Groundwater Flow Simulation by a Stochastic Representation of Soil

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GROUNDWATER FLOW SIMULATION BY A
STOCHASTIC REPRESENTATION OF SOIL
BY
PAUL BRUCE ALDINGER

A THESIS SUBMITTED IN PARTIAL FULFILLMENT OF THE
REQUIREMENTS FOR THE DEGREE OF
DOCTOR OF PHILOSOPHY
IN
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DOCTOR OF PHILOSOPHY DISSERTATION

OF

PAUL BRUCE ALDINGER

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1983
A Monte Carlo technique is utilized to incorporate the uncertainty in media characteristics to the solution of a groundwater flow problem. This technique involves the repetitive solution of a significant number of equiprobable representations of the soil medium. Probability and statistics are utilized to model the soil parameters and study the significance of the output.

An existing computer code was adapted and significantly modified to allow characterization of the medium's hydraulic conductivity (permeability) as autocorrelated and statistically homogeneous. A first order nearest neighbor model was selected to affect the autocorrelation of this parameter within the finite difference mesh. The statistical homogeneity considers that the distribution of hydraulic conductivity values within the mesh comes from a log normal probability density function. The selection of hydraulic conductivity value at any mode of the mesh is stochastic within the framework of the autocorrelation and statistical homogeneity of the mesh aggregate.

The computer code takes the stochastically generated hydraulic conductivity field and the boundary conditions and utilizing an iterative alternating direct implicit solution determines the hydraulic head values at each mode and flow rate through the medium. An array of these results are produced for each of the equiprobable representations of the soil medium.
Mass transport through the region is simulated as a combination of advection and a stochastic simulation of microscopic or particle scale dispersion. A water particle is released from a preselected location along the upgradient boundary. The particle moves toward the downgradient boundary under the influence of advective forces caused by the differences in hydraulic head and the stochastic simulation of microscopic dispersion. This simulation of microscopic dispersion displaces the particle parallel to and perpendicular to the advective transport direction based on laboratory scale dispersivities. The computer code establishes arrays for the particle location at a predetermined time after start as well as the location along the downgradient boundary and total travel time upon completion of transit of the region.

Uniform flow results in most of the regions considered although some alternate configurations were considered. An effective hydraulic conductivity is calculated on the basis of flow rate. After application of a shape factor this value was found to be slightly less but closest to the geometric mean of the hydraulic conductivity distribution thus confirming earlier work. An alternative effective hydraulic conductivity calculated on the basis of travel time was also determined. This value was generally less than the other effective hydraulic conductivity value but again after application of a shape factor the value was best estimated by the geometric mean. These results suggest that the mean flow rate and mean travel time may be estimated by the use of the shape factor from a flow net solution or the method of fragments and the geometric means of the hydraulic conductivity.
The results of the simulations indicate that macroscopic or field scale longitudinal and lateral dispersion is significantly affected by the standard deviation of the hydraulic conductivity distribution. Region size, hydraulic gradient and time interval were found to cause lesser effects.

The techniques utilized provide a means to develop confidence in the output. The effects of the variations in parameters become evident from a review of the results of the equiprobable results. Confidence limits may even be developed in the output where the characteristics of known probability density functions may be utilized. Example problems are presented where confidence limits on the estimates of travel time are developed for the conditions considered.
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Finally I would like to acknowledge the support given me by my wife, Mary Lou and my children who have sacrificed immeasurably over these past seven years.
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This thesis is presented in the manuscript format. Section I, Groundwater Flow in a Stochastic Medium: Model Development and Section II, Groundwater Flow in a Stochastic Medium: Application of Computer Model, will be submitted for publication in the Journal of the Geotechnical Division of the ASCE. Both manuscripts are presented in the format of that journal.

Details of the methods employed including the computer program as well as additional ancillary information are presented in the Appendices in Section III.
SECTION I
GROUNDWATER FLOW IN A STOCHASTIC MEDIUM:
MODEL DEVELOPMENT
by Paul Bruce Aldinger,1 M. ASCE

ABSTRACT: A computer model is developed to simulate groundwater flow in a stochastic porous medium. The hydraulic conductivity (permeability) of the medium is simulated as made up of statistically homogeneous strata which are internally correlated by a two dimensional nearest neighbor model. Dispersion is simulated as a combination of advective transport, and a stochastic simulation of microscopic dispersion. The model utilizes a Monte Carlo technique of repetitively solving equiprobable representations of the medium. Output consisting of hydraulic head, flow rate, travel time and dispersion is then analyzed to allow a measure of significance. A shape factor is developed which may be utilized to calculate an equivalent value of hydraulic conductivity for simplified computation of the mean flux and travel times.

INTRODUCTION
Groundwater flow problems have always been particularly challenging due to their complexity and the uncertainties involved. Increasingly, predictions of flow quantity, direction and/or travel time are necessary to answer questions on risk and safety. This need for establishing the reliability of such predictions has brought investigators from various disciplines within the sciences into this arena. The result is that considerable progress has been achieved in advancing the state of the art in recent years.

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The complexity of these problems is due to many factors. One factor is the difficulty in scaling up and combining the properties of the medium on the microscopic level to the macroscopic scale of the flow region. A related factor is the incomplete knowledge of flow regime caused by the complex conditions during deposition and/or subsequent weathering. Still other factors are the sheer number and range of variables and the limited resources normally available for analysis.

Over the years, numerous techniques have been utilized to solve these groundwater flow problems. Analytical solutions have been developed for many flow situations, however, analytic techniques suffer from a lack of flexibility and the need to make restrictive simplifying assumptions on boundary conditions and media characteristics, thereby limiting their use with many practical problems.

Perhaps the technique most widely used today is that of flow nets (10, 11). Its greatest advantage is its simplicity and ease in use. However, this technique is limited in its ability to vary soil hydraulic conductivity and groundwater surface or free surface.

A similarity with all of these techniques is the lack of flexibility in handling boundary conditions and/or varying soil property characteristics. When these techniques are utilized, the consequences of the required averaging and other approximations are often unknown.

With the recent interest in this area from the multitude of scientific disciplines and with the advancements in computer technology in the last
In the past decade, major changes in the way these flow problems are analyzed have occurred. Investigators have developed numerical solutions which allow much more latitude in setting boundary conditions and input parameters allowing much more complex and realistic characterizations of flow regimes to be considered.

Numerical solutions are approximate solutions to the flow problem. However, when properly executed they result in solutions within almost any desired level of accuracy. The most common types of numerical solutions in use today are the finite element method (FEM) and the finite difference method (FDM). Either of these methods may be used to solve most of the situations encountered, however, one type may have some advantage over the other for particular problems. A review of these methods may be found elsewhere (24, 35).

The FEM and FDM methods have allowed not only more complex boundary conditions and input parameter characterization but also allowed introduction of new types of considerations. Of these, stochastic generation of a correlated hydraulic conductivity distribution to characterize the flow regions, stochastic simulation of microscopic dispersion and the utilization of probability concepts or theory to analyze input and output are major considerations of this work.

The flow region considered in this study is two dimensional. Figure 1 presents the study region with the simplest boundary conditions resulting in predominantly uniform horizontal flow. The flow condition is referred to as uniform flow because flow is largely in one dimension,
Impervious Boundary

Left Boundary has constant Hydraulic head $= H_u$

Right Boundary has constant Hydraulic head $= H_L$

$\frac{\partial h}{\partial y} = 0$

Figure 1 - General Plan of Flow Region
from the left side boundary to the right side boundary. A numerical solution by the finite difference method for steady state flow is used to determine hydraulic heads and flow within the region.

Water particles within the flow region are subject to advective transport forces and microscopic dispersion due to the pore structure. Water particles are released from the upgradient boundary, subjected to advection and a stochastic representation of microscopic dispersion and their travel across the region monitored. This simulation allows a determination of the relative effects of hydraulic conductivity variations on observed dispersivities. It has been recognized that field dispersivities are generally higher than those measured in the laboratory and researchers have attributed this to the effects of heterogeneities.

This paper presents the background for the methodology developed to simulate water flow in a medium with an autocorrelated hydraulic conductivity (permeability) mesh. By a Monte Carlo technique which involves generating numerous equiprobable distributions, a better understanding of the uncertainty in the predictions of flow quantity, dispersion and travel time is obtained. A companion paper will demonstrate its use to solve two types of real groundwater flow problems.(3)

BACKGROUND

The soil parameters required to characterize a flow medium are the hydraulic conductivity (permeability), porosity, and the dispersion
parameters. It should be pointed out that the term hydraulic conductivity is utilized rather that the more common geotechnical engineering term of permeability to avoid confusion with workers in other disciplines. The term permeability is reserved for the medium's flow characteristic without the effects of the pore fluid's characteristics. This is comparable with the work in the geologic and petroleum industries and with similar terminology in such areas as heat, electrical and chemical flow.

The most significant of the soil parameters governing groundwater flow is hydraulic conductivity. The range of values for hydraulic conductivity of normal soil deposits is as much as 13 orders of magnitude. This variation is large for a soil property. By comparison, porosity may only vary between zero and one, unit weights by less than one and dispersivity by two orders of magnitude.

The variation within one single soil type can also be large. A variation of three orders of magnitude within a soil designation, such as sand or silt, is possible. The engineer has, by necessity, to categorize similar soil encountered in soil explorations into various soil strata. The variation in hydraulic conductivity in one soil stratum may be as much as one order of magnitude. This suggests that knowing the order of magnitude of hydraulic conductivity in a soil stratum may be enough and to expect to know the value at one particular point in a soil mass to within one order of magnitude is somewhat presumptive. Indeed we should expect considerable variation within even a "homogeneous" soil.
It is this potential for wide variation and therefore the implied uncertainty which has led engineers and geologists to turn to probability and statistical techniques to characterize hydraulic conductivity. The value of hydraulic conductivity in situ is considered to be a random variable in this methodology. This implies that the exact value at any point cannot be predicted with certainty a priori. There is uncertainty in any estimate prior to experimentation.

A random variable may be described by a probability density function (PDF) which simply relates the value of a variable with its corresponding probability. A Monte Carlo solution is accomplished by generating a significant number of equally probable representations of the flow medium from the PDF, repetitively solving each for the unknown desired results, and analyzing the results to determine the "most probable" results as well as a measure of the magnitude of variation of that result.

