M=1,NEL
420    PRINT 11700,M, (IE(M,I),I=1,3),NND
C
C  MODIFY MATERIAL TYPES FOR SELECTED ELEMENTS, IF NECESSARY.
C
430  IF (MCH.LE.0) GO TO 470
      PRINT 10600
      L=0

```

DATA 820
 DATA 825
 DATA 830
 DATA 835
 DATA 840
 DATA 845
 DATA 850
 DATA 855
 DATA 860
 DATA 865
 DATA 870
 DATA 875
 DATA 880
 DATA 885
 DATA 890
 DATA 895
 DATA 900
 DATA 905
 DATA 910
 DATA 915
 DATA 920
 DATA 925
 DATA 930
 DATA 935
 DATA 940
 DATA 945
 DATA 950
 DATA 955
 DATA 960
 DATA 965
 DATA 970
 DATA 975
 DATA 980
 DATA 985
 DATA 990
 DATA 995
 DATA 1000
 DATA 1005
 DATA 1010
 DATA 1015
 DATA 1020
 DATA 1025
 DATA 1030
 DATA 1035
 DATA 1040
 DATA 1045
 DATA 1050
 DATA 1055
 DATA 1060
 DATA 1065
 DATA 1070
 DATA 1075
 DATA 1080
 DATA 1085
 DATA 1090
 DATA 1095
 DATA 1100
 DATA 1105
 DATA 1110
 DATA 1115
 DATA 1120
 DATA 1125
 DATA 1130
 DATA 1135
 DATA 1140
 DATA 1145
 DATA 1150
 DATA 1155
 DATA 1160
 DATA 1165
 DATA 1170
 DATA 1175
 DATA 1180
 DATA 1185
 DATA 1190

```

440 READ 11000, NI, NTYP, NK
    IE(NI,3) = NTYP
    PRINT 11000, NI, IE(NI,3)
    L = L + 1
    IF (NK.LT.NI) GO TO 460
    NI = NI + 1
    DO 450 NJ=NI, NK
        IE(NJ,3) = NTYP
        PRINT 11000, NJ, IE(NJ,3)
450    L = L + 1
460 IF (L.LT.NCH) GO TO 440
C
C CHECK MATERIAL TYPES FOR EACH ELEMENT.
C
470 DO 480 N=1, NEL
    NTYP=IE(N,3)
    IF (NTYP.GT.0.AND. NTYP.LE.NMAT) GO TO 480
    PRINT 14200, N
    ISTOP=ISTOP+1
480    CONTINUE
    IF (ISTOP.EQ.0) GO TO 490
    PRINT 13700, ISTOP
490 IF (KNSH.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, NI(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 NI(NJ)=NI(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    NI(NI)=XTMP(NJ)
C
C IDENTIFY BOUNDARY MODES.
C
560 CALL SUBP
    DO 570 NP=1, NNP
570    DP(NP)=0.
    IF (NDC.EQ.0) GO TO 640
C
C READ CONSTANT-CONCENTRATION DIRICHLET CONDITIONS DD(NPP) TO BE
C APPLIED AT NODES NPN(NPP).
C
    NPP=0
580 IF (NPP.EQ.NDC) GO TO 610
    IF (NPP.LT.NDC) GO TO 590
    PRINT 13000, NDC
    ISTOP=ISTOP+1
    GO TO 610
590 READ 11900, NI, NNI
600 NPP=NPP+1
    NPN(NPP)=NI
    DD(NPP)=NNI
    GO TO 580
610 PRINT 10700
    DO 620 NPP=1, NDC
620    PRINT 12100, NPN(NPP), DD(NPP)

```

DATA1195
 DATA1200
 DATA1205
 DATA1210
 DATA1215
 DATA1220
 DATA1225
 DATA1230
 DATA1235
 DATA1240
 DATA1245
 DATA1250
 DATA1255
 DATA1260
 DATA1265
 DATA1270
 DATA1275
 DATA1280
 DATA1285
 DATA1290
 DATA1295
 DATA1300
 DATA1305
 DATA1310
 DATA1315
 DATA1320
 DATA1325
 DATA1330
 DATA1335
 DATA1340
 DATA1345
 DATA1350
 DATA1355
 DATA1360
 DATA1365
 DATA1370
 DATA1375
 DATA1380
 DATA1385
 DATA1390
 DATA1395
 DATA1400
 DATA1405
 DATA1410
 DATA1415
 DATA1420
 DATA1425
 DATA1430
 DATA1435
 DATA1440
 DATA1445
 DATA1450
 DATA1455
 DATA1460
 DATA1465
 DATA1470
 DATA1475
 DATA1480
 DATA1485
 DATA1490
 DATA1495
 DATA1500
 DATA1505
 DATA1510
 DATA1515
 DATA1520
 DATA1525
 DATA1530
 DATA1535
 DATA1540
 DATA1545
 DATA1550
 DATA1555
 DATA1560
 DATA1565

```

C
C  APPLY DIRICHLET BOUNDARY SPECIFICATIONS TO THE INITIAL CONDITIONS.
C
      DO 630 NPP=1,NBC
        NP=NPV(NPP)
        630  RI(NP)=BB(NPP)
        640  IF (NST.LE.0) GO TO 660
C
C  READ SURFACE-TERM FLUX LI TO BE APPLIED AT BOUNDARY
C  NODE LI.
C
      NPP=0
      PRINT 10800
      650  IF (NPP.EQ.NST) GO TO 660
      READ 11900,NI,RI
      DP(NI)=RI
      NPP=NPP+1
      NPST(NPP)=NI
      PRINT 12100,NI,RI
      GO TO 650
      660  IF (NST.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
      NPI=0
      NPP=0
      PRINT 10900
      670  IF (NPP.EQ.NST) GO TO 710
      READ 12000,NI
      NPI=NPI+1
      NPP=NPP+1
      NPST(NPP)=NI
      DO 690 NPJ=1,NBEL
        NJ=ISB(NPJ,1)
        IF (NI.NE.NJ) GO TO 690
        NSTE(NPI)=N
        DCOS(NPI)=DCOSB(NPJ)
        DO 680 J=1,2
          680  IS(NPI,J)=ISB(NPJ,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 CONNECTION 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' MORTSETT TIME INTEGRATION INDEX. . . . . ',I5/ 5X,
1' INITIAL-CONDITION CONTROL . . . . . ',I5/ 5X,
1' MESH CONTROL. . . . . ',I5)
1  .30  FORMAT(5X, ' TIME INCREMENT. . . . . ',
1  E10.4/ 5X, ' MULTIPLIER FOR INCREASING DELT. . . . . ',
1  E10.4/ 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 . . . . . ', DATA1945
1 F10.4/ 5X, ' MAXIMUM X-VALUE . . . . . ', DATA1950
1 F10.4/ 5X, ' LOWER FIRST X-INCREMENT . . . . . ', DATA1955
1 F10.4/ 5X, ' UPPER FIRST X-INCREMENT . . . . . ', DATA1960
1 F10.4/ 5X, ' CONSTANT ARC VELOCITY . . . . . ', DATA1965
1 E10.4)
10200 FORMAT (//6X, 'OUTPUT CONTROL') DATA1970
10300 FORMAT (////' MATERIAL-TRANSPORT INPUT TABLE 2.. ', DATA1980
1 ' MATERIAL PROPERTIES'// ' MAT. NO.', 9(3A4)) DATA1985
10400 FORMAT (////' MATERIAL-TRANSPORT TABLE 3.. NODAL-POINT DATA', // DATA1990
1 7X, 'NODE', 8X, 'X') DATA1995
10500 FORMAT (////' MATERIAL-TRANSPORT TABLE 4.. ELEMENT DATA' //11X, DATA2000
1 ' GLOBAL INDICES OF ELEMENT NODES'//X, 'ELEMENT', 3X, '1', 7X, '2', DATA2005
1 6X, 'MATERIAL', 6X, 'NODE DIFF.' ) DATA2010
10600 FORMAT (////' CORRECTIONS TO MATERIAL TYPES FOR SELECTED ELEMENTS'//DATA2015
1 ) DATA2020
10700 FORMAT (////' MATERIAL-TRANSPORT INPUT TABLE 5.. BOUNDARY ', DATA2025
1 ' CONDITIONS OF FORM B=BB' // ' NODE', 7X, 'BB') DATA2030
10800 FORMAT (////' MATERIAL-TRANSPORT INPUT TABLE 6.. SURFACE TERMS', DATA2035
1 ' FLUX=EI AT NODE XI', 'NODE', 7X, 'EI'//) DATA2040
10900 FORMAT (////' MATERIAL-TRANSPORT INPUT TABLE 7.. SEEPAGE-SURFACE', DATA2045
1 ' INFORMATION'//5X//'NO#2'//) DATA2050
11000 FORMAT (16I5) DATA2055
11100 FORMAT (8F10.0) DATA2060
11200 FORMAT (80I1) DATA2065
11300 FORMAT (10X, 10I10) DATA2070
11400 FORMAT (10, 90I2.4) DATA2075
11500 FORMAT (15, 2F10.3) DATA2080
11600 FORMAT (10, 2D15.4) DATA2085
11700 FORMAT (110, 2I8, I10, I15) DATA2090
11800 FORMAT (110, 32X, I10) DATA2095
11900 FORMAT (15, 5X, F10.0) DATA2100
12000 FORMAT (2I5, F10.0) DATA2105
12100 FORMAT (15, 6I5.4) DATA2110
12200 FORMAT (3I5, 5X, 2F10.0) DATA2115
12300 FORMAT (2I5, 2 (1PD15.4)) DATA2120
12400 FORMAT (////33H TOO MANY NODAL POINTS, MAXIMUM =, 15//) DATA2125
12500 FORMAT (////30H TOO MANY ELEMENTS, MAXIMUM =, 15//) DATA2130
12600 FORMAT (////41H TOO MANY CORRECTION MATERIALS, MAXIMUM =, 15//) DATA2135
12700 FORMAT (////36H TOO MANY TIME INCREMENTS, MAXIMUM =, 15//) DATA2140
12800 FORMAT (////29H CHECK VELOCITY INPUT CONTROL//) DATA2145
12900 FORMAT (////30H TOO MANY MATERIALS, MAXIMUM =, 15//) DATA2150
13000 FORMAT (////36H CHECK BOUNDARY CONDITIONS, MAXIMUM=, 15//) DATA2155
13100 FORMAT (////30H CHECK SURFACE TERMS, MAXIMUM=, 15//) DATA2160
13200 FORMAT (////31H CHECK TRANSIENT S.T., MAXIMUM=, 15//) DATA2165
13300 FORMAT (////28H EXECUTION HALTED BECAUSE OF, 15, 13H FATAL ERRORS//) DATA2170
13400 FORMAT (////30H ERROR IN NODAL-POINT CARD NO., 15//) DATA2175
13500 FORMAT (////26H ERROR IN ELEMENT CARD NO., 15//) DATA2180
13600 FORMAT (////36H ERROR IN INITIAL-CONDITION CARD NO., 15//) DATA2185
13700 FORMAT (////45H ASSEMBLY AND SOLUTION WILL NOT BE PERFORMED., 15, DATA2190
1 19H FATAL CARD ERRORS//) DATA2195
13800 FORMAT (////36H ERROR IN FIRST SEEPAGE-SURFACE CARD//) DATA2200
13900 FORMAT (////41H ERROR IN TRANSIENT-SURFACE CARD FOR NODE, 15//) DATA2205
14000 FORMAT (////49H ERROR IN FIRST B=BB TYPE BOUNDARY-CONDITION CARD //DATA2210
1 /) DATA2215
14100 FORMAT (////33H ERROR IN FIRST SURFACE-TERM CARD//) DATA2220
14200 FORMAT (////40H ERROR IN MATERIAL TYPE CODE FOR ELEMENT , 15//) DATA2225
END DATA2230
SUBROUTINE FLUX(P1, V1, B, TH, MAXEL, MAXNP) FLUX 0
C FLUX 5
C FLUX 10
C FUNCTION OF SUBROUTINE--TO DETERMINE MATERIAL FLUX P1(N,IQ) . FLUX 15
C FLUX 20
C FLUX 25
C FLUX 30
IMPLICIT REAL*8 (A-H, Q-Z) FLUX 35
COMMON/GEOM/X(101), BB(2), DCOSB(2), DCOS(2), DELT, CHRG, DELTAY, THAI, FLUX 35
1 IPX(101), IE(100,3), NPB(2), NPST(2), NPST(2), NBE(2), BTSE(2), ISB(2), FLUX 40
1 2), IS(2,2), NBP, NEL, NBAT, IBADD, BDC, BST, NEST, NREL, NTL, NNOB FLUX 45
COMMON/NPROP/PROP(1,5), EXI FLUX 50
DIMENSION DMX(2,2), IQ(2), VI(MAXEL,2), PI(MAXEL,2), R(MAXNP), FLUX 55
1 TH(MAXEL,2) FLUX 60
ISTOP=0 FLUX 65
DO 50 N=1, NEL FLUX 70
C FLUX 75
C FOR EACH ELEMENT N PREPARE VARIABLES IQ(IQ) FOR QND, FLUX 80

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```

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(N,IQ)
      10   XQ(IQ)=X(NP)
        CALL Q4D(DNX,IQ)
C
C FOR EACH NODAL POINT KQ SUM OVER CONTRIBUTIONS FROM EACH BASIS-
C INTERPOLATION FUNCTION N(IQ) TO OBTAIN DERIVATIVES DNX
C OF THE CONCENTRATION R(NP).
C
      DO 40 KQ=1,2
        DNX=0.
        DO 30 IQ=1,2
          NP=IE(N,IQ)
        30   DNX=DNX+DNX(IQ,KQ)*R(NP)
C
C FORM THE DISPERSIVE FLUXES IN FX(N,KQ).
C
        NTYP=IE(N,3)
        AL=PROP(NTYP,3)
        AB=0.
        TAU=0.
        DD=AB*TAU
        VIX=VI(N,KQ)
        DIX=AL*VIX+DD
        FX(N,KQ)=-DIX*DNX
C
C ADD THE ADVECTIVE FLUXES TO FX(N,KQ).
C
        FX(N,KQ)=FX(N,KQ)+VIX*R(NP)
      40   CONTINUE
      50   CONTINUE
      RETURN
      END
      SUBROUTINE Q4D(DNX,.Q)
C
C FUNCTION OF SUBROUTINE--TO COMPUTE X DERIVATIVES DNX(IQ,KQ)
C OF EACH BASIS FUNCTION N(IQ) AT EACH NODE IQ 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,VXU,N,NAKUP,NAKEL,NAIDW,KSS)
C

```