There are several well studied PDF's which have been found to adequately characterize soil properties (6, 20, 24). The Gaussian or normal distribution is one of the most commonly studies PDF's. This distribution is completely defined by the mean and standard deviation. This distribution has been found to model well those processes which are additive of many processes or random variables. This is the premise of the Central Limit Theorem. An example of a soil property which has been found to follow this PDF is porosity.
Another PDF which has been found to model some soil random variables is the log normal distribution. This distribution represents well those processes which are the result of multiplying other random variables. Hydraulic conductivity has been found to be adequately characterized by a log normal PDF (13, 29, 32). A useful identity is that the PDF of the log of a random variable with a lognormal PDF is normal.

The physical processes which result in soil deposits may be quite random and conditions predominating at one time and place will be modified elsewhere. It should be expected, however, to find similarities at adjacent locations when compared to locations separated by some distance. This similarity is often quantified by calculation of the autocorrelation of the random variable.

Techniques to accomplish this spatial autocorrelation include a nearest neighbor model, trend analysis, spectral density and variations of these. The nearest neighbor models develop equations for the dependency of the variable at adjacent locations and solve these equations for model development. This technique is adopted here so that further discussion will follow.

The trend analysis technique was developed at Northwestern University by Krumbein and Whitten (23, 42). The technique assumes that the random variable at any point may be characterized as the summation of a trend component (dependent on location) and a random component. Koch and Link (22) present an excellent introduction to this technique. Tabba and Yong (36) have developed a working model and in a companion paper (37)
demonstrate its application to a real problem. This technique interpolates and extrapolates information on the random variables to all points in the flow media.

The spectral density technique recognizes the Fourier transform pair consisting of the spectral density function of the random variable $S(f)$, and the autocorrelation function, $R(x)$. $S(f)$ describes the frequency information for the process and $R(x)$ the autocorrelation. This approach may describe the variations in soil properties more precisely than the other. However, its inherent complexity and the need for large amounts of data has discouraged its use for real problems in groundwater flow. It's use in solving groundwater flow problems has been demonstrated (4, 16, 17, 18).

The effects of dispersion during advective transport is becoming more critical as interest in tracking movement of pollutants and predicting concentrations in groundwater systems increases. Others have studied the problem of dispersion in groundwater flow stochastically (17, 35, 41). The first and last papers incorporate microscopic dispersion in addition to advective transport. Smith and Schwartz (35) demonstrate that large scale spatial variations in hydraulic conductivity are the major factor causing macroscopic or field scale dispersion in groundwater flow. Microscopic dispersivity is a minor factor. The assumption of normality for the travel time ensemble has not been confirmed. Gelhar, et al (17) indicated that for long travel distances a constant longitudinal dispersivity should be expected.
A methodology to include microscopic dispersion was first developed by Ahlstrom, et al (1) and modified in part by Smith & Schwartz (35). The technique assumes that this movement is a stochastic phenomenon and the magnitude is a function of a microscopic dispersivity term. A similar technique was developed by others (27). An alternate technique by contrast uses spectral analysis assuming a vertical variability of hydraulic conductivity (17).

MODEL INPUT DEVELOPMENT

The methodology presented in this paper adopts the general premise that a soil stratum may be considered statistically homogeneous with the hydraulic conductivity having a lognormal PDF. A result of this premise is that the variation in the soil property may be represented by a curve similar to those presented in Figure 2. The upper curves illustrate PDF's of hydraulic conductivity for two different magnitudes of standard deviation but with the same mean value. These curves have lognormal PDF's. The lower curves illustrate the change in form of these PDF's when the log of hydraulic conductivity for these same two distributions are plotted. These curves have normal PDF's. It should be noted that a convenient aspect of the lognormal distribution is that negative values of the parameter are avoided.

The method selected to achieve the auto-correlation for the hydraulic conductivity values at adjacent nodes in the finite difference mesh is the stochastic nearest neighbor-model originally adapted by Smith (31) for use in groundwater flow applications. The method was utilized by
Mean of Hydraulic Conductivity, $\bar{K} = 5$, Standard Deviation, $\sigma_K = 1$

$\bar{K} = 5, \sigma_K = 5$

Hydraulic Conductivity, ft/day

Figure 2 - Probability Density Function for Hydraulic Conductivity
others in other fields (5, 7, 9, 25, 42). A computer code was written to generate statistically independent realizations of hydraulic conductivity for each of the required Monte Carlo simulations.

Smith (31) presents a detailed development of the stochastic nearest neighbor model and much of this information is also available elsewhere (32, 33, 34). A summary is presented here.

The finite difference method utilized to solve the groundwater flow problem requires as input hydraulic conductivities at regularly spaced grid points. These points or nodes are located at the center of a block of constant hydraulic conductivity, the so-called block centered approach. Figure 3 presents this diagramatically including the numbering system used. The nearest neighbor model uses the following equation to relate the conductivity at one point to all adjacent points.

\[
K_{ij} = \frac{\alpha_x}{4} \left( K_{i,j-1} + K_{i,j+1} \right) + \frac{\alpha_y}{4} \left( K_{i-1,j} + K_{i+1,j} \right)
\]  

(1)

Where

- \( K_{ij} \) = Hydraulic conductivity at nodal point, \( i, j \).
- \( i \) = Row number with range from 1 to \( N_{ROW} \)
- \( j \) = Column Number with range from 1 to \( N_{COL} \)
- \( \alpha_x, \alpha_y \) = Autoregressive parameters which indicate the degree of correlation of hydraulic conductivity in the \( x \) and \( y \) directions. Range is from 0 to 1.

This relationship may be put in matrix form and a stochastic element introduced as follows:

\[
[K] = [W] [K] + \{\varepsilon\}
\]  

(2)
\[ K_{i,j} = \alpha_x / 4 (K_{i-1,j} + K_{i+1,j}) + \alpha_y / 4 (K_{i+1,j} + K_{i,j+1}) \]

- Interior Node -

\[ K_{i,j} = \alpha_x / 3 (K_{i-1,j} + K_{i+1,j}) + \alpha_y / 3 (K_{i,j+1}) \]

- Boundary Node -

Figure 3 - Correlation of Hydraulic Conductivity
In this equation $[W]$ is a weighting matrix consisting of NP rows and columns where NP is the total number of nodal points within the flow region, i.e., $NP = NROW \times NCOL$. The $[W]$ matrix is square while $\{K\}$ and $\{\varepsilon\}$ are column matrices.

The $\{\varepsilon\}$ matrix is a column matrix of random numbers with a preselected mean and standard deviation. The basis for selecting the mean and standard deviation will be discussed later.

Since the $\{K\}$ matrix is the unknown result, we can rearrange this equation by bringing both $\{K\}$ matrices to the left side as below.

$$\{K\} - [W] \{K\} = \{\varepsilon\} \quad (3)$$

We may then utilize the properties of an identity matrix and write

$$([I] - [W]) \{K\} = \{\varepsilon\} \quad (4)$$

Finally, we may solve for $\{K\}$ by multiplying by the inverse of $([I] - [W])$ resulting in

$$\{K\} = ([I] - [W])^{-1} \{\varepsilon\} \quad (5)$$

We now have the necessary matrix equation for this method. We need only develop the Weighting matrix $[W]$, subtract it from the identity matrix, $[I]$, compute an inverse, which may be called the Filter matrix, and multiply by the $\{\varepsilon\}$ matrix.
It should be noted that the Filter matrix contains all the information concerning the autocorrelation of hydraulic conductivities for each block in the flow region. The \( \{ \varepsilon \} \) matrix contains the random component which is incorporated into the system of hydraulic conductivity values.

The nearest neighbor model is easily adapted for developing the \([W]\) matrix for interior nodes. However, boundary nodes are another matter. Smith (31) assumed that the \( \alpha \) term is divided by the number of adjacent nodes. Figure 3 also presents the situation along the upper boundary. Here this approach results in the following equation:

\[
K_{ij} = \alpha x/3 \ K_{i,j-1} + K_{i,j+1} + \alpha y/3 \ K_{i+1,j}
\]  

(6)

Since a log normal distribution of hydraulic conductivity was adopted, the \( \{ \varepsilon \} \) matrix generated for each simulation will have a mean value of 0, a standard deviation of 1 and a normal distribution. A transformation will later be made so that the hydraulic conductivity values will be log normally distributed. Smith (31) demonstrated that if the \( \{ \varepsilon \} \) matrix is multiplied by a constant term, \( \eta \), any desired variance in the hydraulic conductivity values could be effected. He showed that this constant term, \( \eta \), is a function of the desired variance of the conductivity distribution and the square root of a quantity \( G \) defined as:

\[
G = \frac{2}{\alpha_y \rho_y(2)/8 + \alpha_x \rho_x(1,1)/2 + \alpha_y \rho_y(1) - \alpha_x \rho_x(1) + \alpha_y /8}
\]

\[
+ \alpha_x /8 + 1 + \alpha_x \rho_x(2)/8
\]  

(7)
where $\rho_x(1), \rho_y(1)$ are the lag 1 correlation coefficients of $K$ in the $x$ and $y$ directions

$\rho_x(2), \rho_y(2)$ are the lag 1 correlation coefficients of $K$ in the $x$ and $y$ directions

$\rho(1,1)$ are the lag 1 in the $x$ direction and lag 1 in the $y$ direction correlation coefficients of $K$

The assumption of a log normal distribution of hydraulic conductivity requires a transformation of the mean and standard deviation. It should be pointed out that the mean of the distribution of $\ln K$ does not equal the natural log of the mean of $K$. Benjamin and Cornell (6) among others, present this transformation.

\[
\sigma_y^2 = \ln \left( \left( \frac{\sigma_K}{\bar{K}} \right)^2 + 1 \right) \quad (8)
\]

\[
\bar{Y} = \ln \left( \bar{K} \right) - \frac{\sigma_y^2}{2} \quad (9)
\]

where:

$\sigma_y^2$ = variance of $Y$

$\bar{Y}$ = mean of $Y$

$\sigma_K^2$ = variance of $K$

$\bar{K}$ = mean of $K$

$Y$ = $\ln K$

This transformation is performed and the values $\sigma_y$ and $Y$ used with the $[\varepsilon]$ matrix. Following multiplication by the filter matrix and addition of the mean of the $\ln K$, a transformation back to $K$ is made. This transformation erodes some of the correlation although this has not been found to be significant (31).
This method does not produce a distribution of hydraulic conductivity which exactly follows the desired correlation structure each time. This results from the randomness inserted by the random number generator, the exponential transformation, and boundary effects. However, each generated distribution is correlated and follows the desired correlation structure. When the ensemble of all Monte Carlo simulation is studied, a closer approximation to the desired correlation is obtained.

Smith (31) pointed out a problem at the boundary in maintaining the autocorrelation of the \( K \) values. For this work it was decided to "shave off" the outer boundary nodes all around the block region. A \( 7 \times 7 \) region, for example, would have the outer nodes deleted and then be transformed into a \( 5 \times 5 \) region. This technique reduces the boundary effects but also reduces the size of the region which may be considered by this technique in light of the matrix inversion limitations.

This nearest neighbor method was chosen chiefly because it is easy to understand and, based on the work of previous researchers, it appears to represent the problem reasonably. Its major drawback is the amount of computer time needed to invert the weighting matrix, albeit this need only be done once for any region size and autocorrelation parameters and then stored. Indeed there are real limits to the size of the matrix that may realistically be inverted. This drawback effectively sets a limit on the number of nodes and hence influences mesh spacing and may influence the validity of results.

To alleviate this limitation, the flow region may be considered a compo-
site of two or more "blocks" that contain statistically homogeneous and internally correlated hydraulic conductivity meshes. For example, the shaved 5 x 5 region may be systematically added to 3 other statistically equivalent regions resulting in a 10 x 10 region. The computer time to add these regions together is much less than that required for inverting the larger matrix.

The program utilized to solve the flow problem was developed by Reiter (29). This code was adapted from other available work for the two dimensional cross-sectional model (38).

**MASS TRANSPORT SIMULATION**

A computer code was developed to simulate transport across the hydraulic field resulting from a steady state solution. Transport results from hydraulic advection, a stochastic simulation of microscopic dispersion and dispersion resulting from variations in hydraulic conductivity. The major objective of this effort was to analyze the effects of hydraulic conductivity variations on dispersion.

Others (17, 35) have indicated that the variation in porosity is much less than the variation in hydraulic conductivity and probably does not significantly influence dispersion. The value of the porosity has therefore been assumed constant throughout the region.

The finite difference method assumes that the hydraulic head, hydraulic conductivity, porosity and therefore the resulting pore water velocity
are constant within each individual block in the flow region. These velocities are calculated for each conductivity simulation and for each block within the region by the method suggested by Sauty (30).

Microscopic dispersion is incorporated into the model in a manner first described by Ahlstrom, et al (1) and then modified in part by Smith and Schwartz (35). In this method, dispersion is treated as a stochastic phenomenon. The water particle is assumed to undergo a random displacement in the direction of flow and another random displacement perpendicular to flow. These displacements are calculated from the following two equations:

\[
DL = (24 \text{ DLC} \times \text{ DELT})^{1/2} \times (0.5 - \text{ RANOL}) \tag{10}
\]

\[
DT = (24 \text{ DTC} \times \text{ DELT})^{1/2} \times (0.5 - \text{ RANOT}) \tag{11}
\]

In these equations, DL and DT are the displacements in the longitudinal and transverse directions, respectively, relative to the direction of advective transport. DLC and DTC are the longitudinal and transverse dispersion coefficients. RANOL and RANOT are random numbers normally distributed with a mean of zero and a standard deviation of one then divided by six to keep the range of values in the \(-0.5\) to \(+0.5\) area.

Kelly (21) developed a direct relationship, which has been adopted for this study, between grain size and microscopic dispersivity. This relationship may be expressed as:
\[ \delta = 0.08 D_{50} \quad (12) \]

Where \( \delta \) = dispersivity, in meters,

and \( D_{50} \) = mean particle size in millimeters

The longitudinal dispersion coefficient, DLC, is taken equal to the dispersivity times the velocity, \( V_L \), in the direction of flow. The transverse dispersion coefficient, DFC, is taken equal to a percentage of the dispersivity, DSPRAT, times the dispersivity and velocity, \( V_L \). The expressions from Ahlstrom, et al (1) for microscopic dispersion are then modified by these assumptions and units adjusted to obtain the following:

\[
DL = (6.3 \ast D_{50} \ast V_L \ast \text{DELT}) \ast \text{RANOL} \quad (13)
\]
\[
DT = (6.3 \ast D_{50} \ast V_L \ast \text{DELT}) \ast \text{DSPRAT} \ast \text{RANOT} \quad (14)
\]

Since the advective transport direction will not always coincide with the X and Y axes the displacements in the X and Y directions are obtained by a transformation.

The computer code simulates water movement from the upgradient side of the region to the downgradient side. A particle is released from the upgradient boundary and moves across the region as dictated by the
advective displacements and stochastic dispersive displacements. When an impervious boundary is encountered, the particle is reflected back into the region. Eventually the water particle encounters the downgradient boundary. The location, travel time and other data are recorded and available for statistical analysis.

Monte Carlo simulations result in a great deal of output. It was necessary to develop a large data collection and analysis system to deal with the data. Data from this study was stored in disk data files as it was produced and saved for use and analysis later. The Statistical Analysis System (SAS) has been used in the analysis of the data.

The data output to disk files was varied but consists of information on the hydraulic conductivity means and correlation for each simulation, travel times and dispersion, hydraulic head values both mean values and those for selected rows from each simulation. These data are used as input to the SAS programs. SAS programs have been written to perform all types of statistical calculations and checks, as well as to plot results.

RESULTS AND DISCUSSION

A considerable amount of computer simulation was performed during this study. One major limitation immediately encountered was the inordinate amount of computer time required to invert the (I-W) matrix. The size of the matrix increases very rapidly with the region size since a new row and column is added for each new finite difference block in the
region. The results of inverting this matrix for three region sizes, 7 by 7, 12 by 12 and 12 by 22 suggest an exponential relationship between the total number of nodes in the region and the required computer time. The fact that the computer time required to perform the inversion increases so rapidly with an increase in region size effectively sets a practical limit on the region size which could be considered in one block. The largest region considered in this study was a 12 by 22 region which required that a 264 x 264 matrix be inverted. We shall see later that some techniques may be utilized to somewhat relax this limitation.

The arithmetic, geometric and harmonic means of all the simulations of hydraulic conductivity for the numerous Monte Carlo solutions were computed. These mean values were compared to an effective hydraulic conductivity, \( K_q \), calculated on the basis of the flow quantity by the following equation:

\[
K_q = \frac{Q}{h_L} \frac{L \cdot S}{H} = \frac{Q \cdot S}{h_L}
\]

where \( Q \) is the flow quantity, \( h_L \) is the total head loss within the region, \( L \) is the total length over which that head loss occurs, \( H \) is the height of the flow region and \( S \) is a shape factor computed in accordance with a technique suggested by Warren and Price (40) which will be presented later.

The value of \( S \) is a shape factor which may be directly compared with the
shape factor, $N_D/N_F$, in a flow net solution or the form factor in the method of fragments. $N_D$ and $N_F$ are the number of equipotential drops and flow lines respectively in the flow net solution. The results of similar Monte Carlo simulations of flow regions represented by random and uncorrelated hydraulic conductivity meshes have indicated that the geometric mean is a good estimate of the effective hydraulic conductivity (8, 18, 40).

A second measure of the effective hydraulic conductivity in terms of mean travel time was computed for each Monte Carlo simulation. This effective hydraulic conductivity on the basis of travel time, $K_t$, was calculated by making assumptions similar to those used in calculating $K_q$. Figure 4 presents a typical layout of a flow region with approximately horizontal uniform flow from left to right. The flow is not precisely uniform due to the dispersion present in the flow simulation.

The velocity of flow, $v$, may be calculated by the following formula:

$$v = \frac{K_i}{n} = \frac{K}{\bar{h}}$$  \hspace{1cm} (16)

The mean velocity of all flow particles traversing the flow region, $\bar{v}$, may be calculated by dividing the length of the particle travel, $L_T$, by the mean travel time, $\bar{t}$, as below:

$$\bar{v} = \frac{L_T}{\bar{t}}$$  \hspace{1cm} (17)

The effective hydraulic conductivity on the basis of travel time, $K_t$, has been calculated by setting $v$ equal to $\bar{v}$ in the above two equa-
Along left boundary where $J=1$, hydraulic head is maintained constant at value of $H$
Along right boundary where $J=NCOL$, hydraulic head is maintained constant at value $H$.

Mean head loss in flow region = $h_L = H_u - H_L$

Figure 4 - Region of Mass Transport
tions, introducing the height of the region by inserting in both the numerator and denominator and solving for $K_t$ resulting in the following:

$$K_t = \frac{L_t \ nH \ L \ (S_t^{'})}{h_L \ H} = \frac{L_t \ nH}{h_L \ (S_t^{'})}$$  \hspace{1cm} (18)

where $L_t$ is the total length of particle travel and for the uniform flow case will equal $L$, $n$ is the porosity, $t$ is the mean travel time and $L$, $H$ and $h_L$ are as defined above. $S_t^{'}$ is a shape factor dependent on boundary conditions and is computed in a manner similar to $S$ and will be discussed later. $S_t^{''}$ is a modified shape factor which may be compared to the other shape factors, $S$, and the shape factor in the flow net solution or by the method of fragments.

Twenty-five variations of flow region size and characteristics were studied to determine the relationship between these calculated means. Generally for each flow region, 40 Monte Carlo characterizations were done. The means and effective hydraulic conductivities for each of these were computed.