```

PLUX 85
PLUX 90
PLUX 95
PLUX 100
PLUX 105
PLUX 110
PLUX 115
PLUX 120
PLUX 125
PLUX 130
PLUX 135
PLUX 140
PLUX 145
PLUX 150
PLUX 155
PLUX 160
PLUX 165
PLUX 170
PLUX 175
PLUX 180
PLUX 185
PLUX 190
PLUX 195
PLUX 200
PLUX 205
PLUX 210
PLUX 215
PLUX 220
PLUX 225
PLUX 230
PLUX 235
PLUX 240
PLUX 245
PLUX 250
PLUX 255
PLUX 260
Q4D 0
Q4D 5
Q4D 10
Q4D 15
Q4D 20
Q4D 25
Q4D 30
Q4D 35
Q4D 40
Q4D 45
Q4D 50
Q4D 55
Q4D 60
Q4D 65
Q4D 70
Q4D 75
Q4D 80
Q4D 85
Q4D 90
Q4D 95
Q4D 100
Q4D 105
Q4D 110
Q4D 115
Q4D 120
Q4D 125
Q4D 130
Q4D 135
Q4D 140
Q4D 145
Q4D 150
Q4D 155
Q4D 160
Q4D 165
Q4D 170
Q4D 175
Q4D 180
BC 0
BC 5

```


C		BC	10
C	FUNCTION OF SUBROUTINE--TO APPLY CONSTANT-CONCENTRATION	BC	15
C	DIRICHLET CONDITIONS AND CONSTANT-FLUX NEUMANN SURFACE	BC	20
C	BOUNDARY CONDITIONS.	BC	25
C		BC	30
C		BC	35
	IMPLICIT REAL*8 (A-H,O-Z)	BC	40
	REAL*8 KD	BC	45
	COMMON/GEOM/X(101),BB(2),DCOSB(2),DCOS(2),DELTA,CHRG,DELMAX,THAX,	BC	50
	1 IPI(101),IE(100,3),NPN(2),NPST(2),NPTST(2),NBE(2),NTSE(2),ISB(2,	BC	55
	1 2),IS(2,2),NRP,NEL,NHAT,IBAND,NBC,NST,NTST,NBEL,NTI,NHOR	BC	60
	DIMENSION A(MAXNP,1),B(MAXNP,1),R(MAXNP),DP(MAXNP),VIN(MAXEL,2),	BC	65
	1 RP(MAXNP)	BC	70
	INALPB=(IBAND-1)/2	BC	75
	INBP=INALPB+1	BC	80
	IF (NBC.EQ.0) GO TO 140	BC	85
C		BC	90
C	APPLY CONSTANT-CONCENTRATION DIRICHLET BOUNDARY CONDITIONS.	BC	95
C		BC	100
	DO 130 NPP=1,NBC	BC	105
C		BC	110
C	MODIFY ROW NPN(NPP) OF MATRIX B(NP,IB).	BC	115
C		BC	120
	NI=NPN(NPP)	BC	125
	DO 10 IB=1,IBAND	BC	130
10	B(NI,IB)=0.0	BC	135
	B(NI,INBP)=1.0	BC	140
	R(NI)=BB(NPP)	BC	145
C		BC	150
C	MODIFY LOAD VECTOR R(NP) FOR NON-ZERO BB(NPP).	BC	155
C		BC	160
	IF (BB(NPP).EQ.0.0) GO TO 50	BC	165
	DO 20 IB=1,INALPB	BC	170
	NJ=NI-IB	BC	175
	IF (NJ.LT.1) GO TO 30	BC	180
	JB=INBP+IB	BC	185
20	R(NJ)=R(NJ)-BB(NPP)*B(NJ,JB)	BC	190
30	DO 40 IB=1,INALPB	BC	195
	NJ=NI+IB	BC	200
	IF (NJ.GT.NNP) GO TO 50	BC	205
	JB=INBP-IB	BC	210
40	R(NJ)=R(NJ)-BB(NPP)*B(NJ,JB)	BC	215
C		BC	220
C	ZERO COLUMN NPN(NPP) OF MATRIX B(NP,IB).	BC	225
C		BC	230
	50 DO 60 IB=1,INALPB	BC	235
	NJ=NI-IB	BC	240
	IF (NJ.LT.1) GO TO 70	BC	245
	JB=INBP+IB	BC	250
60	B(NJ,JB)=0.0	BC	255
70	DO 80 IB=1,INALPB	BC	260
	NJ=NI+IB	BC	265
	IF (NJ.GT.NNP) GO TO 90	BC	270
	JB=INBP-IB	BC	275
80	B(NJ,JB)=0.0	BC	280
C		BC	285
C	ZERO COLUMN NPN(NPP) OF MATRIX A(NP,IB),	BC	290
C		BC	295
	90 DO 100 IB=1,INALPB	BC	300
	NJ=NI-IB	BC	305
	IF (NJ.LT.1) GO TO 110	BC	310
	JB=IB+1	BC	315
100	A(NJ,JB)=0.0	BC	320
C		BC	325
C	ZERO ROW NPN(NPP) OF MATRIX A(NP,IB).	BC	330
C		BC	335
	110 DO 120 KB=1,INBP	BC	340
	A(NI,KB)=0.0	BC	345
	130 CONTINUE	BC	350
C		BC	355
C	MODIFY LOAD VECTOR FOR SURFACE TERMS OF THE FORM DB/DN=C.	BC	360
C		BC	365
	140 DO 150 NP=1,NRP	BC	370
	150 R(NP)=R(NP)+DP(NP)	BC	375
	160 RETURN	BC	380

C		Q#	30
C		Q#	35
	IMPLICIT REAL*8 (A-H,O-Z)	Q#	40
	REAL*8 N(4),NH,KD,LAMBDA	Q#	45
	DIMENSION QA(2,2),QB(2,2),VIX(2),S(2),V(2),XQ(2),THQ(2),DTHQ(2),	Q#	50
	1 DTHQ(2)	Q#	55
	DATA P / 0.577350269189526 /, S / -1.0D+00, 1.0D+00 /	Q#	60
	RD=1.+KD*RHOB*FOR	Q#	65
	DD=AM*TAU	Q#	70
C		Q#	75
C	INITIALIZE MATRICES QA(IQ,JQ) AND QB(IQ,JQ) .	Q#	80
C		Q#	85
	DO 10 IQ=1,2	Q#	90
	DO 10 JQ=1,2	Q#	95
	QA(IQ,JQ)=0.0	Q#	100
10	QB(IQ,JQ)=0.0	Q#	105
C		Q#	110
C	EVALUATE QUANTITIES FOR USE IN JACOBIAN DJAC, BELOW, NECESSARY	Q#	115
C	FOR TRANSFORMATION FROM GLOBAL TO LOCAL COORDINATES.	Q#	120
C		Q#	125
	X21 = IQ(2) - IQ(1)	Q#	130
	DO 40 KG=1,2	Q#	135
C		Q#	140
C	DETERMINE THE LOCAL COORDINATE SS AND EVALUATE THE JACOBIAN AT	Q#	145
C	EACH GAUSS-INTEGRATION POINT KG.	Q#	150
C		Q#	155
	SS = P*S(KG)	Q#	160
	DJ = X21	Q#	165
	DJAC = 0.5*DJ	Q#	170
	DJI=1./DJ	Q#	175
	SH = 1.0 - SS	Q#	180
	SP = 1.0 + SS	Q#	185
C		Q#	190
C	CALCULATE VALUES OF THE BASIS FUNCTIONS N(IQ) AND THEIR DERIVATIVES	Q#	195
C	V(IQ) W.R.T. X AT GAUSS POINT KG.	Q#	200
C		Q#	205
	V(1)=-DJI	Q#	210
	V(2)=DJI	Q#	215
	N(1)=0.5*SH	Q#	220
	N(2)=0.5*SP	Q#	225
C		Q#	230
C	INTERPOLATE WITH THE BASIS-INTERPOLATION FUNCTIONS N(IQ) TO OBTAIN	Q#	235
C	THE ADVECTIVE VELOCITY AT EACH GAUSS INTEGRATION POINT.	Q#	240
C		Q#	245
	THK=0.	Q#	250
	DTHK=0.	Q#	255
	VIX=0.	Q#	260
	DO 20 IQ=1,2	Q#	265
	THK=THK+N(IQ)*THQ(IQ)	Q#	270
	DTHK=DTHK+N(IQ)*DTHQ(IQ)	Q#	275
20	VIX=VIX+N(IQ)*VIXQ(IQ)	Q#	280
C		Q#	285
C	ACCUMULATE THE SUMS TO EVALUATE THE MATRIX INTEGRALS QA(IQ,JQ)	Q#	290
C	AND QB(IQ,JQ) .	Q#	295
C		Q#	300
	A=DJAC*RD*THK	Q#	305
	DIX=DJAC*(AL*VIX+DD)	Q#	310
	C=DJAC*RD*(DTHK+LAMBDA*THK)	Q#	315
	VIX=VIX+DJAC	Q#	320
	DO 30 IQ=1,2	Q#	325
	DO 30 JQ=1,2	Q#	330
	NH=N(IQ)*N(JQ)	Q#	335
	VV=V(IQ)*V(JQ)	Q#	340
	VN=V(IQ)*N(JQ)	Q#	345
	QA(IQ,JQ)=QA(IQ,JQ)+A*NH	Q#	350
30	QB(IQ,JQ)=QB(IQ,JQ)+DIX*VV+C*NH-VIX*VN	Q#	355
40	CONTINUE	Q#	360
	RETURN	Q#	365
	END	Q#	370
	SUBROUTINE PHANTH(ITN)	PRIN	0
C		PRIN	5
C		PRIN	10
C	FUNCTION OF SUBROUTINE--TO OUTPUT FLOWS, CONCENTRATIONS, MATERIAL	PRIN	15
C	FLUXES, WATER CONTENTS, DARCY VELOCITIES, PRESSURE HEADS, AND	PRIN	20
C	TOTAL HEADS AS SPECIFIED BY THE PARAMETER KJR.	PRIN	25

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C
C
      IMPLICIT REAL*8 (A-H,O-Z)
      REAL*4 PHAT
      COMMON/CTRL/KPGH,KWTR,KWI,KSTRH,KSTRW,ISTOP,KSS,KDIG,KHOUT, KHOUT,
1 KSTP,KROUT,KRCH,KRUP,KANL,KIC,KSTRS
      COMMON/CRVAR/TIME,TH(100,2),TSH(100,2),TSH(100,2),DTH(100,2),
1 VI(100,2),VIP(100,2),VSH(100,2)
      COMMON/GEOM/X(101),BB(2),DCOSB(2),DCOS(2),DELT,CHNG,DELHAX,THAI,
1 IPX(101),IE(100,3),NRP(2),NPST(2),NPTST(2),NBE(2),NTSE(2), ISB(2,
1 2), IS(2,2),NRP,NEL,NHAT,IBAND,NBC,NST,NTST,NBEL,NTI,NHOR
      COMMON/HIVAR/KPR0,KPR(1000),HAIIDIP,HAXEL,HAXNP,HAXHAT,HAXBW,
1 HAXNTI,NUPPH
      COMMON/HVAR/ A(101,2),B(101,3),R(101),RP(101),RI(101),RB(101),
1 DP(101),R1(101),RT(101),ITNP(101),BPLX(101),BPLXP(101), FI(100,2)
1 ,PRATE(10),FLOW(10),TFLOW(10),H,PHAT(3,5)
      KDIG=KDIG+1
      IF (KHOUT.EQ.0) KHOUT=1
      IF (KPR(ITN).EQ.0) RETURN
      IF (ITN.EQ.0) GO TO 10
C
C PRINT DIAGNOSTIC FLOW INFORMATION.
C
      PRINT 10700,KDIG,TIME,DELT
      PRINT 10600, (PRATE(I),FLOW(I),TFLOW(I),I=1,4)
      KHOUT=KHOUT+1
10 IF (KPR(ITN).EQ.1) RETURN
C
C PRINT CONCENTRATIONS.
C
      PRINT 10000,KHOUT,TIME,DELT
      DO 20 NI=1,NRP,8
        NJNN=NI
        NJHX=NINO(NI+7,NRP)
      20 PRINT 10200,NI,(R(NJ),NJ=NJNN,NJNX)
      KHOUT=KHOUT+1
      PRINT 10100,KHOUT,TIME,DELT
      DO 30 NI=1,NRP,8
        NJNN=NI
        NJHX=NINO(NI+7,NRP)
      30 PRINT 10200,NI,(RB(NJ),NJ=NJNN,NJNX)
      IF (KPR(ITN).EQ.2) RETURN
C
C PRINT MATERIAL FLUX.
C
      KHOUT=KHOUT+1
      PRINT 10300,KHOUT,TIME,DELT
      DO 40 NI=1,NEL,4
        NK=NINO(NI+3,NEL)
      40 PRINT 10200,NI,((FI(NJ,IQ),IQ=1,2),NJ=NI,NK)
      IF (KPR(ITN).EQ.3) RETURN
C
C PRINT WATER CONTENTS.
C
      KHOUT=KHOUT+1
      PRINT 10400,KHOUT,TIME,DELT
      DO 50 NI=1,NEL,4
        NK=NINO(NI+3,NEL)
      50 PRINT 10200,NI,((TH(NJ,IQ),IQ=1,2),NJ=NI,NK)
C
C PRINT DARCY VELOCITIES.
C
      KHOUT=KHOUT+1
      PRINT 10500,KHOUT,TIME,DELT
      DO 60 NI=1,NEL,4
        NK=NINO(NI+3,NEL)
      60 PRINT 10200,NI,((VI(NJ,IQ),IQ=1,2),NJ=NI,NK)
      RETURN
10000 FORMAT('////' OUTPUT TABLE',I4,'.. FLUID CONCENTRATIONS AT TIME =',PRIN 370
1 1PD12.4,'',(DELT=' ',1PD12.4,'')'//' ' NODE I',5I, PRIN 375
1 'FLUID CONCENTRATION AT NODES I,I+1,...,I+7'/' PRIN 380
10100 FORMAT('////' OUTPUT TABLE',I4,'.. BULK CONCENTRATIONS AT TIME =', PRIN 385
1 1PD12.4,'',(DELT=' ',1PD12.4,'')'//' ' NODE I',5I, PRIN 390
1 'BULK CONCENTRATION AT NODES I,I+1,...,(I+7)'/' PRIN 395
10200 FORMAT(I7,8(1PD15.4)) PRIN 400

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10300 FORMAT(////' OUTPUT TABLE',I4,'... MATERIAL FLUX AT TIME =',      PRIN 405
1 1PD12.4,'',(DELT =',1PD12.4,')',// 63X,      PRIN 410
1 'FLUX-X AT NODES'/17X,'1',14X,'2',14X      PRIN 415
1 '1',14X,'2',14X,'1',14X,'2',14X,'1',14X,'2',/3X,'ELEMENT',2X,      PRIN 420
1 '.....',5X,      PRIN 425
1 '.....')      PRIN 430
10400 FORMAT(////' OUTPUT TABLE',I4,'... WATER CONTENTS AT TIME =',      PRIN 435
1 1PD12.4,'',(DELT =',1PD12.4,')',// 63X,      PRIN 440
1 'THETA AT NODES'/17X,'1',14X,'2',14X,'1',14X,'2',      PRIN 445
1 14X,'1',14X,'2',14X,'1',14X,'2',/3X,'ELEMENT',2X,      PRIN 450
1 '.....',5X      PRIN 455
1 '.....')      PRIN 460
10500 FORMAT(////' OUTPUT TABLE',I4,'... DARCY VELOCITIES AT TIME =',      PRIN 465
1 1PD12.4,'',(DELT =',1PD12.4,')',// 63X,      PRIN 470
1 'VEL-X AT NODES'/17X,'1',14X,'2',14X,'1',      PRIN 475
1 14X,'2',14X,'1',14X,'2',14X,'1',14X,'2',/3X,'ELEMENT',2X,      PRIN 480
1 '.....',5X,      PRIN 485
1 '.....')      PRIN 490
10600 FORMAT(//5X,' TYPE OF FLOW',35X,'RATE',8X,'INC. FLOW',7X,      PRIN 495
1 'TOTAL FLOW'/5X,' CONSTANT-CONCENTRATION NODE FLOW. . . .',3(      PRIN 500
1 E12.4,5X)/5X,' CONSTANT-FLUX-NODE FLOW . . . . .',3(E12.4,      PRIN 505
1 5X)/5X,' SEEPAGE FLUX-NODE FLOW . . . . .',3(E12.4,5X)/      PRIN 510
1 5X,' NUMERICAL LOSSES. . . . .',3(E12.4,5X)/5X,      PRIN 515
1 ' NET FLOW. . . . .',3(E12.4,5X)/5X,      PRIN 520
1 ' INCREASE IN MATERIAL CONTENT (LIQUID) .',3(E12.4,5X)/5X,      PRIN 525
1 ' INCREASE IN MATERIAL CONTENT (SOLID) .',3(E12.4,5X)/5X,      PRIN 530
1 ' RADIOACTIVE LOSSES (LIQUID AND SOLID) .',3(E12.4,5X))      PRIN 535
10700 FORMAT(////' .....PRIN 540
1 .....PRIN 545
1 .....PRIN 550
1 ' , (DELT =',1PD12.4,')')      PRIN 555
END      PRIN 560
SUBROUTINE STRB      STRB 0
C      STRB 5
C      STRB 10
C FUNCTION OF SUBROUTINE--TO STORE PERTINENT QUANTITIES ON AN AUXILIARYSTRB 15
C DEVICE FOR FUTURE USE, E.G. FOR PLOTTING. WHAT DEVICE IS TO BE      STRB 20
C USED MUST BE SPECIFIED BY APPROPRIATE JOB-CONTROL CARDS.      STRB 25
C      STRB 30
C      STRB 35
C      STRB 40
C      IMPLICIT REAL*8 (A-H,O-Z)      STRB 45
C      REAL*4 PHAT      STRB 50
C      COMMON/PROBID/TITLE(8),NPROB      STRB 55
C      COMMON/CRVAR/TIME,TH(100,2),TNS(100,2),TNW(100,2),DTN(100,2),      STRB 60
1 VX(100,2),VXP(100,2),VXW(100,2)      STRB 65
C      COMMON/GEOM/X(101),BB(2),DCOSB(2),DCOS(2),DELT,CHNG,DELMAX,THAX,      STRB 70
1 IPX(101),IE(100,3),NPN(2),NPST(2),NPTST(2),NBE(2),WTSE(2),ISB(2,      STRB 75
1 2),IS(2,2),NWP,NEL,NHAT,IBAND,NBC,NST,NSTST,NBEL,NTI,NMON      STRB 80
C      COMMON/HRVAR/ A(101,2),B(101,3),R(101),RP(101),RI(101),RB(101),      STRB 85
1 DP(101),R1(101),RT(101),ITSP(101),BPLX(101),BPLXP(101),PX(100,2)      STRB 90
1 ,PRATE(10),FLOW(10),TFLW(10),W,PHAT(3,5)      STRB 95
C      STRB 100
C      .....PRIN 105
C      ENTRY STRBI      STRB 110
C      PUNCH 10000, (TITLE(I),I=1,8)      STRB 115
C      PUNCH 10100,NWP      STRB 120
C      PUNCH 10200, (X(NP),NP=1,NWP)      STRB 125
C      RETURN      STRB 130
C      STRB 135
C      .....PRIN 140
C      .....PRIN 145
C      ENTRY STRBT      STRB 150
C      PUNCH 10200,TIME      STRB 155
C      PUNCH 10200, (R(NP),NP=1,NWP)      STRB 160
C      RETURN      STRB 165
10000 FORMAT(8A8)      STRB 170
10100 FORMAT(16I5)      STRB 175
10200 FORMAT(8E10.4)      STRB 180
END      STRB 185
SUBROUTINE SURP      SURP 0
C      SURP 5
C      SURP 10
C FUNCTION OF SUBROUTINE--TO IDENTIFY BOUNDING NODES THRU THE ARRAY      SURP 15
C ISB(NP,2).      SURP 20

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DO 30 NPP=1,NBP	SPLO 185
S=S+BFLX(NP)	SPLO 190
30 SP=SP+BFLIP(NP)	SPLO 195
PRATE(5)=S	SPLO 200
FLOW(5)=.5*(S+SP)*DELT	SPLO 205
C	SPLO 210
C CONSTANT DIRICHLET BOUNDARY NODES.	SPLO 215
C	SPLO 220
PRATE(1)=0.	SPLO 225
FLOW(1)=0.	SPLO 230
IF (FDC.LE.0) GO TO 50	SPLO 235
S=0.	SPLO 240
SP=0.	SPLO 245
DO 40 NPP=1,NBC	SPLO 250
NP=NPB(NPP)	SPLO 255
S=S+BFLX(NP)	SPLO 260
40 SP=SP+BFLIP(NP)	SPLO 265
PRATE(1)=S	SPLO 270
FLOW(1)=.5*(S+SP)*DELT	SPLO 275
C	SPLO 280
C CONSTANT NEUBANK BOUNDARY NODES.	SPLO 285
C	SPLO 290
50 PRATE(2)=0.	SPLO 295
FLOW(2)=0.	SPLO 300
IF (NST.LE.0) GO TO 70	SPLO 305
S=0.	SPLO 310
SP=0.	SPLO 315
DO 60 NPP=1,NST	SPLO 320
NP=NPST(NPP)	SPLO 325
S=S+BFLX(NP)	SPLO 330
60 SP=SP+BFLIP(NP)	SPLO 335
PRATE(2)=S	SPLO 340
FLOW(2)=.5*(S+SP)*DELT	SPLO 345
C	SPLO 350
C TRANSIENT SERPAGE BOUNDARY NODES.	SPLO 355
C	SPLO 360
70 PRATE(3)=0.	SPLO 365
FLOW(3)=0.	SPLO 370
IF (WTST.LE.0) GO TO 90	SPLO 375
S=0.	SPLO 380
SP=0.	SPLO 385
DO 80 NPP=1,WTST	SPLO 390
NP=NPST(NPP)	SPLO 395
S=S+BFLX(NP)	SPLO 400
80 SP=SP+BFLIP(NP)	SPLO 405
PRATE(3)=S	SPLO 410
FLOW(3)=.5*(S+SP)*DELT	SPLO 415
C	SPLO 420
C NUMERICAL FLOW THROUGH UNSPECIFIED BOUNDARY NODES.	SPLO 425
C	SPLO 430
90 S=0.	SPLO 435
SP=0.	SPLO 440
DO 100 I=1,3	SPLO 445
S=S+PRATE(I)	SPLO 450
100 SP=SP+FLOW(I)	SPLO 455
PRATE(4)=PRATE(5)-S	SPLO 460
FLOW(4)=FLOW(5)-SP	SPLO 465
C	SPLO 470
C CALCULATE THE INCREASES IN THE INTEGRATED MATERIAL CONTENTS FOR THE	SPLO 475
C FLUID AND THE SOLID PHASES AND DETERMINE LOSSES DUE TO RADIOACTIVE	SPLO 480
C DECAY.	SPLO 485
C	SPLO 490
QBP=QB	SPLO 495
QDP=QD	SPLO 500
QLP=QL	SPLO 505
QB=0.	SPLO 510
QD=0.	SPLO 515
QL=0.	SPLO 520
DO 120 N=1,NEL	SPLO 525
NTYP=IE(N,3)	SPLO 530
KD=PROP(NTYP,1)	SPLO 535
RROB=PROP(NTYP,2)	SPLO 540
LAMBDA=0.	SPLO 545
POB=PROP(NTYP,5)	SPLO 550
DO 110 IQ=1,2	SPLO 555

	NP=IE(N,IQ)	SPLO 560
	XQ(IQ)=X(NP)	SPLO 565
110	RQ(IQ)=R(NP)*TH(N,IQ)	SPLO 570
	CALL Q4R(RQ,QRH,XQ)	SPLO 575
	QR=QR+QRH	SPLO 580
	QDH=RHOB*KD*QRH/POB	SPLO 585
	QD=QD+QDH	SPLO 590
	QLH=QRH+QDH	SPLO 595
	QL=QL+LAMBDA*QLH	SPLO 600
120	CONTINUE	SPLO 605
	FLOW(6)=QR-QRP	SPLO 610
	FRATE(6)=FLOW(6)/DELT	SPLO 615
	FLOW(7)=QD-QDP	SPLO 620
	FRATE(7)=FLOW(7)/DELT	SPLO 625
	FRATE(8)=-5*(QL+QLP)	SPLO 630
	FLOW(8)=DELT*FRATE(8)	SPLO 635
	DO 130 I=1,8	SPLO 640
130	TFLOW(I)=TFLOW(I)+FLOW(I)	SPLO 645
	RETURN	SPLO 650
	END	SPLO 655
	SUBROUTINE Q4R(RQ,QRH,XQ)	Q4R 0
C		Q4R 5
C		Q4R 10
C	FUNCTION OF SUBROUTINE--TO EVALUATE THE CONCENTRATION INTEGRAL	Q4R 15
C	OVER THE LENGTH OF ONE ELEMENT.	Q4R 20
C		Q4R 25
C		Q4R 30
	IMPLICIT REAL*8 (A-H,O-Z)	Q4R 35
	REAL*8 N(2)	Q4R 40
	DIMENSION RQ(2),S(2),XQ(2)	Q4R 45
	DATA P / 0.577350269189626 /, S / -1.0D+00, 1.0D+00 /	Q4R 50
C		Q4R 55
C	EVALUATE QUANTITIES FOR USE IN THE JACOBIAN DJAC, BELOW, NECESSARY	Q4R 60
C	FOR TRANSFORMATION FROM GLOBAL TO LOCAL COORDINATES.	Q4R 65
C		Q4R 70
	X21 = XQ(2) - XQ(1)	Q4R 75
	QRH=0.	Q4R 80
	DO 20 KG=1,2	Q4R 85
C		Q4R 90
C	DETERMINE LOCAL COORDINATES SS OF GAUSS-INTEGRATION POINT KG.	Q4R 95
C		Q4R 100
	SS = P*S(KG)	Q4R 105
C		Q4R 110
C	EVALUATE THE JACOBIAN DJAC	Q4R 115
C		Q4R 120
	DJ = X21	Q4R 125
	DJAC = 0.5*DJ	Q4R 130
C		Q4R 135
C	CALCULATE VALUES OF THE BASIS-INTERPOLATION FUNCTIONS N(IQ).	Q4R 140
C		Q4R 145
	SN = 1.0 - SS	Q4R 150
	SP = 1.0 + SS	Q4R 155
	N(1)=0.5*SN	Q4R 160
	N(2)=0.5*SP	Q4R 165
C		Q4R 170
C	INTERPOLATE TO OBTAIN THE CONCENTRATION RQP AT THE GAUSS POINT KG.	Q4R 175
C		Q4R 180
	RQP=0.	Q4R 185
	DO 10 IQ=1,2	Q4R 190
10	RQP=RQP+RQ(IQ)*N(IQ)	Q4R 195
C		Q4R 200
C	ACCUMULATE THE SUM TO EVALUATE THE INTEGRAL QRH.	Q4R 205
C		Q4R 210
	QRH=QRH+RQP*DJAC	Q4R 215
20	CONTINUE	Q4R 220
	RETURN	Q4R 225
	END	Q4R 230
	SUBROUTINE SOLVE(KKK,C,R,NP,INALPB,NAINP,NAIDW)	SOLV 0
C		SOLV 5
C		SOLV 10
C	FUNCTION OF SUBROUTINE--TO SOLVE THE MATRIX EQUATION CX = R,	SOLV 15
C	RETURNING THE SOLUTION X IN R. IT IS ASSUMED THAT THE ARRAY C(NP,IB)	SOLV 20
C	CONTAINS THE FULL BAND OF AN ASYMMETRIC MATRIX.	SOLV 25
C		SOLV 30
C		SOLV 35

IMPLICIT REAL*8 (A-H,O-Z)	SOLV	40
DIMENSION C (MAXNP,MAXBP),R (MAXNP)	SOLV	45
INBP=INALPB+1	SOLV	50
C	SOLV	55
C IF KKK = 1, THEN TRIANGULARIZE THE BAND MATRIX C(NP,IB), BUT	SOLV	60
C IF KKK = 2, THEN SIMPLY SCAVE WITH THE RIGHT-HAND SIDE R(NP)	SOLV	65
C	SOLV	70
IF (KKK.EQ.2) GO TO 50	SOLV	75
C	SOLV	80
C TRIANGULARIZE MATRIX C(NP,IB);-	SOLV	85
C	SOLV	90
NU=INBP-INALPB	SOLV	95
DO 20 NI=1,NU	SOLV	100
PIVOTI=1./C (NI,INBP)	SOLV	105
NJ=NI+1	SOLV	110
IB=INBP	SOLV	115
NK=NI+INALPB	SOLV	120
DO 10 NL=NJ,NK	SOLV	125
IB=IB-1	SOLV	130
A=-C (NL,IB) *PIVOTI	SOLV	135
C (NL,IB)=A	SOLV	140
JB=IB+1	SOLV	145
KB=IB+INALPB	SOLV	150
LB=INBP-IB	SOLV	155
DO 10 NB=JB,KB	SOLV	160
NB=LB+NB	SOLV	165
10 C (NL,NB)=C (NL,NB) +A*C (NI,NB)	SOLV	170
20 CONTINUE	SOLV	175
NR=NU+1	SOLV	180
NU=INBP-1	SOLV	185
NK=INBP	SOLV	190
DO 40 NI=NR,NU	SOLV	195
PIVOTI=1./C (NI,INBP)	SOLV	200
NJ=NI+1	SOLV	205
IB=INBP	SOLV	210
DO 30 NL=NJ,NK	SOLV	215
IB=IB-1	SOLV	220
A=-C (NL,IB) *PIVOTI	SOLV	225
C (NL,IB)=A	SOLV	230
JB=IB+1	SOLV	235
KB=IB+INALPB	SOLV	240
LB=INBP-IB	SOLV	245
DO 30 NB=JB,KB	SOLV	250
NB=LB+NB	SOLV	255
30 C (NL,NB)=C (NL,NB) +A*C (NI,NB)	SOLV	260
40 CONTINUE	SOLV	265
RETURN	SOLV	270
C	SOLV	275
C MODIFY LOAD VECTOR R(NP).	SOLV	280
C	SOLV	285
50 NU=INBP+1	SOLV	290
IBAND=2*INALPB+1	SOLV	295
DO 70 NI=2,INBP	SOLV	300
IB=INBP-NI+1	SOLV	305
NJ=1	SOLV	310
SUM=0.0	SOLV	315
-O 60 JB=IB,INALPB	SOLV	320
SUM=SUM+C (NI,JB) *R (NJ)	SOLV	325
60 NJ=NJ+1	SOLV	330
70 R (NI)=R (NI) +SUM	SOLV	335
IB=1	SOLV	340
NL=INBP+1	SOLV	345
DO 90 NI=NL,INBP	SOLV	350
NJ=NI-INL2+1	SOLV	355
SUM=0.0	SOLV	360
DO 80 JB=IB,INALPB	SOLV	365
SUM=SUM+C (NI,JB) *R (NJ)	SOLV	370
80 NJ=NJ+1	SOLV	375
90 R (NI)=R (NI) +SUM	SOLV	380
C	SOLV	385
C BACK SOLVE.	SOLV	390
C	SOLV	395
R (INBP)=R (INBP) /C (INBP,INBP)	SOLV	400
DO 110 IB=2,INBP	SOLV	405
NI=NU-IB	SOLV	410

	NJ=NI	SOLV 415
	HB=INALPB+IB	SOLV 420
	SUM=0.0	SOLV 425
	DO 100 JB=NL,HB	SOLV 430
	NJ=NJ+1	SOLV 435
100	SUM=SUM+C(NI,JB)*R(NJ)	SOLV 440
110	R(NI)=(R(NI)-SUM)/C(NI,INBP)	SOLV 445
	HB=IBAND	SOLV 450
	DO 130 IB=NL,INBP	SOLV 455
	NI=NI-1	SOLV 460
	NJ=NI	SOLV 465
	SUM=0.0	SOLV 470
	DO 120 JB=NL,HB	SOLV 475
	NJ=NJ+1	SOLV 480
120	SUM=SUM+C(NI,JB)*R(NJ)	SOLV 485
130	R(NI)=(R(NI)-SUM)/C(NI,INBP)	SOLV 490
	RETURN	SOLV 495
	END	SOLV 500
	SUBROUTINE WTR	WTR 0
		WTR 5
		WTR 10
	FUNCTION OF SUBROUTINE--TO DETERMINE ONE-DIMENSIONAL MOISTURE TRANSPORT	WTR 15
	USING THE ANALYTIC METHOD OF PARLANGE.	WTR 20
		WTR 25
		WTR 30
	IMPLICIT REAL*8 (A-H,O-Z)	WTR 35
	REAL*4 PHAT	WTR 40
	COMMON/CTRL/KPGH,KUTR,KVI,KSTRH,KSTRV,ISTOP,KSS,KDGC,KROUT,KWOUT,	WTR 45
	KSTP,KROUT,KSDCH,KDGP,KABL,KIC,KSTRS	WTR 50
	COMMON/CHVAR/TIME,TN(100,2),TNS(100,2),TNH(100,2),DTN(100,2),	WTR 55
	VI(100,2),VIP(100,2),VKH(100,2)	WTR 60
	COMMON/GEOM/I(101),BB(2),DCOSB(2),DCGS(2),DELTA,CHGC,DELEAX,TMAX,	WTR 65
	IPX(101),IE(100,3),NPH(2),NPST(2),KPTST(2),NBE(2),NTSE(2),ISB(2,	WTR 70
	2),IS(2,2),NRP,NEL,NHAT,IBAND,NBC,NST,NYST,NBEL,BTI,NHOS	WTR 75
	COMMON/SIVAR/KPRO,KPR(1000),HAXDIP,BAXEL,BHIMP,BAXHAT,HAXBW,	WTR 80
	HAXTI,NHPPF	WTR 85
	COMMON/HRVAR/ A(101,2),B(101,3),Z(101),RP(101),RI(101),RB(101),	WTR 90
	DP(101),R1(101),RT(101),XTEP(101),BPLI(101),BPLIP(101),PX(100,2)	WTR 95
	1,PRATE(10),FLOW(10),TFLOW(10),N,PHAT(3,5)	WTR 100
	COMMON/BI/ TB1,TN0,TNB,SINEPS	WTR 105
	COMMON/CW1/ W1,V1	WTR 110
	COMMON/HUMITC/ BORDR1,BORDR2,BITP,ITNIB,IGSS,ITHIB,IGSSV(3)	WTR 115
	COMMON/TPLX/TTAB(50),VIN(50),VITAB(50),WITAB(50),UTAB(50),	WTR 120
	TTAB(50),WITAB(50),TEMP(50),IPTTAB(50),BITAB	WTR 125
	COMMON/WPROP/AKPAR(50),CDPAR(50),AKSH(25),ALPK(25),D(25),ALPD(25)	WTR 130
	1,AKSAT,AKSH0,NKPAR,NKSP,NCDPAR,NDSP	WTR 135
	COMMON/XVAR/XSUP1(50),XSUP2(50),TNP(50),ALP(50),VSUP1(50),	WTR 140
	VSUP2(50),P(50),QGA(50),QG(50),TNTHP(50),AKGSS(212),DGSS(212),	WTR 145
	1IPTTH(50),NTH,JTH,NGSS	WTR 150
	EXTERNAL TLPUN,TUPUN,TIFUN,TOPUN,GPUN,GAPUN,GSPUN,G2PUN	WTR 155
	DATA IUD1/0/,TZX/0.025/	WTR 160
		WTR 165
	*****	WTR 170
		WTR 175
	ENTRY NIBL	WTR 180
	KWOUT=0	WTR 185
	NTNP=NTN+1	WTR 190
	NTNB=NTN-1	WTR 195
		WTR 200
	CALCULATE TABULAR FUNCTION OF REDUCED VELOCITY WITAB VS. TIME ITAB.	WTR 205
		WTR 210
	IPP=1	WTR 215
	DO 70 IT=1,NTTAB	WTR 220
	DO 10 I=1,3	WTR 225
	IGSSV(I)=0	WTR 230
10	CONTINUE	WTR 235
	W1=WITAB(IT)	WTR 240
	ZBX=(AKSAT*5*SINEPS-ALPH0)/(TNH*W1)	WTR 245
	IF (ZBX.LT.TZX) GO TO 40	WTR 250
	IF (SINEPS.EQ.0.00) GO TO 40	WTR 255
	TL=0.	WTR 260
	TQ=0.	WTR 265
	TI=0.	WTR 270
	BORDER=BORDER	WTR 275
	DO 20 ITN=1,NTNB	WTR 280