In addition to calculation of mean values for each of the Monte Carlo characterizations, a mean value of all Monte Carlo characterizations was computed. Correlation of the geometric mean, and the two effective hydraulic conductivity values (flow quantity and travel time) were visually observed by plotting and also by computation of correlation coefficients. A typical plot of these results is presented in Figure 5 and the results are summarized in Table 1.
Figure 5 - Correlation of Effective Hydraulic Conductivity with Geometric Mean
### Table 1 - Summary of Flow Simulations

| File | Region Size | Block Size | Auto. Corr. Data | No. of Sims | No. of Time Waves Days | Kolmogorov Stat | Y Coord. at End | Total Travel Time, Days | Means of Hydraulic Conductivity ft/day |
|------|-------------|------------|------------------|-------------|------------------------|----------------|------------------|------------------------|---------------------------------------|
| 1    | 10 X 20     | 10 X 10    | 0.8 0.8 0.68 40  | 1 1.6       | 0.032 60.6             |                |                  | 172.5 5.02 4.63 4.28 4.53 4.44 2.10 |
| 2    | 10 X 20     | 10 X 20    | 0.8 0.4 0.68 40  | 1 1.6       | 0.115 60.4             |                |                  | 168.5 4.84 4.62 4.40 4.59 4.51 1.54 |
| 3    | 10 X 20     | 10 X 20    | 0.8L 0.8L 0.68 40| 1 1.6       | 0.15 59.5              |                |                  | 171.1 5.01 4.65 4.32 4.57 4.44 2.01 |
| 4    | 10 X 10     | 10 X 10    | 0.8 0.8 0.68 40  | 1 0.8       | 0.01 59.7              |                |                  | 39.8 5.13 4.77 4.45 4.75 4.61 1.99  |
| 5    | 5 X 5       | 5 X 5      | 0.8 0.8 0.68 40  | 2 6.4       | 0.01 35.0              |                |                  | 9.5 5.13 4.78 4.46 4.80 5.28 1.90  |
| 6    | 10 X 20     | 10 X 20    | 0.8 0.8 0.68 10  | 4 1.6       | 0.024 58.4             |                |                  | 176.6 4.86 4.51 4.19 4.42 4.30 1.95 |
| 7    | 10 X 20     | 10 X 20    | 0.8 0.8 0.68 44  | 3 1.6       | - 58.6                 |                |                  | 234.3 5.05 4.69 4.36 4.63 4.54 1.99 |
| 8    | 10 X 20     | 10 X 20    | 0.8 0.4 1.0 40   | 1 1.6       | 0.01 60.0              |                |                  | 173.0 5.09 4.60 4.15 4.54 4.39 2.40 |
| 9    | 10 X 20     | 10 X 20    | 0.8 0.8 0.68 40  | 1 1.6       | 0.01 59.9              |                |                  | 169.7 5.04 4.68 4.34 4.62 4.52 2.02 |
| 10   | 10 X 40     | 10 X 20    | 0.8 0.8 0.68 40  | 1 3.2       | 0.01 59.6              |                |                  | 703.4 4.99 4.62 4.28 4.53 4.45 2.02 |
| 11   | 10 X 40     | 10 X 20    | 0.8 0.8 0.68 40  | 1 0.3       | 0.15 60.2              |                |                  | 694.4 5.06 4.68 4.32 4.59 4.51 2.08 |
| 12   | 10 X 40     | 10 X 20    | 0.8 0.8 0.68 40  | 1 6.4       | 0.014 59.2             |                |                  | 702.2 5.02 4.64 4.29 4.54 4.46 2.08 |
| 13   | 10 X 40     | 10 X 10    | 0.8 0.8 0.68 40  | 1 3.2       | 0.04 60.8              |                |                  | 697.0 5.02 4.64 4.29 4.55 4.48 2.08 |
| 14   | 20 X 40     | 10 X 10    | 0.8 0.8 0.68 20  | 1 3.2       | 0.15 111.7             |                |                  | 700.0 4.99 4.61 4.27 4.54 4.46 2.09 |
| 15   | 20 X 40     | 10 X 20    | 0.8 0.8 0.68 20  | 1 3.2       | 0.15 111.2             |                |                  | 699.7 4.98 4.62 4.28 4.55 4.46 2.03 |
| 16   | 10 X 60     | 10 X 20    | 0.8 0.8 0.68 40  | 1 4.8       | 0.15 59.5              |                |                  | 1576.2 5.06 4.67 4.31 4.57 4.49 2.11 |
| 17   | 10 X 60     | 10 X 10    | 0.8 0.8 0.68 40  | 1 4.8       | 0.052 59.5             |                |                  | 1576.7 5.06 - - - - 2.14 |
| 18   | 10 X 20     | 10 X 20    | 1.0 1.0          | 1 40 1.6    | 0.15 60.2              |                |                  | 151.9 5.0 5.0 5.0 5.0 0.0 0.0  |
TABLE 1 - SUMMARY OF FLOW SIMULATIONS (CONTINUED)

| File | Region Size | Block Size | Auto. Corr. | No. of Time | Kol- Y | Total Travel | Means of Hydraulic Conductivity |
|------|-------------|------------|-------------|-------------|--------|--------------|---------------------------------|
|      |             |            | Data        | Wa- Int., D | Coor.  | Time, Days   | ft/day                          |
|      |             |            | x          |             | y      | End          | K_a    | K_g    | K_h   | K_q   | K_t   | K    |
| 19   | 10 X 20     | 10 X 20    | .8         | .2          | 1.0    | 40           | 1.16   | 60.7   | 170.1 | 5.11  | 4.65  | 4.23 | 4.62 | 4.47  | 2.35  |
| 20   | 10 X 20     | 10 X 20    | .8         | .2          | 0.9    | 40           | 1.16   | .15    | 60.2  | 169.8 | 5.005 | 4.64 | 4.23 | 4.6   | 4.7   | 2.04  |
| 21   | 10 X 60     | 10 X 20    | .8         | .8          | .68    | 40           | 1.0    | .048   | 60.3  | 314.5 | 4.96  | 4.58 | 4.23 | 4.48  | 4.41  | 2.05  |
| 22   | 10 X 60     | 10 X 20    | .8         | .8          | .68    | 40           | .44    | .066   | 60.5  | 143.0 | 5.07  | 4.68 | 4.33 | 4.59  | 4.50  | 2.07  |
| 23   | 10 X 20     | 10 X 20    | .8         | .8          | .68    | 40           | 1.16   | -      | 98.4  | 228.0 | 5.12  | 4.72 | 4.36 | 4.62  | 4.50  | 2.12  |
| 24   | 10 X 20     | 10 X 20    | 1.0        | 1.0         | -      | 1            | 1.6    | -      | 133   | 88.7  | 5.0   | 5.0  | 5.0  | 5.0   | 5.0   | 0.0   |
| 25   | 10 X 20     | 10 X 20    | 1.0        | 1.0         | -      | 1            | 1.6    | -      | 98.8  | 200.5 | 5.0   | 5.0  | 5.0  | 5.0   | 5.0   | 0.0   |
| 26   | 10 X 20     | 10 X 20    | 0.8        | 0.4         | .84    | 40           | 1.16   | -      | 60.2  | 173.7 | 4.90  | 4.55 | 4.23 | 4.51  | 4.39  | 1.98  |
| 27   | 10 X 20     | 10 X 20    | 0.8        | 0.3         | .68    | 40           | 1.16   | .01    | 58.8  | 254.91| 5.01  | 3.54 | 2.51 | 3.32  | 3.06  | 4.786 |
| 28   | 10 X 20     | 10 X 20    | 0.8        | 0.8         | .68    | 40           | 1.16   | -      | 60.0  | 153.11| 5.01  | 4.98 | 4.96 | 4.98  | 4.97  | 0.50  |
| 29   | 10 X 40     | 10 X 20    | 0.8        | 0.8         | .68    | 20           | 1.32   | -      | 109.6 | 2058.4| 2.99  | -   | -   | -     | 1.52  | 2.47  |
| 30   | 10 X 20     | 10 X 20    | .4         | .3          | .95    | 40           | 1.16   | .15    | 59.8  | 170.5 | 5.01  | 4.66 | 4.34 | 4.58  | 4.47  | 1.97  |

Note: Uniform flow in all files except 7 and 24 which simulate S Flow and 23 and 25 with cutoff.

Values listed for $K_q$ and $K_t$ have been adjusted by use of the shape factor $S$. 


The results of these computations support the observation that the geometric mean is the best measure of the effective hydraulic conductivity in terms of flow quantity and travel time. The effective hydraulic conductivity calculated both by flow quantity and travel time are relatively close with the flow quantity value generally somewhat larger. These results generally agree with Butler and Gundlach (10) who determined that the equivalent area for flow and travel time were not always equal. Their flow regions were largely one dimensional.

Two boundary flow configurations were considered in addition to uniform flow, i.e., flow from the left boundary to the right boundary of a rectangular region. The two flow configurations are presented in Figure 6. The first flow configuration is described as S flow and consists of flow from the upper three nodes of the left boundary to the lower three nodes of the right boundary. This case could simulate a general two dimensional flow case such as around an obstruction or low hydraulic conductivity occlusion. The second flow configuration is described as cutoff and consists of flow from the left upper boundary to the bottom right boundary. This case is intended to simulate flow beneath a dam by representing one half of the flow region.

Warren and Price (40) have indicated that the geometric mean of the hydraulic conductivity is a good approximation of the effective hydraulic conductivity even for non-uniform flow provided a shape factor is utilized to adjust the value for the shape of the flow region. They suggest that the magnitude of this shape factor, $S$ in equation 15, be determined by first calculating the effective hydraulic conductivity
Figure 6 - Alternate Boundary Conditions
of the flow region using a singular known value of hydraulic conductivity. This effective value of hydraulic conductivity should then be divided into the singular known value and the result is the shape factor. The shape factor is then multiplied by the effective hydraulic conductivity before comparing with the geometric mean. Examples of these computations are presented elsewhere (2).

The results of this study tend to support this technique. For the cases considered, the adjusted values of effective hydraulic conductivity generally fall between the geometric and harmonic means and is closest to the geometric mean as presented in Table 1.

The importance of this finding is that the mean flow rate may be estimated by rearranging equation 15 to solve for the flow rate, Q, as below:

\[ Q = \frac{K h_L}{S} \]  

(19)

The geometric mean should be used for the value of K and the shape factor, S, may be determined by a flow net solution or the method of fragments.

A similar rearrangement of equation 18 and taking \( L_T \) equal to \( L \), results in the following equation for the mean travel time, \( \bar{t} \):

\[ \bar{t} = \frac{L \cdot n \cdot H \cdot S}{K h_L} \]  

(20)

The mean travel time may then be approximated by using the geometric
mean of hydraulic conductivity for $K$ and the shape factor from a flow net solution or the method of fragments. Although this technique has not been theoretically proven and for nonuniform flow $L_T$ may be unknown exactly and may not equal $L$, the results developed here suggest that this technique can provide reasonable estimates of mean travel time.

The stochastic nearest neighbor process model was utilized to generate random meshes of hydraulic conductivity which are autocorrelated. Each of the individual representations within the ensemble of representations making up each Monte Carlo simulation was analyzed to determine the magnitude of correlation by row and column. The formulation below was utilized to calculate this value and may be found in many references, e.g. (32):

$$
\rho(L) = \frac{\sum_{i=1}^{n-L} (K_i - \bar{K})(K_{i+L} - \bar{K})}{\sqrt{\sum_{i=1}^{n} (K_i - \bar{K})^2}} \quad (21)
$$

In this equation $\rho(L)$ is the autocorrelation coefficient for the lag $L$. $L$ is a whole number with the range zero to one minus the number of elements in the row or column considered. $K$ is the value of hydraulic conductivity and $\bar{K}$ is the mean value. The denominator is the variance of the hydraulic conductivity. It may be easily shown that if $L$ equals zero, then $\rho(0)$ equals 1.0.

A graph of a typical result of this computation for lags from one to three is presented in Figure 7. The concept of integral scale as dis-
$\alpha_x = \alpha_y = 0.8$
Block size = 10 Feet

Integral Scale = $\lambda$
\[ \lambda = (1.0 + 0.436 + 0.138 + 0.008)10 \]
\[ = 15.8 \text{ Feet} \]

Figure 7 - Correlation Coefficient Versus Lag Number
cussed by Smith and Freeze (33) is utilized herein to conceptualize the degree of dependency of the hydraulic conductivity value at one node with the value at adjacent nodes. The integral scale has been estimated as the summation of the positive auto-correlation coefficients times the block size. As indicated, the integral scale, $\lambda$, equals 15.8 for the data in Figure 7.

Smith (31) recognized a problem with the autocorrelation resulting from boundary effects. This problem was mitigated somewhat by deleting the boundary blocks of the region after development. Aldinger (2) demonstrates the effects on the autocorrelation coefficients of deleting these boundary blocks. Also presented are the effects on these same autocorrelation coefficients caused by the log transformation to hydraulic conductivity. The results indicate a slight loss of correlation when the boundaries blocks were deleted and some additional loss when the log transformation was completed. This total loss was slight, particularly for the integral scale.

The effect of the region size on the integral scale is demonstrated in Figure 8. It is clear that as the region size increases, the integral scale increases, although at a decreasing rate. This figure also demonstrates the effects of stacking blocks of internally autocorrelated hydraulic conductivity meshes to model larger regions without utilizing a larger FILTR matrix. There is a loss in the integral scale although this loss is relatively small even when the region is increased by three times. The figure also demonstrates that as the region size increases, the integral scale continues to increase even with the same FILTR
Figure 8 - Integral Scale Versus Region Size

Note: Finite Difference Mesh consists of 10 Foot by 10 Foot Sections in all cases.
Sensitivity of Ensemble Means and Variances to the Number of Simulations

Computer computations are relatively inexpensive. However, the practicing engineer does not want to do more computations than are necessary to obtain reliable answers. A study of the number of simulations required to compute reliable mean values of various parameters was then conducted.

Initially consider the mean and standard deviation of the hydraulic conductivity formulations. Figure 9 presents a plot of an accumulating mean of the lag 3 arithmetic mean and standard deviation of the hydraulic conductivity as each new equiprobable representation of the Monte Carlo simulations is calculated. This plot demonstrates that the cumulative mean very rapidly approaches a constant value, in this case after approximately 8 simulations.

The SAS program written to compute the cumulative mean of the lag 3 means and standard deviation is an inexact estimate of the actual mean and standard deviation of all preceding observations. The procedure computes the mean and standard deviation of the previous three observations. A running mean value of these two results is then computed as each new mean and standard deviation is computed for a new observation and the two left from the earlier group of three after deleting the first observation. The results have been found accurate to approximately 3 to 4 decimal places for the mean value. However, the
Figure 9 - Cumulative Mean Values of Mean and Standard Deviation of Hydraulic Conductivity Versus Simulation Number
mean of the cumulative mean of the lag 3 standard deviation computed by this technique may only be used as a qualitative measure of the trend and its stability. A precise measure of the actual standard deviation can only be computed after the entire ensemble is sampled.

Similar plots for the effective hydraulic conductivity in terms of flow quantity, $K_q$, and travel time, $K_t$, respectively have been developed (2). These indicate that a fairly constant value is rapidly approached, usually in less than 10 simulations. This probably results from the fact these are a measure of the variation of the mean hydraulic conductivity in the flow region. The model attempts to set the mean value of hydraulic conductivity equal to the same value for each simulation so that these related mean values should also approach consistent values fairly rapidly. However, the cumulative means of the lag 3 standard deviation for these terms fluctuates considerably. In Figure 9, a truly constant value is not achieved even after the 40 simulations in this ensemble although after the first 20, the fluctuations are greatly reduced.

**Sensitivity of Ensemble Means and Variances to Number of Water Particles**

The number of particles which need to be released and their travel simulated to allow an estimate of the mean and standard deviation of the travel time is another important consideration in the amount of computation time required. A SAS program was written to compute the cumulative mean of the lag 3 mean and standard deviation of the travel time for particle transit. A typical plot for one run is presented in
Figure 10. This figure illustrates that a mean value of travel time is reached after approximately 20 water particles have transited the region. The cumulative mean of the lag 3 standard deviation of the travel time fluctuates 20 or 40 percent after 20 water particles, reaching a fairly consistent, although still slightly decreasing value, after approximately 80 water particles.

Fried (15) gives an expression for the longitudinal dispersion coefficient, $D_L$, assuming that the development of particle concentration at some distant point is normally distributed. He illustrates that this coefficient is directly related to the variance of the travel times. The equation developed for a long travel distance relative to the dispersion is:

$$D_L = \frac{\bar{U}^2 (2\sigma_t)^2}{8 \bar{t}}$$

(22)

where $\bar{U}$ and $\bar{t}$ are the mean velocities and travel time, respectively, and $\sigma_t$ is the standard deviation of the travel time.

The distance, $x$, over which the dispersion occurs equals the product $Ut_{0.5}$ and may be substituted in this equation resulting in the following equation:

$$D_L = \frac{\sigma_t x}{2(\bar{t})^3}$$

(23)
Figure 10 - Cumulative Mean Values of the Mean and Standard Deviation of Travel Times Versus Particle Number
These expressions illustrate the relationship between the standard deviation of the travel time, $\sigma_t$, and the longitudinal dispersion coefficient. The macroscopic or field scale dispersivity, $\delta_f$, may be determined by dividing by the mean velocity to arrive at:

$$\delta_f = \frac{\sigma_t x}{2 t^2} \quad (24)$$

These results and others indicate that the 400 water particles simulated is sufficient to compute a mean and standard deviation for travel time.

The macroscopic or field scale lateral dispersion coefficient, $D_T$, has been similarly shown (15) to be a function of the scatter about the mean ending location after traversing a region. The following equation was given:

$$D_T = \frac{1}{2} \frac{\sigma_y}{x} \frac{\bar{U}}{2} \quad (25)$$

where $\sigma_y$ is the standard deviation of the normalized location perpendicular to the primary direction of flow and $\bar{U}$ and $x$ are as defined earlier.

A record was maintained of the starting and ending y coordinate of each particle. A normalized ending y coordinate was then computed along with a cumulative mean and cumulative mean standard deviation as each new
record of water transport was added. The same was computed for the y coordinate at the estimated time to transit half the region. A typical plot of these results is presented in Figure 11. These results also indicate that the 400 water particles are sufficient to reach a consistent mean value for these variables.

Normality Check on Travel Times

The ensemble of travel times was utilized to plot a breakthrough curve. Figure 12 presents a representative sample of a breakthrough curve. These curves are similar to a concentration versus time curve and their similarity of shape supports the premise of general conformance of normality.

A check for the goodness of fit of the assumption of a normal distribution for the ensemble of travel time records was made. A SAS program was written to test the null hypothesis that the data could be a random sample from a normal distribution. A Kolomogorov D statistic was computed and compared with critical values. A Kolomogorov statistic was utilized rather than the more common chi square check since it is more easily adapted to continuous uncategorized data.

Table 1 presents the results of this check for several flow ensembles. Several of the normality checks support the assumption of a normal distribution with a general tendency to do so as the transit distance increases. Cases 10, 11 and 12 suggest that as the time interval decreases, there is a greater likelihood of acceptance of a normal dis-
Figure 11 - Cumulative Mean of Mean and Standard Deviation of Ending Y Location Versus Particle Number
Figure 12 - Typical Breakthrough Curve
tribution. A Kolomogorov D statistic of 0.10 or greater was considered acceptance of the assumption of normality for this study.

Hydraulic Head Value Sensitivity

The hydraulic head value along two rows was tabulated for each of the simulations. This tabulation was then available to allow computation of mean values and variations resulting from changes in region size, hydraulic gradient, conductivity and other factors.

Figure 13 presents typical results from one of the Monte Carlo simulations. The upper plot presents the mean hydraulic head versus the node number. The averaging over the 40 Monte Carlo simulations results in a fairly smooth straight line relationship. The middle curve in Figure 13 presents the standard deviation and the lower curve the variance of the hydraulic head for the 40 Monte Carlo simulations versus the node number. These plots clearly demonstrate the boundary effects. At the ends of the flow region the head is held constant and therefore the standard deviation is zero at these nodes. At nodes further away, there is less influence from the boundary and therefore the standard deviation and variance are greater.

The number of Monte Carlo simulations required to reach a fairly consistent value of the hydraulic head was also investigated. Figure 14 presents a typical plot of the results of one such investigation at an interior node. This plot indicates that the initial simulation had a value very close to the resulting mean value and after three simulations
Figure 13 - Mean, Standard Deviation and Variance of Hydraulic Head Versus Node Number
Figure 14 - Cumulative Mean of the Head Versus Simulation Number
the mean value was within 3 percent of that value.

The effect of variations in region size is demonstrated in Figure 15. The maximum value of the normalized standard deviation of hydraulic head for any of the nodes in the region increases as the region size increased. The maximum value of the standard deviation of hydraulic head was normalized by dividing each value by the mean head loss in each block or grid.

The effect of variations in hydraulic gradient is demonstrated in Figure 16. The upper plot indicates a gradual increase in the maximum value of the standard deviation of hydraulic head as the hydraulic gradient increases. After normalizing these values by dividing by the mean head loss, however, there is no general trend as is demonstrated by the lower plot.