```

      JTH=JTH+1
      IF (JTH.EQ.NTH) NORDER=NORDER+1
      CALL GAUSS(ALP(JTH),ALP(JTH),TLA,TLFUB,NORDER)
      CALL GAUSS(ALP(JTH),ALP(JTH),TQA,TQFUB,NORDER)
      CALL GAUSS(ALP(JTH),ALP(JTH),TIA,TFUB,NORDER)
      TL=TL+TLA
      T=TQ+TQA
      TI=TI+TIA
25    CONTINUE
      IF (TQ-LT-TL) GO TO 30
      PRINT 10000, VIN(IT)
      GO TO 40
30    TTAB(IT)=TL-TQ
      UTAB(IT)=TTAB(IT)*VITAB(IT)-UITAB(IT)*TND*TL+TND*TI
      GO TO 70
40    IF (IPP.NE.1) GO TO 60
      IPP=0
      TQ=0.
      IGSS=0
      NORDER=NORDER
      DO 50 JTH=1,NTH
        JTH=JTH+1
        IF (JTH.EQ.NTH) NORDER=NORDER+1
        CALL GAUSS(ALP(JTH),ALP(JTH),TQA,TQFUB,NORDER)
        TQ=TQ+TQA
50    CONTINUE
60    WII=1./W1
      TTAB(IT)=-.5*WII*UITAB(IT)
      UTAB(IT)=TTAB(IT)*VITAB(IT)+.5*TND*WII*TL
70    CONTINUE

C
C PUT TABULAR ARRAYS IN ASCENDING ORDER.
C
      CALL DSORT(TTAB,IPTTAB,UTTAB)
      DO 80 IT=1,UTTAB
        IP=IPTTAB(IT)
        TEMP(IT)=UITAB(IP)
80    CONTINUE
      DO 90 IT=1,UTTAB
        VITAB(IT)=TEMP(IT)
90    CONTINUE
      DO 100 IT=1,UTTAB
        IP=IPTTAB(IT)
        TEMP(IT)=VITAB(IP)
100   CONTINUE
      DO 110 IT=1,UTTAB
        VITAB(IT)=TEMP(IT)
110   CONTINUE
      DO 120 IT=1,UTTAB
        IP=IPTTAB(IT)
        TEMP(IT)=VIN(IP)
120   CONTINUE
      DO 130 IT=1,UTTAB
        VIN(IT)=TEMP(IT)
130   CONTINUE
      DO 140 IT=1,UTTAB
        IP=IPTTAB(IT)
        TEMP(IT)=UTAB(IP)
140   CONTINUE
      DO 150 IT=1,UTTAB
        UTAB(IT)=TEMP(IT)
150   CONTINUE

C
C PREPARE TABULAR ARRAY FOR LOG-LOG INTERPOLATION.
C
      DO 160 I=1,UTTAB
        TTAB(I)=DLOG(TTAB(I))
        VITAB(I)=DLOG(VITAB(I))
160   CONTINUE
      RETURN

C
C *****
C
      ENTRY UNINT(V)

```

C	GIVEN T VALUE, INTERPOLATE TO FIND U1VALUE.	UTR	660
C		UTR	665
	IF (T.LT.TTAB(1)) PRINT 10100,T,TTAB(1)	UTR	670
	IF (T.GT.TTAB(NTTAB)) PRINT 10200,T,TTAB(NTTAB)	UTR	675
	TP=DLOG(T)	UTR	680
	WIP=YLAG(TP,TTABL,WITABL,IND1,WITP,ITHR,NTTAB,LEX)	UTR	685
	W1=DEXP(WIP)	UTR	690
	V1=THB*W1-AKSHO	UTR	695
	RETURN	UTR	700
C		UTR	705
C	*****	UTR	710
C		UTR	715
	ENTRY NTIME(T)	UTR	720
	DO 170 I=1,3	UTR	725
	IGSSV(I)=0	UTR	730
170	CONTINUE	UTR	735
	NDRP=NORDER	UTR	740
	IF (SINEPS.EQ.0.DO) GO TO 190	UTR	745
	TL=0.	UTR	750
	TQ=0.	UTR	755
	TI=0.	UTR	760
	DO 180 ITH=1,NTN	UTR	765
	JTH=ITH+1	UTR	770
	IF (ITH.EQ.NTN) NDRP=NORDR1	UTR	775
C		UTR	780
C	RECALCULATE T.	UTR	785
C		UTR	790
	CALL GAUSS(ALP(ITH),ALP(JTH),TLA,TLFUB,NDRP)	UTR	795
	CALL GAUSS(ALP(ITH),ALP(JTH),TQA,TQFUB,NDRP)	UTR	800
	CALL GAUSS(ALP(ITH),ALP(JTH),TIA,TIFUB,NDRP)	UTR	805
	TL=TL+TLA	UTR	810
	TQ=TQ+TQA	UTR	815
	TI=TI+TIA	UTR	820
180	CONTINUE	UTR	825
	TU=TL-TQ	UTR	830
	T=TU	UTR	835
	RETURN	UTR	840
190	TO=0.	UTR	845
	IGSS=0	UTR	850
	W1=1./W1	UTR	855
	DO 200 ITH=1,NTN	UTR	860
	JTH=ITH+1	UTR	865
	IF (ITH.EQ.NTN) NDRP=NORDR1	UTR	870
	CALL GAUSS(ALP(ITH),ALP(JTH),TOA,TOFUB,NDRP)	UTR	875
	TO=TO+TOA	UTR	880
200	CONTINUE	UTR	885
	TU=.5*W1*W1*TO	UTR	890
	RETURN	UTR	895
C		UTR	900
C	*****	UTR	905
C		UTR	910
	ENTRY NTRN1	UTR	915
C		UTR	920
C	CALCULATE FIRST-ORDER POSITIONS AND VELOCITIES.	UTR	925
C		UTR	930
	IGSS=0	UTR	935
	NDRP=NORDER	UTR	940
	ISUP1(NTN)=0.0	UTR	945
	VSUP1(NTN)=V1	UTR	950
	DO 210 ITH=1,NTN	UTR	955
	JTH=ITH+1	UTR	960
	IF (ITH.EQ.NTN) NDRP=NORDR1	UTR	965
	CALL GAUSS(ALP(ITH),ALP(JTH),ISUP1(ITH),VFUB,NDRP)	UTR	970
210	CONTINUE	UTR	975
	DO 220 ITH=1,NTN	UTR	980
	ITH=NTN-ITH	UTR	985
	JTH=ITH+1	UTR	990
	XSUP1(ITH)=ISUP1(JTH)+ISUP1(ITH)	UTR	995
	VSUP1(ITH)=V1	UTR	1000
220	CONTINUE	UTR	1005
	RETURN	UTR	1010
C		UTR	1015
C	*****	UTR	1020
C		UTR	1025
	ENTRY NTRN2	UTR	1030