The relationship between this quantity and the standard deviation of the hydraulic conductivity is of more significance. Figure 17 presents this relationship which indicates a direct relationship. This is significant since the uncertainty in the hydraulic conductivity value directly affects our uncertainty in the value of the hydraulic head value within the region.

**Macroscopic Dispersivity Sensitivity**

The macroscopic or field scale longitudinal dispersivity has been shown to be a function of the standard deviation of the travel time. The
Note: Finite Difference Mesh consists of 10 Foot by 10 Foot sections in all cases.

Figure 15 - Maximum Value of Normalized Standard Deviation of Head Versus Region Size
Figure 16 - Maximum Value of Standard Deviation of Head Versus Hydraulic Gradient
Figure 17 - Maximum Value of Standard Deviation of Head Versus Standard Deviation of Hydraulic Conductivity
macroscopic transverse dispersivity has been shown to be a function of the standard deviation about the mean ending location perpendicular to the general flow direction. For the horizontal uniform flow case this may be taken as the standard deviation in the ending y coordinate. The sensitivity of the macroscopic dispersivities to variations in region size, hydraulic gradient, time interval and standard deviation of hydraulic conductivity was investigated.

Figure 18 presents results of the effect of region size on the macroscopic longitudinal and transverse dispersivity. The upper plot indicates a relatively small change in the longitudinal dispersivity with an increase in region size and no consistent trend. The lower plot indicates a steadily decreasing transverse dispersivity with region size. The values plotted for the macroscopic dispersivities was determined by dividing the dispersion coefficients determined by equations 18 and 21 by the mean particle velocity in the region. These results suggest that a constant value of dispersivity is not reached during the transit of these particles.

Figure 19 presents the effects of a change in hydraulic gradient and Figure 20 the effects of a change in time interval for mass transport on these same parameters. The variation of both macroscopic longitudinal and transverse dispersivity is small and inconsistent due to the change in hydraulic gradient and time interval. The insensitivity of the observed dispersivity due to time interval variation is important since the computer time required to simulate particle transit is dependent on the time interval utilized.
Figure 18 - Macroscopic Dispersivity Versus Region Size
Figure 19 - Macroscopic Dispersivity Versus Hydraulic Gradient
Figure 20 - Macroscopic Dispersivity Versus Time Interval
The effect of a variation in the standard deviation of hydraulic conductivity is much more pronounced than these other variables. The results of a variation of this parameter are presented in Figure 21. A reduction in standard deviation of the hydraulic conductivity from 2 to 0.5 resulted in a reduction from 2.5 to 0.3 in longitudinal dispersivity and from 0.14 to 0.05 on the transverse dispersivity.

The sensitivity of the macroscopic dispersivity on the microscopic dispersivity was also investigated. The typical range of lab or microscopic longitudinal dispersivity has been reported (14) to be in the range of 0.1 to 20 mm for unconsolidated geologic sediments. Lab values of transverse dispersivity have likewise been reported to be 5 to 20 percent of the longitudinal dispersivity. Mass transport in regions of uniform flow with values of dispersivity near the extremes of this range was simulated. The initial simulation with both microscopic dispersivity values equal to zero and a singular constant value of hydraulic conductivity of five resulted in a macroscopic dispersivity of zero. A second simulation with microscopic dispersivities of 0.47 feet (144 mm) and 0.14 feet (43 mm) respectively, resulted in macroscopic dispersivities of 0.16 feet and 0.05 feet respectively. However when these same microscopic dispersivities are compared with the results presented in Figure 21, it is apparent that the variation of the microscopic dispersivities is of secondary importance relative to possible variations in hydraulic conductivity.

The sensitivity of the longitudinal dispersivity to changes in the shape of the flow region was also considered. Generally the greater the
Figure 21 - Macroscopic Dispersivity Versus Standard Deviation of Hydraulic Conductivity
tortuosity of the flow region boundary conditions, the greater the macroscopic dispersivity. The macroscopic longitudinal dispersivity varied from 2.49 feet for the uniform flow case to 2.84 and 3.25 feet for the S flow and cutoff cases respectively. For the three general flow regions considered the variation in macroscopic dispersivity was relatively small when compared to that resulting from a variation in the hydraulic conductivity distribution.

Development of Confidence Limits

The confidence which the engineer has in his prediction of flow quantity, travel times and dispersion is the major reason for utilizing these more sophisticated and complex solutions for field flow problems. If the engineer were not able to increase his confidence in his predictions there would be little reason to utilize these techniques. The nature of the output from this method lends itself to the development of confidence limits on the solution.

A methodology to utilize the knowledge of the variability of the flow region characteristics to establish confidence limits on the output utilizing probability and statistics has been formulated. The emphasis of this methodology is in the quantification of the characteristics of the major input parameter, hydraulic conductivity. Other parameters have been shown to be of lesser importance to the problem solution.

The procedure to develop the site specific soil parameters is essentially unchanged. Field programs are utilized to measure insitu
soil parameters and to secure samples for laboratory testing. The field and laboratory tests will be analyzed so that a probability density function of the hydraulic conductivity may be formulated. Other parameters such as porosity, and laboratory dispersivity characteristics must also be developed.

These parameters are then the input to a Monte Carlo computer solution for flow quantity and travel time. The results of these Monte Carlo computer simulations may then be analyzed utilizing the knowledge of the underlying distribution of these results to develop confidence in the results.

In general the flow quantity and travel time results should be expected to conform to a normal distribution. This assumption is made on the basis of the Central Limit Theorem. The water particle movement may be considered the result of adding up the effects of many individual factors (hydraulic conductivity values). This assumption of normality has been only generally verified in this study, since numerous exceptions were observed.

The mean value of the flow quantity and travel time may then be estimated with confidence by the method described below. The results of one Monte Carlo simulation are presented in Figure 22. The characteristics of the flow region are also presented. The mean and standard deviation of the effective hydraulic conductivity, $K_q$, is 4.57 and 0.230 respectively. The magnitude of error of the mean with 95% confidence may be estimated by the following expression (26):
Figure 22 - Typical Output on Flow and Travel Time
where $t_{a/2}$ is the value of the cumulative distribution function of the student t distribution at $a/2$ significance, $s$ is the value of the standard deviation and $N$ is the sample size.

The mean value would then be expected to lie between the limits of the sample mean (4.57) plus or minus the error (0.07) i.e., 4.50 and 4.64.

The effective hydraulic conductivity, $K_q$, was calculated by dividing the flow by the mean hydraulic gradient and area. The flow rate may then be estimated with confidence limits of 95% by multiplying by these constants. In so doing the flow limits of 38 to 39.5 ft$^3$/day were estimated with 95% confidence limits.

The same methodology may be utilized to develop confidence limits on the travel times. The mean and standard deviation of the travel time is 1576.2 and 146.9 days. The magnitude of error of the mean with 95% confidence may be estimated as:

$$E < t_{a/2} \frac{s}{\sqrt{N}} = 1.96 \cdot \frac{0.230}{\sqrt{40}} = 14.4 \text{ days}$$

The mean value of travel time is therefore expected to lie between 1562 and 1591 days.

The standard deviation of the travel time may also be estimated with confidence by the expressions given below (26):
where $Z_{a/2}$ is the value of the cumulative density function at a significant of $a/2$. Utilizing this equation results in the following:

$$\frac{146.9}{1 + \frac{1.96}{\sqrt{2(400)}}} < \sigma < \frac{146.9}{1 - \frac{1.96}{\sqrt{2(400)}}}$$  \hspace{1cm} (29)

which reduces to:

$$137.4 < \sigma < 157.8$$ \hspace{1cm} (30)

The water particles are expected to follow a normal distribution so that a hypothetical breakthrough curve may be developed for the extremes of these parameters. The result of such an exercise is presented in Figure 23. This allows the engineer to estimate not only the mean arrival time with confidence but also the distribution of travel times.
Figure 23 - Hypothetical Breakthrough Curve with Confidence Limits
CONCLUSIONS

The methodology outlined herein which utilizes a stochastic nearest neighbor model and a log normal PDF technique to simulate the variation in hydraulic conductivity (permeability) is useful in incorporating the variability in flow regions into flow calculations. The following conclusions concerning the results of the Monte Carlo simulations for steady state flow may be drawn:

1. The effects of the boundaries, of stacking blocks of internally autocorrelated subregions and the log transformation necessitated by this technique did not severely erode the integral scale for the cases considered.

2. The geometric mean is the best estimate of the effective hydraulic conductivity value computed either on the basis of flow quantity or travel time. This is true for uniform as well as the more tortuous flow conditions considered after applying a shape factor.

3. The magnitude of the standard deviation of the hydraulic head at any point in the flow region is a function of the standard deviation of the hydraulic conductivity, the region size and the distance from the boundary.

4. The flow quantity and travel time to traverse the region cannot always be assumed normally distributed. This may be due to the limited size of the regions considered in this study. However,
when testing confirms normality, confidence limits for the mean and standard deviation may be developed. These estimates could provide the necessary input for economic studies of alternates when tempered with engineering judgement.

5. The macroscopic lateral and transverse dispersivities did not consistently reach constant values within the distance studied. The magnitude of the macroscopic dispersivity was more dependent on distributions of hydraulic conductivity than other parameters considered including variations in the microscopic dispersivity.
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APPENDIX II - NOTATION

The following symbols are used in this paper:

\( D_{L} \) = macroscopic longitudinal dispersion coefficient

\( D_{T} \) = macroscopic transverse dispersion coefficient

\( D_{50} \) = 50\% particle size or mean particle size

DELT = time increment, days

DL = longitudinal displacement

DLC = microscopic longitudinal dispersion coefficient

DSPRAT = transverse to longitudinal dispersivity ratio

DT = transverse displacement

DTC = microscopic transverse dispersion coefficient

E = magnitude of error

F(K) = probability density function of K

G = variable relating standard deviations of Y to K
h = hydraulic head

h_L = hydraulic head loss

H = height of flow region

H_L = hydraulic head at downgradient boundary

H_u = hydraulic head at upgradient boundary

i = row number of finite difference grid system

I = identity matrix

j = column number of finite difference grid system

K_{ij} = hydraulic conductivity (permeability) at nodal point i,j

\bar{K} = mean hydraulic conductivity

K_a = arithmetic mean of hydraulic conductivity

K_g = geometric mean of hydraulic conductivity

K_h = harmonic mean of hydraulic conductivity

K_q = effective hydraulic conductivity on basis of flow
\( K_t \) = effective hydraulic conductivity on basis of travel time

\( L \) = length over which head loss occurs

\( L_T \) = length over which water travels in flow simulation

\( n \) = porosity

\( N \) = sample size

\( N_D \) = number of equipotential drops in flow net

\( N_F \) = number of flow lines in flow net

\( \text{RANOL, RANOT} \) = random number from normal distribution

\( s \) = sample standard deviation

\( s^/, s'_t, s_t \) = shape factors

\( \bar{t} \) = mean travel time

\( t_{\bar{u}/2} \) = cumulative distribution function of student t distribution at \( \bar{u}/2 \) significance

\( \bar{u} \) = mean particle velocity
\( \nu \) = velocity of water

\( W \) = weighting factor matrix

\( x \) = coordinate

\( X \) = distance of total particle travel

\( y \) = coordinate

\( \alpha_x, \alpha_y \) = autoregressive parameters

\( \delta \) = significance level

\( \delta \) = macroscopic dispersivity

\( \epsilon \) = random number matrix

\( \lambda \) = integral scale

\( \eta \) = constant which relates \( \sigma_k \) to \( \sigma_y \)

\( \rho \) = correlation coefficient

\( \sigma \) = standard deviation
SECTION II

GROUNDWATER FLOW IN A STOCHASTIC MEDIUM:
APPLICATIONS OF COMPUTER MODEL

BY
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ABSTRACT: The use of a computer model which characterizes flow in a porous medium as a stochastic process is demonstrated on two field problems. The computer model allows the hydraulic conductivity (permeability) to be varied within the blocks of the finite difference mesh according to a predetermined autocorrelation structure and a log normal probability density function. Mass transport is simulated as a combination of advection and microscopic or particle scale dispersion. The model allows development of confidence in the flow rate and travel times within the region.

INTRODUCTION

Geotechnical engineers are asked to make predictions of groundwater flow in a variety of boundary conditions and soil media. Sometimes there is considerable data available, but more often the problem is so large, the boundary conditions and soil medium so complex, that the resources available can not be expected to identify in detail the conditions insitu.

Nevertheless, predictions are required. The geotechnical engineer has

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met that need by idealizing boundary conditions and soil media characteristics and making conservative assumptions as necessary to develop predictions. Sensitivity analyses have also been performed to study the effects varying of input parameters have on predictions.

Recently new techniques have been introduced which allow more complex and realistic input parameter characterization. In addition, other techniques have been utilized to analyze the results of numerical simulations. One of these tools, the use of probability and statistics, is utilized to estimate confidence limits for the prediction resulting from such analyses.

A word of caution is always necessary when discussing the use of probability and statistics in engineering problems. Too often the user forgets that these results are only estimates and that uncertainty still exists. These techniques do help develop confidence in one's predictions, but like all engineering tools, they must be weighted with engineering judgement.

This paper is the second of two papers. The first paper detailed the development of a computer model which uses a Monte Carlo technique, a finite difference numerical solution and a stochastic representation of the soil medium to simulate groundwater flow (1). This paper presents two applications of this computer model to study a typical groundwater flow problem. The first application is an actual situation in Rhode Island, the second is a hypothetical problem.
BACKGROUND

A two dimensional characterization of the flow region has been chosen for several reasons. The practicing engineer rarely has sufficient information to make a three-dimensional model worth the expense of developing it. The practicing engineer is therefore more familiar with two dimensional representations. In addition, the computational effort required for stochastic three dimensional solutions would be enormous. Perhaps the techniques will be expanded to the three-dimensional case when further advances in computers allow and researchers consider the effort worthwhile.

For problems considered in this paper, steady state conditions are assumed. The first considers flow beneath a dike and the second flow away from a waste disposal lagoon. The flow region has been assumed rectangular for simplicity although other region shapes could be utilized.

The practicing engineer's primary analysis techniques until quite recently have been analytical solutions and flow nets. Analytical solutions are exact solutions to the flow conditions and have been developed to solve many flow situations (6). Where appropriate, these techniques provide reliable answers. These techniques suffer from their lack of flexibility and the need to make restrictive simplifying assumptions for boundary conditions and media parameters. In general, regions must be assumed homogeneous and isotropic. Anisotropy can generally be included by performing a transformation.
Perhaps the technique most widely used today is the flow net. This technique has been available for nearly half a century and been utilized extensively (3, 4). Its greatest advantage is its simplicity and ease of use. The technique suffers from its limited capacity to vary the soil's hydraulic conductivity and freewater surface, however.

Numerical methods allow more realistic problem formulations. In most cases, however, the problem must be simplified into regions where the soil media have constant hydraulic conductivity. The companion paper (2) discusses the problems with this type of approach as well as other more realistic modifications.

The computer model discussed in the companion paper (2) requires input information normally required in any of the foregoing techniques as well as some additional information. Initially the soil medium must be divided into similar strata. Boundary conditions must also be evaluated and locations for constant head and no flow or impervious boundaries identified.

The hydraulic conductivity of the soil medium is presumed to be characterized stochastically by a log normal probability density function (PDF). An estimate of the mean and standard deviation of the hydraulic conductivity must be determined. The method of estimating these values is to compile all the data available and assign weighting factors for the various sources and test procedures used. Perhaps more weight will be given to insitu tests than lab tests or correlations from other measured parameters. An estimate of the integral scale or distance over
which the value of hydraulic conductivity is positively correlated must also be determined. This may be done by plotting the discrete values of hydraulic conductivity from samples taken in close proximity vertically and laterally, computing correlation coefficients and the resulting integral scale. (10)

Other data required are median grain size, the ratio of lateral to longitudinal microscopic or particle scale dispersivity and soil porosity. The median grain size may be determined from grain size distribution curves. Soil porosity may be estimated from standard penetration tests and soil descriptions. Figure 1 presents a correlation between standard penetration test results and porosity for different soils types. This figure is adapted from Navfac DM 7 (8). On the right ordinate scale the results of information were superimposed correlating density descriptions with standard penetration results from Peck (9).

The methodology to be described herein and presented in detail in the companion paper (2) can best be illustrated by example. The following two examples will demonstrate its use in solving real flow problems.

FLOW BENEATH A DIKE EXAMPLE

The State of Rhode Island is presently planning the construction of the Big River Reservoir in central Rhode Island. The reservoir will inundate approximately 7 square miles of land in two towns, Coventry and West Greenwich. Figure 2 presents a plan of the general area of the site.
Figure 1 - Relationship Between Grain Size, Standard Penetration Test and Porosity, (8,9)
Figure 2 - Big River Reservoir Project Area
Interstate Route 95 traverses this area and will divide the impounded water resulting in a reservoir on both sides of the road. For the eastern pool, this interstate highway will essentially form the northern boundary of the reservoir and Division Street will be flooded. Figure 3 presents a plan of the area with the groundwater contours reported in the preliminary geotechnical investigation (7). A groundwater divide is indicated near the proposed alignment of dikes along the southern side of Route 95 near Division Street, effectively separating existing groundwater flow patterns between those flowing south westerly into Carr Pond from those flowing northerly into Lake Mishnock. At the present time, as a consequence of the groundwater divide, the hydraulic gradient of the groundwater from the proposed dike alignment near Division Street to Lake Mishnock is nearly flat and we would expect very little groundwater flowing northerly into Lake Mishnock from the Division Street area. Apparently, the major groundwater contributions to this lake are presently from the east and west.

The design reservoir pool elevation is at 300 feet (91.5 meters) NGVD (National Geodetic Vertical Datum). The ground elevation along Route 95 in this area is approximately 310 feet (94.5 meters) NGVD. The ground surface drops off rapidly to the north in the direction of Lake Mishnock where the ground and water elevation is approximately 250 feet (76.2 meters) NGVD.

Upon completion and filling of the proposed Big River Reservoir and if no mitigating measures are taken, a rather large hydraulic gradient between the reservoir to the south of Route 95 and Lake Mishnock would
Figure 3 - Division Street Dike Vicinity Plan
be set up. This would increase seepage into Lake Mishnock perhaps increasing water levels on a lake already ringed with homes only a few feet above water levels. Other homes between the reservoir and the lake might be similarly affected.

The site is underlain by relatively pervious glacial deposits consisting mostly of sand and silt. They are mapped as undifferentiated sand and gravel deposit and a kame terrace (10). The soils have clearly defined stratification which is visible in borrow cuts in the area but not easily recognized in boring samples. The uniform grain size and stratification suggests that it may have been deposited in a glacial lakebed with some thin coarser outwash deposits near the surface.

Figure 4 from KAME (7) presents a hydrogeologic section along the approximate alignment of the dikes. A deep valley was encountered in the area of boring D5 which coincides with the area of the steepest predicted hydraulic gradient under post construction conditions.

Figure 5 from KAME (7) presents a similar hydrogeologic section oriented perpendicular to that in Figure 4 and presents a section across the dike and along the location of potential leakage from the reservoir.

The major problem confronting the design engineer in this area is to quantify potential leakage from the reservoir if an impervious dike were constructed along the proposed alignment. Seepage losses beneath an impervious dike must be estimated with confidence. In addition, design alternatives to reduce leakage to acceptable levels need to be developed
LEGEND:

D-1  Boring Number
---  Existing Groundwater
-----  Proposed Reservoir Elev.

Note: For Location, see Figure 3

SECTION A - A

Figure 4 - Generalized Hydrogeologic Profile Number 1
Proposed Reservoir Pool Elevation

Proposed New Dike and Slope Treatment

Lake Mishnock Area

Figure 5 - Generalized Hydrogeologic Profile Number 2
and their effects on the seepage losses quantified with confidence.

An idealized soil profile assuming a singular stratum of soil was sufficient to characterize the soil profile was developed and is presented in Figure 6. The soil properties were estimated from the results of a series of laboratory tests. The mean and standard deviation of hydraulic conductivity and mean particle size were estimated from a series of grain size analyses on this soil. The autoregressive parameters were assumed equivalent to the results of field studies based on similar stratified soil by Smith (11). The porosity was estimated from soil descriptions and standard penetration test results.