```

C
C DETERMINE CORRECTIVE FRACTION P.
C
  QCA(1)=0.0
  IGSS=0
  NRDPR=NORDER
  DO 230 ITH=1,NTN
    JTH=ITH+1
    IF (ITH.EQ.NTN) NRDPR=NORDR1
    CALL GAUSS(ALP(ITH),ALP(JTH),DQ,CAPUN,NRDPR)
    QCA(JTH)=QCA(ITH)+DQ
230  CONTINUE
  IGSS=0
  NRDPR=NORDER
  QC(NTN)=0.
  DO 240 ITH=1,NTN
    JTH=ITH+1
    IF (ITH.EQ.NTN) NRDPR=NORDR1
    CALL GAUSS(ALP(ITH),ALP(JTH),QC(ITH),GSPUN,NRDPR)
240  CONTINUE
  DO 250 ITH=1,NTN
    ITJ=NTN-ITH
    JTH=ITH+1
    QC(ITH)=QC(JTH)+QC(ITJ)
250  CONTINUE
  DMI=1./QCA(NTN)
  F(1)=0.
  DO 260 ITH=2,NTN
    F(ITH)=(QCA(ITH)+ALP(ITH)*QC(ITH))*DMI
260  CONTINUE
C
C CALCULATE SECOND-ORDER POSITIONS AND VELOCITIES.
C
  IGSS=0
  ITHIN=1
  NRDPR=NORDER
  XSUP2(NTN)=0.0
  VSUP2(NTN)=V1
  DO 270 ITH=1,NTN
    JTH=ITH+1
    IF (ITH.EQ.NTN) NRDPR=NORDR1
    CALL GAUSS(ALP(ITH),ALP(JTH),XSUP2(ITH),G2FUN,NRDPR)
270  CONTINUE
  DO 280 ITH=1,NTN
    ITN=NTN-ITH
    JTH=ITH+1
    XSUP2(ITH)=XSUP2(JTH)+XSUP2(ITN)
    VSUP2(ITH)=ZND*V1*F(ITH)-AKSHO
280  CONTINUE
  RETURN
C
C *****
C
  ENTRY EULINK
C
C DETERMINE LINKAGE VARIABLES VI AND TH.
C
  CALL DSORT(XSUP2,IPTH,NTN)
  DO 290 NP=1,NTN
    NPI=IPTH(NP)
    THTP(NPI)=VSUP2(NP)
290  CONTINUE
  INI=XSUP2(NTN)
  VEN=THTP(NTN)
  IXIN=1
  DO 310 NP=1,NBP
    IF (I(NP).LT.INI) GO TO 300
    ITNP(NP)=VEN
    GO TO 310
300  ITNP(NP)=YLAG(I(NP),XSUP2,THTP,IND1,NITP,IXIN,NTN,INI)
310  CONTINUE
  DO 320 N=1,NEL
    DO 320 IQ=1,2
      NP=IS(N,IQ)
      VI(N,IQ)=THTP(NP)

```

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UTH 1035
UTH 1040
UTH 1045
UTH 1050
UTH 1055
UTH 1060
UTH 1065
UTH 1070
UTH 1075
UTH 1080
UTH 1085
UTH 1090
UTH 1095
UTH 1100
UTH 1105
UTH 1110
UTH 1115
UTH 1120
UTH 1125
UTH 1130
UTH 1135
UTH 1140
UTH 1145
UTH 1150
UTH 1155
UTH 1160
UTH 1165
UTH 1170
UTH 1175
UTH 1180
UTH 1185
UTH 1190
UTH 1195
UTH 1200
UTH 1205
UTH 1210
UTH 1215
UTH 1220
UTH 1225
UTH 1230
UTH 1235
UTH 1240
UTH 1245
UTH 1250
UTH 1255
UTH 1260
UTH 1265
UTH 1270
UTH 1275
UTH 1280
UTH 1285
UTH 1290
UTH 1295
UTH 1300
UTH 1305
UTH 1310
UTH 1315
UTH 1320
UTH 1325
UTH 1330
UTH 1335
UTH 1340
UTH 1345
UTH 1350
UTH 1355
UTH 1360
UTH 1365
UTH 1370
UTH 1375
UTH 1380
UTH 1385
UTH 1390
UTH 1395
UTH 1400
UTH 1405

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320      CONTINUE
      DO 330 NP=1,NTH
        NPI=IPTH(NP)
        THTP(NPI)=THP(NP)
330      CONTINUE
      THNN=THTP(NTH)
      IXNN=1
      DO 350 NP=1,NHP
        IF (X(NP).LT.IXNN) GO TO 340
        XTHP(NP)=THNN
        GO TO 350
340      XTHP(NP)=YLAG(X(NP),K SUP2,THNNP,IND1,NITP,IXNN,NTH,ICX)
350      CONTINUE
      DO 360 N=1,NEL
        DO 360 IQ=1,2
          NP=IE(N,IQ)
          TH(N,IQ)=XTHP(NP)
360      CONTINUE
      RETURN
10000  FORMAT(' NOTICE: A NUMERICAL ERROR OCCURRED IN THE TABULAR '
1 ' TIME CALCULATION FOR #IN =',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 DATAN
C
C
C
C FUNCTION OF SUBROUTINE--TO READ, PRINT, AND CHECK WATER-TRANSPORT
C VARIABLES PERTAINING TO SOIL PROPERTIES, BOUNDARY-INITIAL CONDITIONS,
C NODAL POSITIONS IN BOTH TIME AND WATER CONTENTS, AND MISCELLANEOUS
C OTHER INFORMATION.
C
C
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON/CTRL/KPGH,KUTH,KVI,KSTNN,KSTRN,ISTOP,KSS,KDIG,KROUT,KNOUT,
1 KSTP,KROUT,KSMCB,KBUPP,KANL,KIC,KSTRS
      COMMON/PROP/PROP(1,5),VII
      COMMON/ZI/TH1,TH0,THB,SINEPS
      COMMON/HUNITG/NORDR1,NORDR2,NITP,ITMNN,IGSS,ITHIN,IGSSV(3)
      COMMON/TP/LX/TTAB(50),VIN(50),VITAB(50),NITAB(50),UTAB(50),
1 TTAB(50),NITAB(50),TRHP(50),IPTTAB(50),NTTAB
      COMMON/TTN/T(50),NT
      COMMON/WPROP/ALPAR(50),COPAR(50),AKSN(25),ALPK(25),D(25),ALPD(25)
1 ,AKSAT,AKSHO,NKPAR,NKSP,NCOPAR,NDSP
      COMMON/XVAR/XSUP1(50),XSUP2(50),THP(50),ALP(50),VSUP1(50),
1 VSUP2(50),P(50),QCA(50),QC(50),THTP(50),AKGSS(212),DGSS(212),
1 IPTTH(50),NTH,JTH,NGSS
      EXTERNAL DUMPOH
      DIMENSION NORDRA(2)
      DATA PI/3.1415926536D0/
C
C *****
C
      ENTRI: DINW
C
C I/O OF NON-ARRAY INTEGER AND REAL PARAMETERS.
C
      READ 10000,KUTH,NTTAB,NT,NTH,NKPAR,NCOPAR,NORDRA(1),NORDRA(2),
1 NITP,KSTRN,KRESH,KANL
      IF (KSTRN.EQ.0) KSTRN=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
      NORDR1=NORDRA(1)
      NORDR2=NORDRA(2)
      IF (KPGH.EQ.2) KUTH=2
      PRINT 10300,KUTH,NTTAB,NT,NTH,NKPAR,NCOPAR,NORDR1,NITP,
1 KSTRN,KRESH,KANL

```

READ 10400, TH0, TH1, EPS, DALP1	DATA 245
PRINT 10500, TH0, TH1, EPS, DALP1	DATA 250
THB=TH1-TH0	DATA 255
DTH1=THB*DALP1	DATA 260
SINEPS=DSIN(EPS*(PI/180.00));	DATA 265
IF (EPS.EQ.0.00) SINEPS=0.00	DATA 270
C	DATA 275
C I/O OF SOIL PROPERTIES.	DATA 280
C	DATA 285
READ 10400, (AKPAR(I), I=1, NKPAB)	DATA 290
PRINT 10600, (AKPAR(I), I=1, NKPAB)	DATA 295
READ 10400, (CDPAR(I), I=1, NCDPAB)	DATA 300
PRINT 10700, (CDPAR(I), I=1, NCDPAB)	DATA 305
C	DATA 310
C I/O OF TABULAR END-POINT DARCY VELOCITIES IN UNITS OF SATURATED	DATA 315
C CONDUCTIVITY.	DATA 320
C	DATA 325
READ 10400, (VIN(I), I=1, NVTAB)	DATA 330
PRINT 10800, (VIN(I), I=1, NVTAB)	DATA 335
C	DATA 340
C CONDITIONAL I/O OF THE TIME VALUES.	DATA 345
C	DATA 350
30 IF (KPGH.NE.2) GO TO 40	DATA 355
IF (KNTB.EQ.0) GO TO 40	DATA 360
READ 10400, (T(I), I=1, NT)	DATA 365
PRINT 10100, (T(I), I=1, NT)	DATA 370
40 RETURN	DATA 375
C	DATA 380
C *****	DATA 385
C	DATA 390
ENTRY PUCAL	DATA 395
C	DATA 400
C PRELIMINARY WATER-TRANSPORT CALCULATIONS.	DATA 405
C	DATA 410
C	DATA 415
C GENERATION OF THE WATER CONTENTS.	DATA 420
C	DATA 425
NTNB=NTB-1	DATA 430
THB=TH1-TH0	DATA 435
DTH1=THB*DALP1	DATA 440
IF (KABL.EQ.0) DUNNY=SPROPI(DUNNY)	DATA 445
IF (KABL.NE.0) DUNNY=SPANLI(DUNNY)	DATA 450
DTH=(TH1-TH0)/DLOAT(NTNB)	DATA 455
THP(1)=TH0	DATA 460
THP(NTB)=TH1	DATA 465
IF (KRESH.NE.0) GO TO 60	DATA 470
DO 50 I=2, NTNB	DATA 475
THP(I)=THP(I-1)+DTH	DATA 480
50 CONTINUE	DATA 485
GO TO 80	DATA 490
60 NV=NTNB	DATA 495
NV=N-1	DATA 500
DTHAV=DTH	DATA 505
SDTH=2.0*(DTHAV-DTH1)/DLOAT(NV)	DATA 510
DTHI=DTH1	DATA 515
DO 70 JV=1, NV	DATA 520
IV=NTB-JV	DATA 525
THP(IV)=THP(IV+1)-DTHI	DATA 530
DTHI=DTHI+SDTH	DATA 535
70 CONTINUE	DATA 540
THP(1)=TH0	DATA 545
80 DO 90 I=1, NTB	DATA 550
ALP(I)=(THP(I)-TH0)/THB	DATA 555
90 CONTINUE	DATA 560
C	DATA 565
C CALCULATION OF TABULAR VELOCITIES.	DATA 570
C	DATA 575
DO 100 I=1, NVTAB	DATA 580
100 VITAB(I)=VIN(I)*AKSAT	DATA 585
DO 110 I=1, NVTAB	DATA 590
110 NITAB(I)=(VITAB(I)+AKSH0)/THB	DATA 595
C	DATA 600
C PREPARATION OF THE GAUSS GRID OF SOIL PROPERTIES.	DATA 605
C	DATA 610
IGSS=0	DATA 615

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      NDRP=NBDRP
      DO 120 ITH=1,NTM
        JTH=ITH+1
        IF (ITH.EQ.NTM) NDRP=NBDRP1
        CALL GAUSS(ALP(ITH),ALP(JTH),DUMY,DUMPS,NDRP)
120    CONTINUE
      NGSS=IGSS
      IF (KPGH.EQ.5) GO TO 130
      IF (KPGH.EQ.7) GO TO 130
      IF (KSRCH.NE.0) PRINT 16200
C
C   OUTPUT OF THE WATER CONTENTS.
C
      PRINT 10900, (THP(I),I=1,NTM)
      PRINT 11000, (ALP(I),I=1,NTM)
130  RETURN
C
10000 FORMAT(16I5)
10100 FORMAT(/' T: '/(2E15.7))
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/RESAT: '/(8E15.7))
10900 FORMAT(/' THP: '/(8E15.7))
11000 FORMAT(/' ALP: '/(8E15.7))
11100 FORMAT(20A4)
11200 FORMAT(1H0,20A4)
      END
      SUBROUTINE DSORT(IPT,IPT,NPT)
C
C
C   FUNCTION OF SUBROUTINE--TO TRANSFORM ARRAY IPT INTO ASCENDING
C   ORDER AND OBTAIN THE PERMUTATIVE TRANSFORMATION IPT.
C
C
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION IPT(1),IPT(1)
      DO 10 I=1,NPT
10    IPT(I)=I
      L=NPT
      L=L/2
      IF (L.EQ.0) RETURN
      K=NPT-L
      J=1
30  I=J
40  IL=I+L
      IF (IPT(I).LE.IPT(IL)) GO TO 50
      TEMP=IPT(I)
      IPT(I)=IPT(IL)
      IPT(IL)=TEMP
      IPT(IL)=IPT(IL)
      IPT(IL)=TEMP
      I=I-L
      IF (I.LE.1) GO TO 40

```

```

DATA 620
DATA 625
DATA 630
DATA 635
DATA 640
DATA 645
DATA 650
DATA 655
DATA 660
DATA 665
DATA 670
DATA 675
DATA 680
DATA 685
DATA 690
DATA 695
DATA 700
DATA 705
DATA 710
DATA 715
DATA 720
DATA 725
DATA 730
DATA 735
DATA 740
DATA 745
DATA 750
DATA 755
DATA 760
DATA 765
DATA 770
DATA 775
DATA 780
DATA 785
DATA 790
DATA 795
DATA 800
DATA 805
DATA 810
DATA 815
DATA 820
DATA 825
DATA 830
DATA 835
DATA 840
DATA 845
DATA 850
DATA 855
DSOR 0
DSOR 5
DSOR 10
DSOR 15
DSOR 20
DSOR 25
DSOR 30
DSOR 35
DSOR 40
DSOR 45
DSOR 50
DSOR 55
DSOR 60
DSOR 65
DSOR 70
DSOR 75
DSOR 80
DSOR 85
DSOR 90
DSOR 95
DSOR 100
DSOR 105
DSOR 110
DSOR 115
DSOR 120
DSOR 125
DSOR 130

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50 J=J+1                                DSOR 135
   IF (J.GT.K) GO TO 20                 DSOR 140
   GO TO 30                             DSOR 145
   END                                  DSOR 150
   FUNCTION SPROP(DUMMY)                SPRO  0
C                                         SPRO  5
C                                         SPRO 10
C FUNCTION OF ROUTINE--INTERPOLATION TO DETERMINE BOTH      SPRO 15
C CONDUCTIVITY AND DIFFUSIVITY.         SPRO 20
C                                         SPRO 25
C                                         SPRO 30
C                                         SPRO 35
      IMPLICIT REAL*8(A-H,O-Z)          SPRO 40
      COMMON/BI/ TH1,TH0,THB,SINEPS    SPRO 45
      COMMON/HUNIT/ MORDR1,MORDER,NITP,ITHIN,IGSS,ITHIN, IGSSV(3) SPRO 50
      COMMON/UPROP/ AKPAR(50),CDPAR(50),AKSH(25),ALPK(25),D(25),ALPD(25) SPRO 55
      1 ,AKSAT,AKSH0,NKPAR,NKSP,MCDPAR,NDSP SPRO 60
      COMMON/XVAR/ XSUP1(50),XSUP2(50),THP(50),ALP(50),VSUP1(50), SPRO 65
      1 VSUP2(50),F(50),QGA(50),QG(50),THTRP(50),AKGSS(212), DGSS(212), SPRO 70
      1 LPTTH(50),NTH,JTH,NGSS SPRO 75
      DATA ALP0/0.0D0/,ALP1/1.0D0/,IND1/0/ SPRO 80
C                                         SPRO 85
C ***** SPRO 90
C ENTRY SPROPI(DUMMY)                   SPRO 95
C                                         SPRO 100
C SECTION SPROPI INITIALIZES THE SOIL-PROPERTY ARRAYS.    SPRO 105
C                                         SPRO 110
      NKSP=NKPAR/2                      SPRO 115
      NDSP =MCDPAR/2                   SPRO 120
C                                         SPRO 125
C EXTRACT CONDUCTIVITY VARIABLES FROM INPUT ARRAY AKPAR.  SPRO 130
C                                         SPRO 135
      J=0                               SPRO 140
      DO 10 I=1,NKPAR,2                SPRO 145
        J=J+1                          SPRO 150
        THT=AKPAR(I)                   SPRO 155
        ALPK(J)=(THT-TH0)/THB          SPRO 160
        AK=AKPAR(I+1)                  SPRO 165
        AKSH(J)=DLOG(AK)               SPRO 170
      10 CONTINUE                      SPRO 175
C                                         SPRO 180
C INTERPOLATE TO FIND AKSH0 AT ALP = 0. SPRO 185
C                                         SPRO 190
      IKSH=1                           SPRO 195
      AK=YLAG(ALP0,ALPK,AKSH,IND1,NITP,IKSH,NKSP,IRX) SPRO 200
      AK0=DEXP(AK)                     SPRO 205
      AKSH0=AK0*SINEPS                 SPRO 210
      IKSH=1                           SPRO 215
      AK=YLAG(ALP1,ALPK,AKSH,IND1,NITP,IKSH,NKSP,IRX) SPRO 220
      AKSAT=DEXP(AK)                   SPRO 225
C                                         SPRO 230
C EXTRACT DIFFUSIVITY VARIABLES FROM INPUT ARRAY CDPAR.  SPRO 235
C                                         SPRO 240
      J=0                               SPRO 245
      DO 20 I=1,MCDPAR,2                SPRO 250
        J=J+1                          SPRO 255
        THT=CDPAR(I)                   SPRO 260
        ALPD(J)=(THT-TH0)/THB          SPRO 265
        D(J)=DLOG(CDPAR(I+1))          SPRO 270
      20 CONTINUE                      SPRO 275
      RETURN                            SPRO 280
C                                         SPRO 285
C ***** SPRO 290
C                                         SPRO 295
C ENTRY AKFUN(ALPG)                     SPRO 300
C                                         SPRO 305
C INTERPOLATE TO DETERMINE CONDUCTIVITY AT ARBITRARY ALPG. SPRO 310
C                                         SPRO 315
      IKSH=1                           SPRO 320
      AK=YLAG(ALPG,ALPK,AKSH,IND1,NITP,IKSH,NKSP,IRX) SPRO 325
      AK=DEXP(AK)                      SPRO 330
C                                         SPRO 335
C DETERMINE REDUCED CONDUCTIVITY--SINE VARIABLE.         SPRO 340
C                                         SPRO 345
      AKFUN=(AK-AK0)*SINEPS/THB       SPRO 350

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```

      RETURN
C
C .....
C
      ENTRY DFUN(ALPG)
C
C INTERPOLATE TO DETERMINE DIFFUSIVITY AT ARBITRARY ALPG.
C
      IDHIN=1
      DF=YLAG(LPG,ALPD,D,IND1,NITP,IDHIN,NDSP,IE1)
      DFUN=DEXP(DF)
      RETURN
      END
      FUNCTION SPANL(DUMMY)
C
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,TH0,THB,SINEPS
      COMMON/WPROP/AKPAR(50),CDPAR(50),AKSN(25),ALPK(25),D(25),ALPD(25)
      1 ,AKSAT,AKSNC,HKPAR,HKSP,HCDPAR,NDSP
      COMMON/XVAR/XSUP1(50),XSUP2(50),THP(50),ALP(50),VSUP1(50),
      1 VSUP2(50),P(50),QGA(50),QG(50),THTHP(50),AKGSS(212),DGSS(212),
      1 IPTTH(50),MTH,JTH,NGSS
      THETA(ALP)=THB*ALP+TH0
      GPF(TH)=(TH1-TH)/(TH1+TH)
C
C INVERSE OF KING WATER-CONTENT FORM FACTOR.
C
      HF(GP)=H0*(DLOG((G/GP)+DSQRT((G/GP)**2-1.)))*BI
C
C GARDNER CONDUCTIVITY FORM FACTOR.
C
      AKP(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
      HKSP=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)
      H0=CDPAR(2)
      B=CDPAR(3)
      BI=1./B
      G=GPF(TH0)
      CB=2.*B*G*TH1/H0
C
C FIND AKSN0 AT ALP=0.
C
      AK0=0.
      AKSN0=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 .....

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SPRO 355
SPRO 360
SPRO 365
SPRO 370
SPRO 375
SPRO 380
SPRO 385
SPRO 390
SPRO 395
SPRO 400
SPRO 405
SPRO 410
SPRO 415
SPAN 0
SPAN 5
SPAN 10
SPAN 15
SPAN 20
SPAN 25
SPAN 30
SPAN 35
SPAN 40
SPAN 45
SPAN 50
SPAN 55
SPAN 60
SPAN 65
SPAN 70
SPAN 75
SPAN 80
SPAN 85
SPAN 90
SPAN 95
SPAN 100
SPAN 105
SPAN 110
SPAN 115
SPAN 120
SPAN 125
SPAN 130
SPAN 135
SPAN 140
SPAN 145
SPAN 150
SPAN 155
SPAN 160
SPAN 165
SPAN 170
SPAN 175
SPAN 180
SPAN 185
SPAN 190
SPAN 195
SPAN 200
SPAN 205
SPAN 210
SPAN 215
SPAN 220
SPAN 225
SPAN 230
SPAN 235
SPAN 240
SPAN 245
SPAN 250
SPAN 255
SPAN 260
SPAN 265
SPAN 270
SPAN 275
SPAN 280
SPAN 285
SPAN 290
SPAN 295
SPAN 300
SPAN 305

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C	ENTRY AKANL(ALPG)	SPAN 310
C		SPAN 315
C	DETERMINE CONDUCTIVITY AT ARBITRARY ALPG.	SPAN 320
C		SPAN 325
C	IF (ALPG.NE.1.) GO TO 10	SPAN 330
	AK=AKS	SPAN 335
	GO TO 20	SPAN 340
10	TH=THETA(ALPG)	SPAN 345
	GP=GPF(TH)	SPAN 350
	H=HF(GP)	SPAN 355
	AK=AKF(H)	SPAN 360
C		SPAN 365
C	DETERMINE REDUCED CONDUCTIVITY-SINE VARIABLE.	SPAN 370
C		SPAN 375
20	AKANL=(AK-AK0)*SINERS/THB	SPAN 380
	RETURN	SPAN 385
C		SPAN 390
C	*****	SPAN 395
C		SPAN 400
C	ENTRY DANL(ALPG)	SPAN 405
C		SPAN 410
C	CALCULATE DIFFUSIVITY AT ARBITRARY ALPG.	SPAN 415
C		SPAN 420
C	IF (ALPG.NE.1.) GO TO 30	SPAN 425
	TH=TH1	SPAN 430
	AK=AKS	SPAN 435
	C=CC*TH	SPAN 440
	GO TO 40	SPAN 445
30	TH=THETA(ALPG)	SPAN 450
	GP=GPF(TH)	SPAN 455
	H=HF(GP)	SPAN 460
	AK=AKF(H)	SPAN 465
	X=H/H0	SPAN 470
	XB=X**B	SPAN 475
	XB1=XB/X	SPAN 480
	C=CH*XB1*DSINH(XB)/(DCOSH(XB)+C)**2+CC*TH	SPAN 485
40	DANL=AK/C	SPAN 490
	RETURN	SPAN 495
C		SPAN 500
C	*****	SPAN 505
C		SPAN 510
C	ENTRY HANL(ALPG)	SPAN 515
C		SPAN 520
C	CALCULATE THE PRESSURE HEAD AT ARBITRARY ALPG.	SPAN 525
C		SPAN 530
C	IF (ALPG.NE.1.) GO TO 50	SPAN 535
	H=0.	SPAN 540
	GO TO 60	SPAN 545
50	TH=THETA(ALPG)	SPAN 550
	GP=GPF(TH)	SPAN 555
	H=HF(GP)	SPAN 560
60	HANL=H	SPAN 565
	RETURN	SPAN 570
C		SPAN 575
C	*****	SPAN 580
C		SPAN 585
C		SPAN 590
C		SPAN 595
C	CALCULATE THE WATER CAPACITY AT ARBITRARY ALPG.	SPAN 600
C		SPAN 605
C	ENTRY CANL(ALPG)	SPAN 610
	IF (ALPG.NE.1.) GO TO 70	SPAN 615
	TH=TH1	SPAN 620
	C=CC*TH	SPAN 625
	GO TO 80	SPAN 630
70	TH=THETA(ALPG)	SPAN 635
	GP=GPF(TH)	SPAN 640
	H=HF(GP)	SPAN 645
	X=H/H0	SPAN 650
	XB=X**B	SPAN 655
	XB1=XB/X	SPAN 660
	C=CH*XB1*DSINH(XB)/(DCOSH(XB)+C)**2+CC*TH	SPAN 665
80	CANL=C	SPAN 670
	RETURN	SPAN 675
	END	SPAN 680

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      FUNCTION PUNS(ALPG)
      PUNS 0
C      PUNS 5
C      PUNS 10
C      PURPOSE OF ROUTINE--TO PROVIDE A COLLECTION OF FUNCTIONS TO BE USED
C      IN THE PARLANGE-TYPE WATER-TRANSPORT CALCULATION.
C      PUNS 15
C      PUNS 20
C      PUNS 25
C      PUNS 30
      IMPLICIT REAL*8 (A-H,O-Z)
      PUNS 35
      COMMON/CTRL/KPGH,KCTR,KVI,KSTRH,KSTRW,ISTOP,KSS,KDIG,KHOUT, KHOUT,
      PUNS 40
      1 KTSTP,KROUT,KSMCH,KBUFP,KANL,KIC,KSTRS
      PUNS 45
      COMMON/CN1/ W1,V1
      PUNS 50
      COMMON/HUNITG/ NORDER1,NORDER,N TTP,ITHIN,IGSS,ITHIN, IGSSV(3)
      PUNS 55
      COMMON/TPLX/TTAB(50),VIN(50),VIPAB(50),WITAB(50),UTAB(50),
      PUNS 60
      1 TTAB(50),WITAB(50),TBRP(50),IPTTAB(50),WITAB
      PUNS 65
      COMMON/XVAR/XSUP1(50),XSUP2(50),TNP(50),ALP(50),VSUP1(50),
      PUNS 70
      1 VSUP2(50),P(50),QGA(50),QG(50),THTNP(50),AKGSS(212), DGSS(212),
      PUNS 75
      1 IPTYN(50),NTH,JTH,DGSS
      PUNS 80
      DATA END1/0/
      PUNS 85
      PUNS 90
C      *****
C      PUNS 95
C      PUNS 100
      ENTRY TLPUN(ALPG)
      PUNS 105
C      PUNS 110
C      EVALUATE LOGARITHM-TYPE TIME INTEGRAND.
      PUNS 115
C      PUNS 120
      IGSSV(1)=IGSSV(1)+1
      PUNS 125
      IGSS=IGSSV(1)
      PUNS 130
      AKSH=AKGSS(IGSS)
      PUNS 135
      D=DGSS(IGSS)
      PUNS 140
      P1=ALPG*D/(AKSH*AKSH)
      PUNS 145
      P2=DLOG((AKSH+W1)/W1)
      PUNS 150
      TLPUN=P1*P2
      PUNS 155
      RETURN
      PUNS 160
C      PUNS 165
C      *****
C      PUNS 170
C      PUNS 175
      ENTRY TQPUN(ALPG)
      PUNS 180
C      PUNS 185
C      DETERMINE QUOTIENT-TYPE TIME INTEGRAND.
      PUNS 190
C      PUNS 195
      IGSSV(2)=IGSSV(2)+1
      PUNS 200
      IGSS=IGSSV(2)
      PUNS 205
      AKSH=AKGSS(IGSS)
      PUNS 210
      D=DGSS(IGSS)
      PUNS 215
      P1=ALPG*D/AKSH
      PUNS 220
      P2=1./(AKSH+W1)
      PUNS 225
      TQPUN=P1*P2
      PUNS 230
      RETURN
      PUNS 235
C      PUNS 240
C      *****
C      PUNS 245
C      PUNS 250
      ENTRY TOPUN(ALPG)
      PUNS 255
C      PUNS 260
C      EVALUATE THE TIME INTEGRAL FOR SINEPS=0.
      PUNS 265
C      PUNS 270
      IGSS=IGSS+1
      PUNS 275
      D=DGSS(IGSS)
      PUNS 280
      TOPUN=ALPG*D
      PUNS 285
      RETURN
      PUNS 290
C      PUNS 295
C      *****
C      PUNS 300
C      PUNS 305
      ENTRY TIPUN(ALPG)
      PUNS 310
C      PUNS 315
C      DETERMINE INTEGRAND ARISING FROM INFINITE VELOCITY LIMIT.
      PUNS 320
C      PUNS 325
      IGSSV(3)=IGSSV(3)+1
      PUNS 330
      IGSS=IGSSV(3)
      PUNS 335
      AKSH=AKGSS(IGSS)
      PUNS 340
      D=DGSS(IGSS)
      PUNS 345
      TIFUN=ALPG*D/AKSH
      PUNS 350
      RETURN
      PUNS 355
C      PUNS 360
C      *****
C      PUNS 365
C      PUNS 370

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      ENTRY GFUN(ALPG)                                PUNS 375
C                                                    PUNS 380
C DETERMINE POSITION INTEGRAND FOR FIRST-ORDER CALCULATION. PUNS 385
C                                                    PUNS 390
      IGSS=IGSS+1                                     PUNS 395
      AKSH=AKGSS(IGSS)                               PUNS 400
      D=DGSS(IGSS)                                   PUNS 405
      GFUN=D/(AKSH+U1)                               PUNS 410
      RETURN                                           PUNS 415
C                                                    PUNS 420
C *****PUNS 425
C                                                    PUNS 430
      ENTRY GAFUN(ALPG)                              PUNS 435
C                                                    PUNS 440
C CALCULATE INTEGRAND OF FIRST FUNCTION USED IN CORRECTION FRACTION F. PUNS 445
C                                                    PUNS 450
      IGSS=IGSS+1                                     PUNS 455
      AKSH=AKGSS(IGSS)                               PUNS 460
      D=DGSS(IGSS)                                   PUNS 465
      GAFUN=D*ALPG/(AKSH+U1)**2                     PUNS 470
      RETURN                                           PUNS 475
C                                                    PUNS 480
C *****PUNS 485
C                                                    PUNS 490
      ENTRY GSPUN(ALPG)                              PUNS 495
C                                                    PUNS 500
C CALCULATE INTEGRAND OF SECOND FUNCTION USED IN CORRECTION FRACTION F. PUNS 505
C                                                    PUNS 510
      IGSS=IGSS+1                                     PUNS 515
      AKSH=AKGSS(IGSS)                               PUNS 520
      D=DGSS(IGSS)                                   PUNS 525
      GSPUN=D/(AKSH+U1)**2                           PUNS 530
      RETURN                                           PUNS 535
C                                                    PUNS 540
C *****PUNS 545
C                                                    PUNS 550
      ENTRY G2FUN(ALPG)                              PUNS 555
C                                                    PUNS 560
C EVALUATE POSITION INTEGRAND FOR SECOND-ORDER CALCULATION. PUNS 565
C                                                    PUNS 570
      IGSS=IGSS+1                                     PUNS 575
      AKSH=AKGSS(IGSS)                               PUNS 580
      D=DGSS(IGSS)                                   PUNS 585
      PP=YLAC(ALPG,ALP,F,IND1,HITP,ITHRIN,UTH,IRX)   PUNS 590
      G2FUN=D/(AKSH+U1*PP)                           PUNS 595
      RETURN                                           PUNS 600
C                                                    PUNS 605
C *****PUNS 610
C                                                    PUNS 615
      ENTRY DUNFUN(ALPG)                             PUNS 620
C                                                    PUNS 625
C CONSTRUCT GAUSS GRID OF SOIL PROPERTIES.          PUNS 630
C                                                    PUNS 635
      IGSS=IGSS+1                                     PUNS 640
      IF (KABL-EQ.0) AKGSS(IGSS)=AKFUN(ALPG)         PUNS 645
      IF (KABL-NE.0) AKGSS(IGSS)=AKABL(ALPG)         PUNS 650
      IF (KABL-EQ.0) DGSS(IGSS)=DFUN(ALPG)           PUNS 655
      IF (KABL-NE.0) DGSS(IGSS)=DABL(ALPG)           PUNS 660
      DUNFUN=1.                                       PUNS 665
      RETURN                                           PUNS 670
      END                                             PUNS 675
      SUBROUTINE PRINTU                                PRIH 0
C                                                    PRIH 5
C                                                    PRIH 10
C FUNCTION OF SUBROUTINE—TO OUTPUT WATER-TRANSPORT VARIABLES, I. E. A PRIH 15
C TABLE OF THE END-POINT VELOCITY AS A FUNCTION OF TIME AND TABLES OF PRIH 20
C POSITIONS AND VELOCITIES AS FUNCTIONS OF WATER CONTENT. PRIH 25
C                                                    PRIH 30
C                                                    PRIH 35
C                                                    PRIH 40
      IMPLICIT REAL*8 (A-H,O-Z)                     PRIH 45
      COMMON/CTRL/KPGH,KUTH,KVI,KSTRH,KSTRN,ISROP,KSS,KDIC,KHOUT, KHOUT, PRIH 50
      1 KSTP,KROUT,KSOCH,KRUPP,KABL,KIC,KSTRS        PRIH 55
      COMMON/TPX/TTAB(50),V1H(50),V1TAB(50),V2TAB(50),UTAB(50), PRIH 60
      1 TTAB(50),H1TAB(50),THRP(50),IPTTAB(50),HTTAB PRIH 65
      COMMON/TUTR/T(50),BT

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COMMON/XVAR/XSUP1(50),XSUP2(50),THP(50),ALP(50),VSUP1(50),
1 VSUP2(50),F(50),QGA(50),QG(50),THTNP(50),MAGSS(212), DGSS(212),
1 IPTTH(50),NTH,JTH,MGSS
C
C
C .....
C ENTRY PRTTAB
C
C PRINT VELOCITY-TIME INTERPOLATION TABLE.
C
  KWOUT=KWOUT+1
  PRINT 10100,KWOUT
  PRINT 10000
  DO 10 ITH=1,NTH
    PRINT 10600,TTAB(ITH),WITAB(ITH),VITAB(ITH),V1H(ITH),UTAB(ITH)
10  CONTINUE
  RETURN
C
C .....
C ENTRY PRTW1(ITH)
C
C PRINT FIRST-ORDER POSITION AND VELOCITY VARIABLES.
C
  KWOUT=KWOUT+1
  TIME=T(ITH)
  PRINT 10200,KWOUT,TIME
  DO 20 ITH=1,NTH,8
    JTHNN=ITH
    JTHNX=MIN0(ITH+7,NTH)
    PRINT 10700,ITH,(XSUP1(JTH),JTH=JTHNN,JTHNX)
20  CONTINUE
  KWOUT=KWOUT+1
  PRINT 10300,KWOUT,TIME
  DO 30 ITH=1,NTH,8
    JTHNN=ITH
    JTHNX=MIN0(ITH+7,NTH)
    PRINT 10700,ITH,(VSUP1(JTH),JTH=JTHNN,JTHNX)
  CONTINUE
  RETURN
  ENTRY PRTW2(ITH)
C
C PRINT SECOND-ORDER POSITION AND VELOCITY VARIABLES.
C
  KWOUT=KWOUT+1
  TIME=T(ITH)
  PRINT 10400,KWOUT,TIME
  DO 40 ITH=1,NTH,8
    JTHNN=ITH
    JTHNX=MIN0(ITH+7,NTH)
    PRINT 10700,ITH,(XSUP2(JTH),JTH=JTHNN,JTHNX)
40  CONTINUE
  KWOUT=KWOUT+1
  PRINT 10500,KWOUT,TIME
  DO 50 ITH=1,NTH,8
    JTHNN=ITH
    JTHNX=MIN0(ITH+7,NTH)
    PRINT 10700,ITH,(VSUP2(JTH),JTH=JTHNN,JTHNX)
  CONTINUE
50  RETURN
10000 FORMAT(/T12,'TTAB',T30,'WITAB',T49,'VITAB',T67,'V1/AKSAT', T86,
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 =',IPD12.4// ' NODE I',5X,'POSITIONS ',
1 'AT THETA NODES I,I+1,...,I+7'/)
10300 FORMAT(////' WATER-TRANSPORT OUTPUT TABLE',I4,'.. FIRST-',
1 'ORDER VELOCITIES AT TIME =',IPD12.4// ' 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 =',IPD12.4// ' NODE I',5X,'POSITIONS ',
1 'AT THETA NODES I,I+1,...,I+7'/)
10500 FORMAT(////' WATER-TRANSPORT OUTPUT TABLE',I4,'.. SECOND-',

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1 'ORDER VELOCITIES AT TIME =' ,1PD12.4// ' HOWE I' ,5X,
1 'VELOCITIES AT THETA MODES I,I+1,...,I+7' /)
10600 FORMAT(5(4X,E15.7))
10700 FORMAT(17,8(1PD15.4))
END
SUBROUTINE STRU
C
C
C FUNCTION OF SUBROUTINE--TO STORE PERTINENT WATER-TRANSPORT
C QUANTITIES ON AN AUXILIARY DEVICE.
C
C
C IMPLICIT REAL*8 (A-H,O-Z)
C COMMON/PROBID/TITLE(8),NPROB
C COMMON/CRVAR/TIME,TH(100,2),TNN(100,2),TNN(100,2),DTH(100,2),
1 VX(100,2),VIP(100,2),VW(100,2)
C COMMON/TPLI/TTAB(50),VIN(50),VITAB(50),WITAB(50),UTAB(50),
1 TTAB(50),WITAB(50),TEMP(50),IPTTAB(50),MTAB
C COMMON/TWTR/T(50),NT
C COMMON/XVAR/XSUP1(50),XSUP2(50),THP(50),ALP(50),VSUP1(50),
1 VSUP2(50),P(50),QGA(50),QG(50),THHP(50),AKGSS(212),DGSS(212),
1 IPTTH(50),NTH,JTH,NGSS
C
C *****
C
C ENTRY STRU1
C PUNCH 10000,(TITLE(I),I=1,8)
C PUNCH 10100,NT
C PUNCH 10100,NTH
C PUNCH 10200,(ALP(I),I=1,NTH)
C PUNCH 10200,(THP(I),I=1,NTH)
C RETURN
C
C *****
C
C ENTRY STRU2
C PUNCH 10200,TIME
C PUNCH 10200,(XSUP2(I),I=1,NTH)
C PUNCH 10200,(VSUP2(I),I=1,NTH)
C 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
C IMPLICIT REAL*8 (A-H,O-Z)
C COMMON/CTBL/CPGN,KUTR,KVI,KSTRM,KSTRU,ISTOP,KSS,KDIG,KHOUT,KVOUT,
1 KTSPP,KROUT,KSDCH,KBUFP,KABL,KIC,KSTRS
C COMMON/TWTR/T(50),NT
C COMMON/KIV/KYIL(5),KYIU(5),KYI(5),KXI,KXE
C COMMON/KIV/KI(100,5),KX(100,5),YI(100,5),DYI(100,5),IT(100),IX(5)
1 ,IUTL(5),IUTU(5)
C COMMON/SIP/SP,KPRS,KIFUN,ICONV,KSCY,IPA(5,20)
C COMMON/SRP/ DELT0,CBIS,ACC,BED,TOLSTP,TOLFUN,P(20),PH(20),PL(20),
1 DELP(20),PLO(20),PHO(20)
C DATA PD/1.D50/
C
C INPUT AND OUTPUT NON-ARRAY INTEGER AND REAL PARAMETERS.
C
C READ 10000,ND,KPRS,KIFUN,KUT,NTI,KBD, KSCY,KSTRS
C IF (KSCY.LE.0) KSCY=1
C IF (KSTRS.NE.0) KSTRS=1
C PRINT 10200,ND,KPRS,KIFUN,KUT,NTI,KBD,KSCY,KSTRS
C READ 10100,ACC,BED,TOLSTP,TOLFUN,BDP,CUT
C PRINT 10300,ACC,BED,TOLSTP,TOLFUN,BDP,CUT
C
C READ AND PRINT INITIAL PARAMETERS P AND THEIR LIMITS PH AND PL.

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C	READ 10100, (P(IP), IP=1, NP)	DATA 155
	IF (MSCY-LE.0) GO TO 20	DATA 160
	DO 10 ISCY=1, MSCY	DATA 165
	READ 10000, (IPA (ISCY, IP), IP=1, NP)	DATA 170
10	CONTINUE	DATA 175
20	IF (KBND-LE.0) GO TO 30	DATA 180
	READ 10100, (PH(IP), IP=1, NP)	DATA 185
	READ 10100, (PL(IP), IP=1, NP)	DATA 190
	GO TO 50	DATA 195
30	DO 40 IP=1, NP	DATA 200
	PL(IP)=-P0	DATA 205
	PH(IP)=P0	DATA 210
40	CONTINUE	DATA 215
50	DO 60 IP=1, NP	DATA 220
	PLW(IP)=PL(IP)	DATA 225
	PHO(IP)=PH(IP)	DATA 230
	DELP(IP)=BDP*P(IP)	DATA 235
60	CONTINUE	DATA 240
C		DATA 245
C	INPUT EXPERIMENTAL DATA. NOTE THAT YX = TXI	DATA 250
C	IN THE WATER-TRANSPORT CASE AND THAT YX = RX	DATA 255
C	IN THE MATERIAL-TRANSPORT CASE.	DATA 260
C		DATA 265
	READ 10100, (TX(ITM), ITM=1, NTX)	DATA 270
	IF (KPCN-NE.5) GO TO 80	DATA 275
	NT=NTX	DATA 280
	DO 70 ITM=1, NT	DATA 285
70	T(ITM)=TX(ITM)	DATA 290
80	READ 10000, (NYX(ITM), ITM=1, NTX)	DATA 295
	DO 90 ITM=1, NTX	DATA 300
	NYXL(ITM)=1	DATA 305
90	NYXU(ITM)=NYX(ITM)	DATA 310
	PRINT 10600	DATA 315
	NT=0	DATA 320
	DO 230 ITM=1, NTX	DATA 325
	NI=NYX(ITM)	DATA 330
	NI=NI+1	DATA 335
	READ 10100, (IX(IX, ITM), IX=1, NI)	DATA 340
	READ 10100, (YX(IX, ITM), IX=1, NI)	DATA 345
	IF (KWT-GE.2) READ 10100, (DYX(IX, ITM), IX=1, NI)	DATA 350
	IF (KWT-GE.3) READ 10100, (XUTL(ITM), XUTU(ITM))	DATA 355
	IF (XUTU(ITM)-LE.XVPL(ITM)) XUTU(ITM)=XI(NI, ITM)	DATA 360
		DATA 365
C		DATA 370
C	CALCULATE STATISTICAL WEIGHTS.	DATA 375
C		DATA 380
	IF (KWT-GE.0) GO TO 110	DATA 385
	DO 100 IX=1, NI	DATA 390
	DYX(IX, ITM)=0.	DATA 392
	IF (YX(IX, ITM)-GT.0.DG) DYX(IX, ITM)=DSJNT(YX(IX, ITM))	DATA 394
	WT=0.	DATA 398
	IF (DYX(IX, ITM)-NE.0.DG) WT=1./DYX(IX, ITM)**2	DATA 400
100	WY(IX, ITM)=WT	DATA 402
	GO TO 190	DATA 405
110	IF (KWT-GE.1) GO TO 130	DATA 410
	DO 120 IX=1, NI	DATA 415
	DYX(IX, ITM)=CWT*YX(IX, ITM)	DATA 420
	WT=0.	DATA 422
	IF (DYX(IX, ITM)-NE.0.DG) WT=1./DYX(IX, ITM)**2	DATA 424
120	WY(IX, ITM)=WT	DATA 426
	GO TO 190	DATA 430
130	DO 140 IX=1, NI	DATA 435
	WT=0.	DATA 438
	IF (DYX(IX, ITM)-NE.0.DG) WT=1./DYX(IX, ITM)**2	DATA 440
140	WY(IX, ITM)=WT	DATA 442
	IF (KWT-LE.2) GO TO 190	DATA 445
	NI=0	DATA 450
	DO 150 IX=1, NI	DATA 455
	NI=NI+1	DATA 460
	IF (IX(IX, ITM)-GE.XUTL(ITM)) GO TO 160	DATA 465
	WY(IX, ITM)=0.	DATA 470
150	CONTINUE	DATA 475
160	NYXL(ITM)=NI	DATA 480
	NI=NI+1	DATA 485
	DO 170 JI=1, NI	DATA 490


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IX=IX1-JX
NX=NX-1
IF (IX(IX,ITM)-LE.XTU(ITM)) GO TO 180
WX(IX,ITM)=0.
170 CONTINUE
180 NYX(IX,ITM)=NX
NXT=NXT+NYX*(IX,ITM)-NYX(IX,ITM)+1
190 PRINT 10700,IX(ITM)
C
C NORMALIZE EXPERIMENTAL POINTS.
C
    NXL=NYXL(ITM)
    NXU=NYXU(ITM)
    SUM=0.
    DO 200 IX=NXL,NXU
        SUM=SUM+YX(IX,ITM)
    200 AB=100./SUM
    ABS=AB*AB
    DO 210 IX=1,NX
        YX(IX,ITM)=AB*YX(IX,ITM)
        DYX(IX,ITM)=AB*DYX(IX,ITM)
    210 WX(IX,ITM)=WX(IX,ITM)/ABS
C
C OUTPUT EXPERIMENTAL DATA, INCLUDING WEIGHTS.
C
    DO 220 IX=1,NX
        WX(IX,ITM)=DABS(WX(IX,ITM))
    220 PRINT 10500,IX,IX,IX,ITM,YX(IX,ITM),WX(IX,ITM)
    230 CONTINUE
    IF (KUT.EQ.3) GO TO 250
    NIT=0
    DO 240 ITM=1,NIX
        NIT=NIT+NYX(ITM)
    240
    250 RETURN
C
C *****
C
    ENTRY SHPREP (ISCT)
C
C PREPARE AND PRINT STEP SIZES DELP AND PARAMETER BOUNDS PH AND PL.
C
    DO 260 IP=1,NP
        DELP(IP)=BDP*P(IP)
    260
    DO 270 IP=1,NP
        PH(IP)=PH0(IP)
        PL(IP)=PL0(IP)
        IF (IPA(XSCY,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.PL(IP)) GO TO 280
        THP=PH(IP)
        PH(IP)=PL(IP)
        PL(IP)=THP
    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/I5X DATA 810
1' DIAGNOSTIC PRINTER CONTROL . . . . .',I5/I5X DATA 815
1' MAXIMUM CHI-SQUARED EVALUATIONS . . . . .',I5/I5X DATA 820
1' WEIGHT-CONTROL INTEGER . . . . .',I5/I5X DATA 825
1' NUMBER OF EXPERIMENTAL TIME NODES . . . . .',I5/I5X DATA 830
1' PARAMETER BOUNDS CONTROL . . . . .',I5/I5X DATA 835
1' NUMBER OF SEARCH CYCLES . . . . .',I5/I5X DATA 840
1' AUXILIARY STORAGE CONTROL . . . . .',I5/I5X DATA 845
10300 FORMAT(5X,' ACCELERATION PARAMETER . . . . .',
1' E10.4/I5X ' REDUCTION PARAMETER . . . . .',
1' E10.4/I5X ' STEP-SIZE TOLERANCE . . . . .',
1' E10.4/I5X ' CHI-SQUARE ACCEPTANCE FACTOR. . . . .',

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1 E10.4/5X ' PARAMETER STEP-LENGTH FRACTION. . . . . ', DATA 870
1 E10.4/5X ' WEIGHTING CONSTANT. . . . . ', DATA 875
1 E10.4) DATA 880
10400 FORMAT(////' SEARCH INPUT TABLE 2.. ', DATA 885
1 ' INITIAL VALUES OF PARAMETERS, LIMITS, AND INCREMENTS'//T9,'IP', DATA 890
1 T25,'P',T45,'PH',T65,'PL',T85,'DP') DATA 895
10500 FORMAT(I10,4E20.5) DATA 900
10600 FORMAT(////' SEARCH INPUT TABLE 3.. EXPERIMENTAL DATA') DATA 905
10700 FORMAT(/5X' TABLE AT TIME =',E10.4//T9,'IX', T25,'IX',T45,'YI', DATA 910
1 T65,'YI') DATA 915
END DATA 920
SUBROUTINE PRINTS(ITH) PRINT 0
C PRINT 5
C PRINT 10
C FUNCTION OF SUBROUTINE--TO OUTPUT RESULTS OF PARAMETER SEARCH PRINT 15
C INCLUDING PARAMETER VALUES AND A TABLE OF CORRESPONDING EXPERIMENTAL PRINT 20
C AND THEORETICAL VARIABLES. PRINT 25
C PRINT 30
C PRINT 35
C IMPLICIT REAL*8 (A-H,O-Z) PRINT 40
REAL*4 PHAT PRINT 45
COMMON/CTRL/KPGH,KVTR,KVI,KSTRH,KSTRH,ISTOP,KSS,KDIG,KHOUT, KHOUT, PRINT 50
1 KTSTP,KSOUT,KSCHN,KDUFF,KABL,KIC,KSTBS PRINT 55
COMMON/GEOM/X(101),BB(2),DCOSB(2),DCOS(2),DELT,CHNG,DELHAI,THAI, PRINT 60
1 IPX(101),IE(100,3),BPH(2),BPST(2),BPTST(2),BDE(2),BTSE(2), ISB(2, PRINT 65
1 2), IS(2,2),BHP,BEL,BHAT,IBAND,BSC,BST,BTST,BDEL,BTI,BHOR PRINT 70
COMMON/HRVAR/ A(101,2),B(101,3),B(101),BP(101),BI(101),BB(101), PRINT 75
1 DP(101),B1(101),BT(101),XTRP(101),BPLX(101),BPLXP(101), PX(100,2) PRINT 80
1 ,PRATE(10),FLOW(10),TFLW(10),W,PHAT(3,5) PRINT 85
COMMON/XY/XYX(5),XYXU(5),YIX(5),YIXI,XYT PRINT 90
COMMON/IRV/IX(100,5),IXI(100,5),IXI(100,5),DTX(100,5), YT(100),TX(5) PRINT 95
1 ,XITL(5),XITU(5) PRINT 100
COMMON/SIP/SP,KPRS,HIPUN,ICONV,NSCT,IPA(5,20) PRINT 105
COMMON/SRP/ DELTO,CHIS,ACC,BED,TOLSTP,TOLPUN,P(20), PH(20),PL(20), PRINT 110
1 DELP(20),PLO(20),PHO(20) PRINT 115
KSOUT=KSOUT+1 PRINT 120
PRINT 10100,KSOUT PRINT 125
C PRINT 130
C PRINT FINAL PARAMETER VALUES. PRINT 135
C PRINT 140
DO 10 IP=1,NP PRINT 145
10 PRINT 10200,IP,P(IP),PH(IP),PL(IP),DELP(IP) PRINT 150
C PRINT 155
C OUTPUT EXPERIMENTAL AND THEORETICAL PROFILES. PRINT 160
C PRINT 165
KSOUT=KSOUT+1 PRINT 170
PRINT 10300,KSOUT PRINT 175
IX=XYX(ITH) PRINT 180
PRINT 10400,IX(ITH) PRINT 185
DO 20 IX=1,NI PRINT 190
20 PRINT 10200,IX,IX(IX,ITH),YIX(IX,ITH),YT(IX),DTX(IX,ITH) PRINT 195
IF (ITH.NE.NTX) GO TO 30 PRINT 200
C PRINT 205
C OUTPUT CHI/(MODAL POINT). PRINT 210
C PRINT 215
RES=CHIS/DFLOAT(NIT) PRINT 220
RES=DSQRT(RES) PRINT 225
PRINT 10500,RES PRINT 230
30 RETURN PRINT 235
10000 FORMAT(I5,5X,E10.4) PRINT 240
10100 FORMAT(////' SEARCH OUTPUT TABLE ',I4, PRINT 245
1 ' .. FINAL VALUE OF PARAMETERS, BOUNDS, AND INCREMENTS'//T9,'LP', PRINT 250
1 T25,'P',T45,'PH',T65,'PL',T85,'DP') PRINT 255
10200 FORMAT(I10,4E20.5) PRINT 260
10300 FORMAT(////' SEARCH OUTPUT TABLE',I4, PRINT 265
1 ' .. EXPERIMENTAL DATA AND THEORETICAL PFX') PRINT 270
10400 FORMAT(/5X' TABLE AT TIME =',E10.4//T9,'IX', T25,'IX',T45,'YI', PRINT 275
1 T65,'YI',T85,'DTX') PRINT 280
10500 FORMAT(/5X' AVERAGE POINT RESIDUAL =',E12.4) PRINT 285
END PRINT 290
SUBROUTINE STBS(ITH) STBS 0
C STBS 5
C STBS 10
C FUNCTION OF SUBROUTINE--TO STORE NORMALIZED EXPERIMENTAL STBS 15
C AND THEORETICAL PROFILES AS OBTAINED FOR THE EXPERIMENTAL STBS 20

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C SPACE GRID SO THAT SUCH QUANTITIES MAY BE PLOTTED. STRS 25
C STRS 30
C STRS 35
  IMPLICIT REAL*8 (A-H,O-Z) STRS 40
  REAL*4 PHAT STRS 45
  COMMON/PROBID/TITLE(8),NPROB STRS 50
  COMMON/CTRL/KPGM,KUTR,KVI,KSTRM,KSTRU,ISTOP,KSS,KDIC,KROUT, KROUT, STRS 55
1 KTSIP,KSOOT,KSDCH,KBOFF,KANL,KIC,KSTRS STRS 60
  COMMON/GEOM/X(101),BB(2),DCOSB(2),DCOS(2),DELTA,CHNG,DELHAY,THAY, STRS 65
1 IPX(101),IX(100,3),NPH(2),NPST(2),NPTST(2),NBE(2),NTSE(2), ISB(2, STRS 70
1 2),IS(2,2),NBP,NEL,NBAT,IBAND,NBC,NST,NYST,NBEL,NTI,NBOR STRS 75
  COMMON/NEVAR/ A(101,2),B(101,3),R(101),R2(101),RI(101),RB(101), STRS 80
1 DP(101),B1(101),BT(101),ITMP(101),BPLX(101),BPLIP(101), FX(100,2) STRS 85
1 ,PRATE(10),FLOW(10),TFLOW(10),W,PHAT(3,5) STRS 90
  COMMON/XIV/XYL(5),XYU(5),XYI(5),WTX,WTY STRS 95
  COMMON/XRV/XX(100,5),XXI(100,5),YI(100,5),DYI(100,5), YT(100),TX(5) STRS 100
1 ,XUTL(5),XUTU(5) STRS 105
  IF (ITL.GT.1) GO TO 10 STRS 110
  PUNCH 10000, (TITLE(I),I=1,8) STRS 115
  PUNCH 10100, WTX STRS 120
  IF (KPGM.EQ.2) NBP=0 STRS 125
  PUNCH 10100, (WTX(I),I=1,WTX),NBP STRS 130
10 PUNCH 10200,TX(ITB) STRS 135
  XI=WTX(ITB) STRS 140
  PUNCH 10200, (XI(IX,ITB),IX=1,XX) STRS 145
  PUNCH 10200, (YT(IX),IX=1,XI) STRS 150
  PUNCH 10200, (YI(IX,ITB),IX=1,XX) STRS 155
  PUNCH 10200, (DYI(IX,ITB),IX=1,XX) STRS 160
  IF (KPGM.EQ.2) PUNCH 10200, (X(NP),NP=1,NBP) STRS 165
  IF (KPGM.EQ.2) PUNCH 10200, (BB(NP),NP=1,NBP) STRS 170
  RETURN STRS 175
10000 FORMAT(8A8) STRS 180
10100 FORMAT(16I5) STRS 185
10200 FORMAT(8E10.4) STRS 190
  END STRS 195
  SUBROUTINE NEVAL(P,CHIS) NEVA 0
C NEVA 5
C FUNCTION OF SUBROUTINE--TO EVALUATE CHI-SQUARED FOR THE NEVA 10
C MATERIAL-TRANSPORT CASE. NEVA 15
C NEVA 20
C NEVA 25
C NEVA 30
  IMPLICIT REAL*8 (A-H,O-Z) NEVA 35
  REAL*4 PHAT NEVA 40
  COMMON/CTRL/KPGM,KUTR,KVI,KSTRM,KSTRU,ISTOP,KSS,KDIC,KROUT, KROUT, NEVA 45
1 KTSIP,KSOOT,KSDCH,KBOFF,KANL,KIC,KSTRS NEVA 50
  COMMON/CEVAR/TIME,TN(100,2),THN(100,2),TNN(100,2),DTN(100,2), NEVA 55
1 VIX(100,2),VIXP(100,2),VEN(100,2) NEVA 60
  COMMON/GEOM/X(101),BB(2),DCOSB(2),DCOS(2),DELTA,CHNG,DELHAY,THAY, NEVA 65
1 IPX(101),IX(100,3),NPH(2),NPST(2),NPTST(2),NBE(2),NTSE(2), ISB(2, NEVA 70
1 2),IS(2,2),NBP,NEL,NBAT,IBAND,NBC,NST,NYST,NBEL,NTI,NBOR NEVA 75
  COMMON/NEVAR/ A(101,2),B(101,3),R(101),RP(101),RI(101),RB(101), NEVA 80
1 DP(101),B1(101),BT(101),ITMP(101),BPLX(101),BPLIP(101), FX(100,2) NEVA 85
1 ,PRATE(10),FLOW(10),TFLOW(10),W,PHAT(3,5) NEVA 90
  COMMON/XIV/XYL(5),XYU(5),XYI(5),WTX,WTY NEVA 95
  COMMON/XRV/XX(100,5),XXI(100,5),YI(100,5),DYI(100,5), YT(100),TX(5) NEVA 100
1 ,XUTL(5),XUTU(5) NEVA 105
  COMMON/SRP/ DELTO,CHISO,ACC,BED,TOLSTP,TOLPUN,P0(20), PH(20), NEVA 110
1 PL(20),DELP(20),PBO(20),PBD(20) NEVA 115
  DIMENSION P(1) NEVA 120
  DATA IND1/0/ NEVA 125
C NEVA 130
C CORRELATE SEARCH PARAMETERS WITH PHYSICAL PARAMETERS. NEVA 135
C NEVA 140
  CALL BUFRN(P) NEVA 145
  CHIS=0. NEVA 150
C NEVA 155
C TIME SEQUENCE CALCULATION. NEVA 160
C NEVA 165
  TIME=0. NEVA 170
  CALL HIBL NEVA 175
  IF (KPGM.LE.3) CALL PRINTN(0) NEVA 180
  DELT=DELTO NEVA 185
  TIME=DELTO NEVA 190
  ITN=1 NEVA 195

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      ITX=1
10  IF (TIME-GE. TX(ITX)) GO TO 20
C
C  GENERATE RESULTS FOR INTERMEDIATE STEPS.
C
      CALL MTRAN
      IF (KPGH.LE.3) CALL PRINTB(ITH)
      DELT=DELT*(1.+CHNG)
      DELT=DMIN1(DELT,DELMAX)
      TIME=TIME+DELT
      ITH=ITH+1
      GO TO 10
C
C  CALCULATE CONCENTRATION 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 (KPGH.LE.3) CALL PRINTB(ITH)
      NX=NYX(ITX)
      IXMIN=1
      SUM=0.
      NXL=NYXL(ITX)
      NIU=NYIU(ITX)
      DO 30 IX=1,NX
          YT(IX)=YLAG(IX(IX,ITH),X,IB,IND1,2,IXMIN,NX,IX)
          IF (IX.LT.NXL) GO TO 30
          IF (IX.GT.NIU) 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+WI(IX,ITX)*(YT(IX)-YI(IX,ITH))**2
40  CONTINUE
      CHISO=CHIS
      IF (KPGH.GT.3) GO TO 50
      CALL PRINTS(ITX)
      IF (KSTRS.EQ.1) CALL STAS(ITX)
50  IF (ITX-GE.NTX) GO TO 60
      ITX=ITX+1
      DELT=DELTP
      TIME=TIME+DELT
      ITH=ITH+1
      GO TO 10
60  RETURN
      END
      SUBROUTINE BUEVAL(P,CHIS)
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
      IMPLICIT REAL*8 (A-H,O-Z)
      REAL*4 PHAT
      COMMON/CTRL/KPGH,KUTR,KVI,KSTRH,KSTHV,ISTOP,KSS,KDIG,KHOUT, KHOUT,
1  KSTP,KSOUP,KSCCH,KBUFP,KANL,KIC,KSTRS
      COMMON/CRVAR/TIME,TH(100,2),TTH(100,2),TTH(100,2),DTH(100,2),
1  VX(100,2),VXP(100,2),VXV(100,2)
      COMMON/GEOM/X(101),BB(2),DCOSB(2),DELT,CHNG,DELMAX,TMAX,
1  IPX(101),IB(100,3),NPA(2),NPST(2),NPTST(2),NDB(2),NTSE(2),
1  ISB(2),IS(2,2),NUP,NEL,NHAP,IBAND,NBC,NST,NTST,NDEL,NTI,NHOR
      COMMON/NPROP/PRQP(1,5),FXI
      COMMON/SEVAR/ A(101,2),B(101,3),R(101),RP(101),RI(101),RB(101),
1  DP(101),R1(101),RT(101),XTNP(101),BFLX(101),BFLXP(101), FX(100,2)

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NEVA 200
 NEVA 205
 NEVA 210
 NEVA 215
 NEVA 220
 NEVA 225
 NEVA 230
 NEVA 235
 NEVA 240
 NEVA 245
 NEVA 250
 NEVA 255
 NEVA 260
 NEVA 265
 NEVA 270
 NEVA 275
 NEVA 280
 NEVA 285
 NEVA 290
 NEVA 295
 NEVA 300
 NEVA 305
 NEVA 310
 NEVA 315
 NEVA 320
 NEVA 325
 NEVA 330
 NEVA 335
 NEVA 340
 NEVA 345
 NEVA 350
 NEVA 355
 NEVA 360
 NEVA 365
 NEVA 370
 NEVA 375
 NEVA 380
 NEVA 385
 NEVA 390
 NEVA 395
 NEVA 400
 NEVA 405
 NEVA 410
 NEVA 415
 NEVA 420
 NEVA 425
 NEVA 430
 NEVA 435
 NEVA 440
 NEVA 445
 NEVA 450
 NEVA 455
 NEVA 460
 NEVA 465
 NEVA 470
 NEUV 0
 NEUV 5
 NEUV 10
 NEUV 15
 NEUV 20
 NEUV 25
 NEUV 30
 NEUV 35
 NEUV 40
 NEUV 45
 NEUV 50
 NEUV 55
 NEUV 60
 NEUV 65
 NEUV 70
 NEUV 75
 NEUV 80
 NEUV 85
 NEUV 90
 NEUV 95

1	PRATE(10),FLOW(10),TFLOW(10),W,PRAT(3,5)	882V	100
	COMMON/CH1/ W1,V1	882V	105
	COMMON/XIV/XYXL(5),XYXU(5),XYX(5),WTK,WXT	882V	110
	COMMON/XRV/IX(100,5),WX(100,5),IX(100,5),DYX(100,5),YT(100),TX(5)	882V	115
1	XUTL(5),XUTU(5)	882V	120
	COMMON/SRP/ DELTO,CHISO,ACC,RED,TOLSTP,TOLPUW,P0(20), PH(20),	882V	125
1	PL(20),DELP(20),PLO(20),PHO(20)	882V	130
	DIMENSION P(1)	882V	135
	DATA INU:0/	882V	140
C		882V	145
C	CORRELATE SEARCH PARAMETERS WITH PHYSICAL PARAMETERS.	882V	150
C		882V	155
	CALL BUPPH(P)	882V	160
	CHIS=0.	882V	165
C		882V	170
C	TIME SEQUENCE CALCULATION.	882V	175
C		882V	180
	TIME=0.	882V	185
	CALL HINL	882V	190
	IF (KPGH.LL.3) CALL PRINTH(0)	882V	195
	DELT=DELTO	882V	200
	TIME=DELTO	882V	205
	ITN=1	882V	210
	ITX=1	882V	215
10	V1P=V1	882V	220
	IF (TIME.GT.TX(ITX)) GO TO 40	882V	225
	IF (TIME.GT.TMAX) GO TO 80	882V	230
C		882V	235
C	GENERATE RESULTS FOR INTERMEDIATE STEPS.	882V	240
C		882V	245
	CALL NTRAN	882V	250
	IF (KPGH.LL.3) CALL PRINTH(ITN)	882V	255
	IF (ITSTP.NE.0) GO TO 20	882V	260
	DELT=DELT*(1.+CHNG)	882V	265
	GO TO 30	882V	270
20	IF (ITN.EQ.1) TCON=DELT*V1**(.1+CHNG)	882V	275
	DELT=TCON/V1**(.1+CHNG)	882V	280
30	DELT=DMIN1(DELT,DELMAX)	882V	285
	TIME=TIME+DELT	882V	290
	ITN=ITN+1	882V	295
	GO TO 10	882V	300
C		882V	305
C	CALCULATE CONCENTRATION PROFILE AT TIME STEP FOR WHICH EXPERIMENTAL	882V	310
C	DATA IS GIVEN.	882V	315
C		882V	320
40	DELT=DELT	882V	325
	DELT=DELT-(TIME-TX(ITX))	882V	330
	TIME=TX(ITX)	882V	335
	CALL NTRAN	882V	340
	IF (KPGH.LL.3) CALL PRINTH(ITN)	882V	345
	W=XYX(ITX)	882V	350
	IXMIN=1	882V	355
	SUM=0.	882V	360
	WXL=XYXL(ITX)	882V	365
	W XU=XYXU(ITX)	882V	370
	DO 50 IX=1,WX	882V	375
	YT(IX)=YLAG(WX(IX,ITX),X,RS,IND1,2,IXMIN,W,IX)	882V	380
	IF (IX.LT.WXL) GO TO 50	882V	385
	IF (IX.GT.WXU) GO TO 50	882V	390
	SUM=SUM+YT(IX)	882V	395
50	CONTINUE	882V	400
C		882V	405
C	NORMALIZE THEORETICAL POINTS.	882V	410
C		882V	415
	AN=100./SUM	882V	420
	DO 60 IX=1,WX	882V	425
	YT(IX)=AN*YT(IX)	882V	430
C		882V	435
C	COLLECT CHI-SQUARE.	882V	440
C		882V	445
	CHIS=CHIS+W(X,ITN)*(YT(IX)-YX(IX,ITN))**2	882V	450
60	CONTINUE	882V	455
	CHISO=CHIS	882V	460
	IF (KPGH.GT.3) GO TO 70	882V	465
	CALL PRINTH(ITN)	882V	470

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      IF (KSTAS.EQ.1) CALL STNS(ITX)
70  IF (ITX.GE.NTX) GO TO 90
      ITX=ITX+1
      DELT=DELTP
      TIME=TIME+DELT
      ITH=ITH+1
      GO TO 10
80  PRINT 10000
90  RETURN
10000 FORMAT(////' MAXIMUM TIME EXCEEDED')
      END
      SUBROUTINE HVAL2(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*8 PHAT
      COMMON/CTEL/KPGH,KWTR,KVI,KSTRH,KSTRW,ISTOP,KSS,KDIG,KHOUT,KWOUT,
1  KSTP,KROUT,KSRCH,KBUFF,KARL,KIC,KSTES
      COMMON/CRVAR/TIME,TH(100,2),TWH(100,2),DTH(100,2),
1  VX(100,2),VXF(100,2),VXH(100,2)
      COMMON/GEOM/X(101),BB(2),DCOSB(2),DCOS(2),DELT,CHNG,DELRAX,THLX,
1  IPI(101),IR(100,3),RPH(2),RPS*(2),RPTST(2),RBE(2),RTSE(2),ISB(2),
1  2),IS(2,2),RHP,BEL,HHAT,ISAND,WBC,WST,WTST,HBEL,WTI,HHOR
      COMMON/RPROP/PROP(1,5),WII
      COMMON/HVAR/ A(101,2),B(101,3),R(101),RP(101),RI(101),RB(101),
1  DP(101),R1(101),RT(101),XTHP(101),BPLX(101),BPLIP(101),FX(100,2)
1  ,FRATE(10),FLOW(10),TFLOW(10),W,PHAT(3,5)
      COMMON/CH1/ W1,V1
      COMMON/XIV/HIX1(5),HIXU(5),HIX(5),WTX,WTY
      COMMON/XRV/YI(100,5),XI(100,5),YI(100,5),DYI(100,5),YT(100),TX(5)
1  ,XUTL(5),XUTU(5)
      COMMON/SRP/ DELT,CHISO,ACC,BED,TOLSTP,TOLFUN,P0(20),PH(20),
1  PL(20),DELP(20),PLO(20),PNO(20)
      DIMENSION P(1)
      DATA IND1/0/
C
C  CORRELATE SEARCH PARAMETERS WITH PHYSICAL PARAMETERS.
C
      CALL BUFRH(P)
      CALL BUFRH(P)
C
C  SET UP SOIL PROPERTIES.
C
      CALL PUCAL
      CALL H1UL
      CHIS=0.
C
C  TIME SEQUENCE CALCULATION.
C
      TIME=0.
      CALL H1UL
      IF (KPGH.LE.3) CALL PRINTH(0)
      DELT=DELTO
      TIME=DELTO
      ITH=1
      ITX=1
10  V1P=V1
      IF (TIME.GE.TX(ITX)) GO TO 40
      IF (TIME.GT.THAX) GO TO 80
C
C  GENERATE RESULTS FOR INTERMEDIATE STEPS.
C
      CALL HTRH
      IF (KPGH.LE.3) CALL PRINTH(ITH)
      IF (KSTP.NE.0) GO TO 20
      DELT=DELT*(1.+CHNG)
      GO TO 30

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20 IF (ITN.EQ.1) V1P=V1
   DELT=(1.+(1.+CHMS)*(V1P/V1-1.))*DELT
30 DELT=DMIN1(DELT,DELMAX)
   TIME=TIME+DELT
   ITN=ITN+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 STRAN
   IF (KPGH.LE.3) CALL PRINTN(ITN)
   NX=NYX(ITX)
   IXMIN=1
   SUM=0.
   NYL=NYXL(ITX)
   NYU=NYXU(ITX)
   DO 50 IX=1,NX
     YT(IX)=YLAG(NX(IX,ITX),X,IB,IND1,2,IXMIN,NX,IX)
     IF (IX.LT.NXL) GO TO 50
     IF (IX.GT.NXU) 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+NX(IX,ITX)*(YT(IX)-YX(IX,ITA))*2
60   CONTINUE
   CHIS0=CHIS
   IF (KPGH.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
   ITN=ITN+1
   GO TO 10
80 PRINT 10000
90 RETURN
10000 FORMAT(////' MAXIMUM TIME EXCEEDED')
END
SUBROUTINE BUFP4(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
C IMPLICIT REAL*8 (A-H,O-Z)
C DIMENSION P(1)
C COMMON/BIVAR/KPRO,KPR(1000),HAXIDIP,HAXEL,HAXIMP,HAXSAT,HAXBW,
1 HAXYTI,HXPPM
C COMMON/BI/ TM1,TM0,TM3,SINERS
C COMMON/PROP/PROP(1,5),XXI
C REAL*8 K',LAMBDA
C NTYP=1

C
C PROPERTIES ARE P(I), PROP(I) = KD, RHOB, AL,
C THETAB, AND POR.
C
C
DO 10 IP=1,HXPPM
  PROP(NTYP,IP)=P(I)
10 CONTINUE

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HXVA 320
 HXVA 325
 HXVA 330
 HXVA 335
 HXVA 340
 HXVA 345
 HXVA 350
 HXVA 355
 HXVA 360
 HXVA 365
 HXVA 370
 HXVA 375
 HXVA 380
 HXVA 385
 HXVA 390
 HXVA 395
 HXVA 400
 HXVA 405
 HXVA 410
 HXVA 415
 HXVA 420
 HXVA 425
 HXVA 430
 HXVA 435
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 HXVA 450
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 HXVA 460
 HXVA 465
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 HXVA 510
 HXVA 515
 HXVA 520
 HXVA 525
 HXVA 530
 HXVA 535
 HXVA 540
 HXVA 545
 HXVA 550
 HXVA 555
 HXVA 560
 HXVA 565
 HXVA 570
 BUFP 0
 BUFP 5
 BUFP 10
 BUFP 15
 BUFP 20
 BUFP 25
 BUFP 30
 BUFP 35
 BUFP 40
 BUFP 45
 BUFP 50
 BUFP 55
 BUFP 60
 BUFP 65
 BUFP 70
 BUFP 75
 BUFP 80
 BUFP 85
 BUFP 90
 BUFP 95
 BUFP 100
 BUFP 105
 BUFP 110
 BUFP 115


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C                                     SUPR 105
      NX=NYX(ITH)                                     SUPR 110
      CALL DSORT(XSUP2,IPATH,NTM)                     SUPR 115
C                                     SUPR 120
C ORDER WATER-CONTENT VALUES CORRESPONDINGLY.       SUPR 125
C                                     SUPR 130
      DO 10 ITH=1,NTM                                  SUPR 135
        JTM=IPATH(ITH)                                SUPR 140
        THTMP(JTM)=THT(ITH)                          SUPR 145
      10 CONTINUE                                     SUPR 150
C                                     SUPR 155
C INTERPOLATE ON THE EXPERIMENTAL POSITION GRID.       SUPR 160
C                                     SUPR 165
      SUM=0.                                           SUPR 170
      NXL=NYXL(ITH)                                   SUPR 175
      NYU=NYUO(ITH)                                   SUPR 180
      NXI=XSUP2(NTM)                                  SUPR 185
      THNM=THTMP(NTM)                                SUPR 190
      IXIM=1                                           SUPR 195
      DO 40 IX=1,NX                                    SUPR 200
        I=XX(IX,ITH)                                  SUPR 205
        IF (X.LT.IX) GO TO 20                          SUPR 210
        THT=THNM                                       SUPR 215
        GO TO 30                                       SUPR 220
      20 THT=TLAG(X,XSUP2,THTMP,IND1,NITP,IXIM,NTM,IEI) SUPR 225
      30 YT(IX)=THT-THO                                SUPR 230
        IF (IX.LT.NXL) GO TO 40                        SUPR 235
        IF (IX.GT.NXU) GO TO 40                        SUPR 240
        SUM=SUM+YT(IX)                                SUPR 245
      40 CONTINUE                                     SUPR 250
C                                     SUPR 255
C NORMALIZE THEORETICAL POINTS.                      SUPR 260
C                                     SUPR 265
      AN=100./SUM                                     SUPR 270
      DO 50 IX=1,NX                                    SUPR 275
      50 YT(IX)=AN*YT(IX)                             SUPR 280
      RETURN                                           SUPR 285
      END                                             SUPR 290
      SUBROUTINE BUFPN(P)                               BUFP  0
C                                     BUFP  5
C                                     BUFP 10
C FUNCTION OF SUBROUTINE—TO MAKE THE CORRESPONDENCE BUFP 15
C BETWEEN THE ARBITRARY PARAMETERS OF ARRAY P AND BUFP 20
C THE PHYSICAL WATER-TRANSPORT PARAMETERS. THIS ROUTINE BUFP 25
C MUST BE MODIFIED BY THE USER SO AS TO MATCH HIS BUFP 30
C SPECIFICATION OF THE PHYSICAL PARAMETERS IN SPROP. BUFP 35
C                                     BUFP 40
C                                     BUFP 45
      IMPLICIT REAL*8 (A-H,O-Z)                       BUFP 50
      DIMENSION P(1)                                  BUFP 55
      COMMON/CTRL/KPGM,KWTR,KWI,KSTRB,KSTRV,ISTOP,KSS,KDIG,KHOUT, KHOUT, BUFP 60
      1 KTSTP,KSOUP,KSDCH,KBUFP,KANL,KIC,KSTRS        BUFP 65
      COMMON/BIVAR/KPRO,KPR(1000),MAXDIP,MAXEL,MAXMP,MAXHAT,MAXBW, BUFP 70
      1 MAXTI,MBPPH                                     BUFP 75
      COMMON/BPROP/PROP(1,5),NXX                      BUFP 80
      COMMON/BI/ TH1,TMO,TNB,SINRPS                   BUFP 85
      COMMON/UPROP/AKPAR(50),CDPAR(50),AKSH(25),ALPK(25),D(25), ALPD(25) BUFP 90
      1 ,AKSAT,AKSH0,MEPAR,UKSP,UCDPAR,UDSP          BUFP 95
      IPP=0                                             BUFP 100
C                                     BUFP 105
C IF KBUFP IS NON-ZERO, THEN THE WATER-TRANSPORT PARAMETERS FOLLOW THE BUFP 110
C MBPPH MATERIAL-TRANSPORT QUANTITIES.              BUFP 115
C                                     BUFP 120
      IF (KBUFP.NE.0) IPP=MBPPH                      BUFP 125
      DO 10 IP=1,3                                     BUFP 130
        IPP=IPP+1                                     BUFP 135
        AKPAR(IP)=P(IP)                              BUFP 140
        IP3=IPP+3                                     BUFP 145
        CDPAR(IP)=P(IP3)                             BUFP 150
      10 CONTINUE                                     BUFP 155
      IF (KBUFP.NE.0) GO TO 20                        BUFP 160
      IP=IP3+1                                         BUFP 165
      TH0=P(IP)                                       BUFP 170
      IP=IP+1                                         BUFP 175
      TH1=P(IP)                                       BUFP 180

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      RETURN
20  NTYP=1
      THO=PROP(NTYP,4)
      TH1=PROP(NTYP,5)
      RETURN
      END
      DOUBLE PRECISION FUNCTION YLAG(XI,X,Y,IND1,M1,IMIN,IMAX,IEX)
C  PROGRAM AUTHORS  A. A. BROOKS AND E.C. LECG.
C  COMPUTING TECHNOLOGY CENTER, UNION CARBIDE CORP., NUCLEAR DIV.,
C  OAK RIDGE, TENN.
C
C      LAGRANGIAN INTERPOLATION
C      XI IS INTERPOLATED ENTRY INTO X-ARRAY
C      M IS THE ORDER OF LAGRANGIAN 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
C      DIMENSION X(1),Y(1)
C      DOUBLE PRECISION P,D,S,XD,XI,X,Y,YLAG
C      IND=IND1
C      M=M1
C      IEX=0
C      IF (M.LE.IMAX) GO TO 10
C      M=IMAX
C      IEX=M
10  IF (IND.GT.0) GO TO 40
C      DO 20 J = IMIN,IMAX
C          IF (XI-X(J)) 30,130,20
20  CONTINUE
C      IEX=1
C      GO TO 70
30  IND=J
C      IMIN = J
40  IF (IND.GT.1) GO TO 50
C      IEX=-1
50  INL=IND-(M+1)/2
C      IF (INL.GT.0) GO TO 60
C      INL=1
60  INU=INL+M-1
C      IF (INU.LE.IMAX) GO TO 80
70  INL=IMAX-M+1
C      INU=IMAX
80  S=0.
C      P=1.
C      DO 110 J=INL,INU
C          P=P*(XI-X(J))
C          D=1.
C          DO 100 I=INL,INU
C              IF (I.NE.J) GO TO 90
C              XD=XI
C              GO TO 100
90          XD=X(J)
100         D=D*(XD-X(I))
110         S=S+Y(J)/D
C      YLAG=S*P
120 RETURN
130 YLAG=Y(J)
C      IMIN = J+1
C      GO TO 120
C      END
C      SUBROUTINE SEARCH(M,P,PB,PH,PL,ACC,RED,ROLSTP,TOLPUN,DELP,KPMS,
C      1 EVAL,NIPUN,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 BRISMAN AND WOOD (1966) IS USED.
C
C  PROGRAM AUTHOR G. M. WESLEY
C  COMPUTING TECHNOLOGY CENTER, UNION CARBIDE CORP., NUCLEAR DIV.,

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      BOFF 185
      BOFF 190
      BOFF 195
      BOFF 200
      BOFF 205
      BOFF 210
      YLAG 0
      YLAG 5
      YLAG 10
      YLAG 15
      YLAG 20
      YLAG 25
      YLAG 30
      YLAG 35
      YLAG 40
      YLAG 45
      YLAG 50
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      YLAG 255
      YLAG 260
      YLAG 265
      YLAG 270
      YLAG 275
      YLAG 280
      YLAG 285
      YLAG 290
      SEAR 0
      SEAR 5
      SEAR 10
      SEAR 15
      SEAR 20
      SEAR 25
      SEAR 30
      SEAR 35
      SEAR 40
      SEAR 45

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C	OAK RIDGE, TENN.	SEAR	50
C		SEAR	55
C		SEAR	60
	REAL*8 P(1), PL(1), P3(1), DELP(1), BP(20), ACC, MED, TOLSTP, TOLFUN, FB,	SEAR	65
	1 PP, FBP, STOR, TEMP, PAT, KVAL	SEAR	70
	INTEGER*4 NVS(20)	SEAR	75
	IF (KPRS.GT.0) PRINT 10600, BP, NXPUN, ACC, MED, TOLSTP, TOLFUN,	SEAR	80
	1 (PH(1), P(1), PL(1), I=1, NP)	SEAR	85
	ICONV = 0	SEAR	90
	IEIP=0	SEAR	95
	DO 10 I=1, NP	SEAR	100
	IF (P(I).GT.PH(I)) P(I) = PH(I)	SEAR	105
	IF (P(I).LT.PL(I)) P(I) = PL(I)	SEAR	110
	IF (PH(I).EQ.PL(I)) DELP(I) = 0.00	SEAR	115
10	BP(I)=P(I)	SEAR	120
	NFUN=1	SEAR	125
	CALL EVAL(P, FB)	SEAR	130
	FP=FB	SEAR	135
	FBP=FB	SEAR	140
20	NBPAL=0	SEAR	145
	IF (NFUN.GE.NXPUN) GO TO 220	SEAR	150
	IF (KPRS.GT.0) PRINT 11000, NFUN	SEAR	155
	IF (KPRS.GT.0) PRINT 10700, FBP, (BP(I), I=1, NP)	SEAR	160
	IF (KPRS.GT.0) PRINT 11700, (DELP(I), I=1, NP)	SEAR	165
C		SEAR	170
C	START THE EXPLORATORY LOOP. IF IEIP = 1, THEN IT FOLLOWS A	SEAR	175
C	PATTERN MOVE. IF IT IS 0, THEN IT FOLLOWS A BASE POINT.	SEAR	180
C		SEAR	185
	IF (KPRS.GT.1) PRINT 10000	SEAR	190
	DO 120 I=1, NP	SEAR	195
	NVS(I) = 0	SEAR	200
	IF (DELP(I).EQ.0.000) GO TO 110	SEAR	205
	STOR = P(I)	SEAR	210
C		SEAR	215
C	INCREMENT THE I-TH VARIABLE BY ITS CURRENT STEP AND CHECK FOR	SEAR	220
C	ANY RANGE LIMITATIONS. CHECK THE FUNCTION VALUE AT THIS	SEAR	225
C	NEW POINT AGAINST FP FOR IMPROVEMENT.	SEAR	230
C		SEAR	235
	P(I)=P(I) + DELP(I)	SEAR	240
	IF (P(I).GT.PH(I).OR.P(I).LT.PL(I)) GO TO 40	SEAR	245
	IF (KPRS.GT.1) PRINT 10100	SEAR	250
	NFUN=NFUN + 1	SEAR	255
	CALL EVAL(P, FB)	SEAR	260
	IF (KPRS.GT.1) PRINT 10800, I, FB, (P(J), J=1, NP)	SEAR	265
	IF (FB.GE.FP-TOLFUN*DABS(FP)) GO TO 40	SEAR	270
	IF (IEIP.NE.0) GO TO 30	SEAR	275
	IF (KPRS.GT.1) PRINT 10200	SEAR	280
	DELP(I)=DELP(I)*ACC	SEAR	285
30	FP=FB	SEAR	290
	GO TO 120	SEAR	295
40	P(I) = STOR - DELP(I)	SEAR	300
C		SEAR	305
C	DECREMENT THE I-TH VARIABLE AFTER A FAILURE OF THE INCREMENT	SEAR	310
C	PROCEDURE TO GIVE ANY IMPROVEMENT. PROCEED AS ABOVE.	SEAR	315
C		SEAR	320
	IF (P(I).GT.PH(I).OR.P(I).LT.PL(I)) GO TO 60	SEAR	325
	IF (KPRS.GT.1) PRINT 10300	SEAR	330
	NFUN=NFUN + 1	SEAR	335
	CALL EVAL(P, FB)	SEAR	340
	IF (KPRS.GT.1) PRINT 10900, I, FB, (P(J), J=1, NP)	SEAR	345
	IF (FB.GE.FP-TOLFUN*DABS(FP)) GO TO 60	SEAR	350
	IF (IEIP.NE.0) GO TO 50	SEAR	355
	IF (KPRS.GT.1) PRINT 10300	SEAR	360
	DELP(I) = DELP(I) * ACC	SEAR	365
50	NVS(I) = 1	SEAR	370
C		SEAR	375
C	THE REVERSE STEP YIELDED AN IMPROVEMENT, SO TRY THIS DIRECTION	SEAR	380
C	FIRST ON THE NEXT PASS.	SEAR	385
C		SEAR	390
	GO TO 30	SEAR	395
60	P(I) = STOR	SEAR	400
	IF (IEIP.EQ.1) GO TO 120	SEAR	405
C		SEAR	410
C	VARIABLE INCREMENTING AND DECREMENTING FAILED TO YIELD ANY IM-	SEAR	415
C	PROVEMENT. REDUCE THE STEP SIZE AND TEST AGAINST	SEAR	420

```

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.DO-TEMP) 70,80,100
70  DELP(I)=DELP(I)*TEMP
80  TEMP=1.D-10/DABS(DELP(I))
    IF (1.DO-GE-TEMP) GO TO 110
90  DELP(I)=DELP(I)*TEMP
    GO TO 110
100 TEMP=1.D-10/DABS(DELP(I))
    IF (1.DO-TEMP) 90,110,120
110 HNPAL=HNPAL + 1
120 CONTINUE
    IF ((FBP-PP).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, HNPAL
    DO 130 I=1,NP
    IF (RVS(I).EQ.0) GO TO 130
    DELP(I) = -DELP(I)
130 CONTINUE
    FBP=PP
    DO 140 I=1,NP
    PAT=BP(I)
    BP(I)=P(I)
    P(I) = 2.DO * BP(I) - PAT
    P(I)=DMAX1(P(I),PL(I))
140 P(I)=DMIN1(P(I),PH(I))
    HNPAL=HNPAL + 1
    CALL EVAL(P,PP)
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 PP.
C
    IF (KPRS.GT.2) PRINT 11300, PP,(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 (HNPAL.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
    PP = FBP
    DO 180 I=1,NP
180 P(I) = BP(I)
    IF (KPRS.GT.2) PRINT 11600
    GO TO 20
190 IF (PP.LE.FBP) GO TO 210
C
C THE PROGRAM ASSUMES THAT IF HAS FOUND A LOCAL MINIMUM SINCE
C EACH VARIABLE HAS REACHED ITS MINIMUM STEP SIZE.
C
    PP=FBP
    DO 200 I=1,NP
200 P(I)=BP(I)
210 IF (KPRS.GT.0) PRINT 11400, PP,(P(I),I=1,NP)
    FB = PP
    IF (KPRS.GT.0) PRINT 11000, HNPAL

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SEAR 790
SEAR 795

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      GO TO 240
220  ICONV = 1
      IF (KPRS.GT.0) PRINT 11400, NFUN
      IF (KPRS.GT.C) 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 HAS 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 ,13,5X,K4, 13X,F7.4,4X, F7.4,4X,D10.3,3X, D10.3/
1 11X, 'PB', 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', 12,D15.7,2X,7D15.7/ (' ' ,18X,7D15.7))
10900 FORMAT(' R', 12,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(' DEL-',16X,7D15.7/(1H ,19X,7D15.7))
      END
      SUBROUTINE GAUSS(A,P,RGAUSS,Y,H)
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),Z2(63),NF(15)
      DIMENSION WT1(33),WT2(30),Z1(33),Z22(30)
      EQUIVALENCE (WT(1),WT1(1)),(WT(34),WT2(1))
      EQUIVALENCE (Z2(1),Z1(1)),(Z2(34),Z22(1))
C
C   H SHOULD BE IN (2,16) EXCEPT H=15.
C   Y(Z) IS FUNCTION SUBROUTINE FOR THE INTEGRAND.
C
C   GAUSS-LEGENDRE ABSCISSAS.
C
      DATA Z1 / .57735026918963D+00, .77459666924148D+00,
1 .00000000000000D+00, .86113631159405D+00, .33998104358486D+00,
1 .90617984593866D+00, .5384693110568D+00, .00000000000000D+00,
1 .93246951420315D+00, .66120938646626D+00, .23861918608320D+00,
1 .94910791234276D+00, .74153118559939D+00, .40584515137740D+00,
1 .00000000000000D+00, .86028985649754D+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, .83339539412925D+00, .14887433898163D+00,
1 .97822865814606D+00, .88706259976810D+00, .73015200557405D+00,
1 .51909612920681D+00/
      DATA Z2 / .26954315595234D+00, .00000000000000D+00,
1 .98154063424672D+00, .00411725637047D+00, .76990267119430D+00,
1 .58731795428662D+00, .26723149899818D+00, .12523340851147D+00,
1 .98418305471859D+00, .01759839922298D+00, .80157809073331D+00,
1 .64234933944034D+00, .04849275103645D+00, .2304583.595513D+00,
1 .00000000000000D+00, .8628380069681D+00, .92843488366357D+00,
1 .82720131506976D+00, .68729290481168D+00, .51524863635815D+00,
1 .31911236892789D+00, .10805494870734D+00, .98940093499165D+00,

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1 - .74457502307323D+00, -.06563120238783D+00, -.755+0+40835500D+00, GAUS 190
1 - .61787624440264D+00, -.45801677765723D+00, -.28160355077326D+00, GAUS 195
1 - .75012509037637D-01, GAUS 200
C GAUSS-LEGENDRE WEIGHTS. GAUS 205
C GAUS 210
C GAUS 215
DATA WT1 / -.10000000000000D+01, -.5555555555556D+00, GAUS 220
1 - .88888888888889D+00, -.34785484513745D+00, -.65214515486255D+00, GAUS 225
1 - .23692688505619D+00, -.47862867049937D+00, -.5688888888889D+00, GAUS 230
1 - .17132449237917D+00, -.36076157304814D+00, -.46791393457269D+00, GAUS 235
1 - .12948496616887D+00, -.27970539148728D+00, -.38183005050512D+00, GAUS 240
1 - .41795918367347D+00, -.10122853629038D+00, -.22238103445337D+00, GAUS 245
1 - .31370664587789D+00, -.36268378337836D+00, -.81274338361574D-01, GAUS 250
1 - .18064816069486D+00, -.26061069640294D+00, -.31234707704000D+00, GAUS 255
1 - .33023935500126D+00, -.66671344308688D-01, -.14945134915058D+00, GAUS 260
1 - .21508636251598D+00, -.26926671931000D+00, -.29552422471475D+00, GAUS 265
1 - .55668567116174D-01, -.12558036946490D+00, -.18629021092773D+00, GAUS 270
1 - .23319376459199D+00, GAUS 275
DATA WT2 / -.26280454451025D+00, -.27292508677790D+00, GAUS 280
1 - .47175336386512D-01, -.10693932599532D+00, -.16007832854335D+00, GAUS 285
1 - .20316742672307D+00, -.23349253453835D+00, -.24914704581340D+00, GAUS 290
1 - .40484004765316D-01, -.92121499837728D-01, -.13887351021979D+00, GAUS 295
1 - .17814598076194D+00, -.20781604753689D+00, -.22628318026290D+00, GAUS 300
1 - .23255155323087D+00, -.35119460331752D-01, -.80158087159760D-01, GAUS 305
1 - .12151857068790D+00, -.15720316715819D+00, -.18553839747794D+00, GAUS 310
1 - .20519846372130D+00, -.21526385346316D+00, -.27152459411754D-01, GAUS 315
1 - .62253523938648D-01, -.95158511682493D-01, -.12462837125553D+00, GAUS 320
1 - .14959598881658D+00, -.16915651939500D+00, -.18260341504492D+00, GAUS 325
1 - .18945061045507D+00, GAUS 330
C GAUS 335
C GAUS 340
C GAUS 345
DATA BPT/ 0, 1, 3, 5, 8, 11, 15, 19, 24, 29, 35, 41, 48, 55, 55 / GAUS 350
AB=(B-A)*.5 GAUS 355
ABH=(B+A)*.5 GAUS 360
NP=N GAUS 365
BPT0=BPT(NP-1) GAUS 370
G=0. GAUS 375
J=1 GAUS 380
10 NP=J GAUS 385
D=AB GAUS 390
IF (NP+NP-LE.NP) GO TO 20 GAUS 395
NP=NP-NP+1 GAUS 400
D=-D GAUS 405
20 NP=BPT0+NP GAUS 410
W=WT(NP)*AB GAUS 415
Z=ZZ(NP)*D+ABH GAUS 420
30 G=Y(Z)*W+G GAUS 425
J=J+1 GAUS 430
IF (J.LE.NP) GO TO 10 GAUS 435
BGAUSS=G GAUS 440
RETURN GAUS 445
END GAUS 450

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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(1)	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 + NEUC if either of the latter is nonzero.
NMAT	Number of different types of soils comprising system.
NCM	Number of correction materials.
NIT	Number of time increments.
NBC	Number of Dirichlet boundary conditions.
NSI	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.
KISTP	Time-step control. Via this parameter the time step is varied either exponentially, KISTP = 0, or as a power law of the end-point Darcy velocity V_L , KISTP $\neq$ 0.
NELL	Number of elements for which $x < X_0$.
NEUC	Number of elements for which $x > X_0$.

- NNOR** Time integration parameter. If $NNOR = 1$, then integration proceeds as described in Chapter IV, Section 5. Otherwise Norsett integration $O(\Delta t^{**}(NNOR+1))$ is used. Acceptable values are $NNOR = 1, 2, 3$, and 5 .
- KIC** Initial-condition control. If $KIC \neq 0$, 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 .
- XMN** Variable-mesh parameter. Length of chromatographic column ... L .
- DXLI** Variable-mesh parameter. X-increment immediately below point $X0$... L .
- DXUI** Variable-mesh parameter. X-increment immediately above point $X0$... L .
- VX1** Space- and time-independent Darcy velocity ... L/T .
4. **KPRO** Printer control for steady-state and initial conditions. If $KPRO = 0$, there is no output. If $KPRO = 1$, only integrated flow variables pertaining to the material balance are printed. If $KPRO = 2$, then both bulk and fluid concentrations are output. If $KPRO = 3$, material fluxes and those variables mentioned previously are printed. Finally, if $KPRO \geq 4$, then water contents and Darcy velocities are also output.
- KPR(I,M)** Printer control similar to **KPRO** 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, $PROP(I,1) = k$, $PROP(I,2) = \rho$, $PROP(I,3) = a_1$, $PROP(I,4) = \theta$, 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. **MLMK** Element numbers.
- MTYP** Material-type index.
10. **NJ** Nodal number.
- R(NJ)** Fluid or bulk concentration c or $c_s \dots M \cdot L^{**3}$.
11. See definitions for item 10.
12. **NI** Nodal number.
- BBI** Fluid concentration of boundary node NI $\dots M \cdot L^{**3}$.
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 $\dots M \cdot L^{**2} \cdot T$.
14. **VX(MI,IQ)** Darcy velocity at node IQ of element MI $\dots L \cdot T$.
15. **TH(MI,IQ)** Water content at node IQ of element MI $\dots L^{**3} \cdot L^{**3}$.
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 $t(W_i)$ is obtained. If $KWTR = 1$, then, additionally, the first-order calculations for $x^{(1)}$ and $V^{(1)}$ are determined.
- NTTAB** Number of evaluations of the tabular function $t(W_i)$.

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) , $i \leq NTH$. 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 $\alpha(NTH-1) = 1 - DALPI$, 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).
DALPI	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_e 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^* 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 ≥ 2 experimental errors are input. For KWT = 3, the statistical weights obtained from the experimental errors are set to zero for all $XX < XWL$.
- NIX 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.
- KSIRS Control parameter for storage of optimized profiles on auxiliary storage (tape or disk). If KSIRS = 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. $\Delta p(\text{new}) = \text{ACC} * \Delta p(\text{old})$. ACC = 1.2 is typical ... (dimensionless).
- RED Reduction parameter for the step size, i.e. $\Delta p(\text{new}) = \text{RED} * \Delta p(\text{old})$. RED = 0.1 is typical ... (dimensionless).
- TOLSTP Step-size tolerance. Generally, the search is terminated whenever $|\Delta p_i| < \text{TOLSTP}$ for all parameters i . TOLSTP = 0.001 is typical ... (dimensionless).
- TOLFUN Tolerance in the function X . Generally, the search is terminated whenever the $|\Delta X| < \text{TOLFUN}$. TOLFUN = 0.001 is typical ... (dimensionless).
- RDP Step-size parameter. Initially the search step sizes are taken to be $\Delta p_i = \text{RDP} * p_i$ 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_a , ρ , a_1 , θ_1 , and n , in that order, for $IP = 1(1)5$.^{*} If $KPGM = 5$, then **P** contains only the water-transport variables K , h , d , β' , h' , d' , $\theta_1 = \theta$, and $\theta_1 = \theta$, 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_a , ρ , a_1 , θ_1 , and n for $IP = 1(1)5$ and quantities k , h , d , β' , h' , 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**.

^{*}For example,

^{*}The notation $IP = 1(1)5$ means that $IP = 1, 2, \dots, 5$.

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 $n = \text{PROP}(1,5)$ 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

$$\text{DELT} = \text{DELT} * (1 + \text{CHNG}), \text{KTSTP} = 0$$

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

$$\text{DELT} \sim 1. \text{VI}^{**}(1 + \text{CHNG}), \text{KTSTP} \neq 0$$

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 $x = X_0$. Here integers NELL and NELU (above) and real quantities X_0 , X_{MX} , $DXL1$, and $DXU1$ (card-set 3) are operative. Their meanings are apparent from the figure below.

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Note on initial conditions. If $KIC = 0$, then $R = c$, the fluid concentration, in card-set 9. If, however, $KIC \neq 0$, then $R = c_s$, the bulk concentration in card-set 9.

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

List: DELT,CHNG,DELMAX,TMAX,W,X0,XX,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 [$O(\Delta t^2)$, at most] and the intermediate time $t_i = t + \omega \Delta t$ for which time-dependent coefficients are evaluated. If, however, $NNOR > 1$, then Norsett integration [Norsett, 1974] is used, which is accurate to $O(\Delta t^{2(NNOR+1)})$. 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: 8011

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: 15,5X,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: $M1, (IE(M1, I), I=1,3), MODL$

Format: 1615

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 $M1$ 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: $M1, MTYP, MK$

Format: 1615

However, in those cases where numbers of the affected elements range from a lower limit $M1$ 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 $KMESH \neq 2$. In the most general case there is one card per node, a total of NNP cards.

List: $NJ, R(NJ)$

Format: 15,5X,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: $N1, BBI$

Format: 15,5X,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: $NLEI$

Format: $15,5X,F10.0$

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,NORDERI,NIIP,
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_1 is not necessarily equal to θ'_1 . If, on the other hand, KANL $\neq$ 0, then array AKPAR contains the parameters K_s , 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 DALPI (below). The resulting mesh will begin $\alpha_{NTH} = 1$, $\alpha_{NTH-1} = 1 - DALPI$. 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,DALPI

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: (VIN(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 $CWT \cdot YX$, and again the statistical weight, $WX = 1/(CWT \cdot YX)^2$, is internally generated. If $KWT \geq 2$, 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 $XX < XWTL$ and for all $XX > XWTU$.

Note on parameter constraints. If $KBND \neq 0$, 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