A second soil profile which characterizes the soil conditions by using two soil strata is presented in Figure 7. The deeper soil stratum has a higher hydraulic conductivity and thus may act as a conduit for flow beneath the dike. Its thickness is limited to one row of the finite difference mesh located along the bottom of the section.

Both profiles have assumed an impervious barrier for the upper boundary for simplicity. The groundwater would actually flow upward somewhat after travelling beneath the impervious dike. In these examples, a stochastically generated mesh of autocorrelated hydraulic conductivity values are input to the numerical model while heads and resulting flow rate are determined. Subsequently mass transport is simulated by particles released from the upper left area of the region which eventually reach the right boundary. The main interest in this problem
Figure 6 - Computer Simulated Profile Number 1
Flow Region Characteristics:
K is lognormally distributed with
\( K = 5.5 \text{ ft/day}, \sigma_K = 5.0 \text{ ft/day} \) (upper stratum)
\( K = 19.1 \text{ ft/day}, \sigma_K = 17.4 \text{ ft/day} \) (lower stratum)
\( \alpha_x = 0.4, \alpha_y = 0.3 \)
Porosity, \( n = 0.3 \), 360 grid points in upper stratum
40 grid points in lower stratum

Figure 7 - Computer Simulated Profile Number 2
is the calculation of flow rate. Dispersion and travel times are of less concern.

The flow region and boundary conditions in this example do not result in uniform flow so a shape factor must be applied to the effective hydraulic conductivities. The technique to determine this shape factor was included in the companion paper (2).

The results of 40 Monte Carlo simulations for these two flow situations are summarized in Table 1. In addition to the two soil profiles already discussed is a third profile, profile 1A, which has the same layout but the soil is assumed to have a constant value for the hydraulic conductivity of 5.5 feet per day.

The intermediate coordinates during transit and travel time values listed are the mean values for all 400 particles which flow through the region. The reference to percentage of the region are as presented in Figure 6 and merely are a tabulation of time to get to that point in the region. Since an equal number of water particles are released from each of the 10 nodes which are release points, there is a bias in the travel times. More on this later.

These results demonstrate that the presence of the lower stratum of higher hydraulic conductivity increases flow by about 25 percent and lowers the mean value of the exiting y coordinate by approximately twelve feet. The median y coordinate at the end dropped approximately 12 feet. For Profile 2, the median water particle exits within this
### TABLE 1

**SUMMARY OF RESULTS - DIKE EXAMPLE**

|                                | Profile 1 | Profile 1A | Profile 2 |
|--------------------------------|-----------|------------|-----------|
| **Mean Values of Hyd. Conductivity (Ft/Day)** |           |            |           |
| Arithmetic                      | 5.52      | 5.50       | 7.21      |
| Geometric                       | 4.10      | 5.50       | 4.74      |
| Harmonic                        | 3.07      | 5.50       | 3.31      |
| Effective, Hydraulic (After Applying Shape Factor) | 4.41      | 6.37       | 5.43      |
| Effective, Travel Time (After Applying Shape Factor) | 3.26      | 5.04       | 4.99      |
| Std. Deviation of Hyd. Conductivity | 5.00      |            | 0         |
| **Flow Quantity (Cubic Ft/Day) - Mean** |           |            |           |
|                                 | 56.5      | 81.6       | 69.6      |
| **Standard Deviation**           |           |            |           |
| Porosity                        | 3.4       | -          | 4.4       |
|                                 | 0.3       | 0.3        | 0.3       |
| **Mean Coordinates After 191 Days (x)** | 194.8     | 272.2      | 205.4     |
| **Mean y Coordinate at End**     | 122.2     | 122.3      | 135.3     |
| **Median y Coordinate at End**   | 131.5     | -          | 151.2     |
| **Mean Travel Time (Days)**      |           |            |           |
| 50% Region                      | 404.0     | -          | 273.9     |
| 60% Region                      | 454.6     | -          | 305.1     |
| 70% Region                      | 504.8     | -          | 336.0     |
| 80% Region                      | 555.4     | -          | 366.2     |
| 90% Region                      | 605.9     | -          | 397.0     |
| 100% Region                     | 656.2     | 417.7      | 428.5     |
| **Std. Deviation of Travel Time (Days)** |           |            |           |
| 50%                             | 290.9     | -          | 122.9     |
| 60%                             | 292.5     | -          | 114.9     |
| 70%                             | 292.8     | -          | 109.1     |
| 80%                             | 292.2     | -          | 105.0     |
| 90%                             | 292.0     | -          | 103.3     |
| 100%                            | 292.3     | 148.9      | 104.7     |
lower stratum.

The adjusted mean values of the effective hydraulic conductivity fall within the expected range relative to the mean values calculated for the stochastic mesh of values for Profile 1. The effective hydraulic conductivity values are fairly close to the geometric mean, although somewhat lower. The effective value determined by flow is larger than that determined by travel time. No similar comparison was possible for Profile 2 because of the different stratification.

Figure 8 presents a plot of the x and y locations for each water particle after 191 days. The upper plot is for the Profile 1 case, the lower plot for Profile 2. It is clear that the influence of the lower stratum in Profile 2 has caused the water particles to move downward while traversing toward the low head boundary at the right. Figure 9 presents a plot for the starting x coordinate versus the ending y locations for the two cases. This figure also demonstrates the skewing effect of the lower stratum in Profile 2.

Figure 10 presents the time to traverse the region versus the starting x coordinate. Profile 1 results in a clear relationship of decreasing travel time with increasing starting x coordinate. This should be anticipated since we would expect a higher velocity as well as a shorter route for those particles starting closest to the dike.

The flow rate for Profile 1 was computed as 56.5 cubic ft/day per linear foot with a standard deviation of 3.4 cubic ft/day. Figure 11 presents
Figure 8 - X and Y Coordinates of Particles After 191 Days
Figure 9 - Starting X Coordinate Versus Y Coordinate at End of Region
Figure 10 - Total Travel Time Versus Starting X Coordinate
Figure 11 - Cumulative Mean of the Mean and Lag 3 Standard Deviation of Effective Hydraulic Conductivity Versus Simulation Number - Profile 1
the cumulative mean of the mean and lag 3 standard deviation of the effective hydraulic conductivity for this profile. As was indicated in the companion paper (2), the cumulative mean of the lag 3 standard deviation may only be used as a qualitative measure of the trend and stability of the standard deviation. The true measure of the standard deviation would require calculation of that term for all preceding values after each new observation is added. The effective hydraulic conductivity equals a constant times the flow rate. Figure 11 demonstrates that the mean value is very rapidly approached; in fact, there is very little fluctuation after 6 simulations. The mean of the lag 3 standard deviation reaches a fairly consistent level after approximately 26 simulations. A check for normality using the Kolmogorov D statistic indicates that the distribution of flow cannot be accepted as normally distributed to a high enough significance. Confidence limits can therefore not be predicted with accuracy. Even a quick observation of Figure 11, however, would certainly lead one to believe that the mean value of 56.5 cubic ft/day is a fairly good estimate of the flow rate.

Figure 12 presents similar results for Profile 2. The mean value of 69.6 ft/day is also reached very rapidly after only a few simulations. The value of the mean of the lag 3 standard deviation does not appear to reach a consistent mean value except perhaps in the last 4 or 5 simulations. The standard deviation of the flow rate was calculated to be 4.4 cubic ft./day. Again, normality could not be accepted by the calculation of Kolmogorov D statistic but the figure clearly indicates a
Figure 12 - Cumulative Mean of the Mean and Lag 3 Standard Deviation of Effective Hydraulic Conductivity Versus Simulation Number - Profile 2
consistent trend in predicted flow rates.

This analysis would assist the geotechnical engineer in making predictions of groundwater flow beneath the proposed dike. It would also demonstrate that the determination of the presence of the high hydraulic conductivity stratum overlying the bedrock would be an important one. In any case, this flow rate is likely to produce an increase in the groundwater levels around Lake Mishnock which is an unacceptable result.

The next step in the analysis which could be completed would be to study the effect of mitigating measures on the flow rate. A seepage blanket could be simulated extending the left boundary and thereby increasing the flow path. An alternative would be a partially pentrating cutoff wall to increase the travel path of the water downward and around the wall. Similar results would then provide the geotechnical engineer with sufficient information on the predicted flow rates and variations so that the decision on which alternatives to utilize may be made.

GROUNDWATER IN THE VICINITY OF A LANDFILL EXAMPLE

The second example considered was for flow in the vicinity of a waste landfill. The example is for a hypothetical landfill although landfills with similar conditions exist. This landfill has been sited upgradient from a waterbody approximately 600 linear feet (183 meters) as depicted in Figure 13. The landfill was initially begun by excavating to or somewhat below the water table to allow excavation of cover material. The landfill materials were then dumped in the excavation and this
Figure 13 - Landfill Vicinity Plan
dumping has continued for several years.

Monitor wells down gradient from the landfill were installed recently and have indicated some contamination. An investigation into the extent of this contamination, the time required for this contamination to reach the stream, as well as the estimated flow quantity is desired.

The soil profile consists of a stratified fine sand and silt with the same properties as the earlier example. Its thickness is 150 feet (45.5 meters) overlying a crystalline bedrock. The upper and lower boundaries are considered no flow boundaries with the exception of the small area within the landfill itself. The left boundary is a constant head boundary and the right boundary is a no flow boundary beneath the stream indicating a groundwater divide there. Figure 14 presents the soil profile utilized by the computer program to simulate the flow problem.

Table 2 presents the results of the analysis of this simulation. A shape factor was again determined as before to adjust the values of the effective hydraulic conductivities. The adjusted values again indicate that the geometric mean is the best predictor of the travel time and flow rate.

The mean flow quantity for the 40 simulations was calculated at 43.2 cubic ft/day flowing into the stream. The quantity of leachate present would be a part of this total quantity determined by the characteristic of the leachate generation process at the landfill. Assuming no change in the hydraulic head at this point, the results of the travel time
Flow Region's Characteristics:

- \( K \) is lognormally distributed with \( \bar{K} = 5.5 \text{ ft/day} \) and \( \sigma_K = 5.0 \text{ ft/day} \), \( \alpha_x = 0.4 \), \( \alpha_y = 0.3 \)
- Porosity, \( n = 0.3 \), 400 Grid Points

Constant Head = 100'
and Particles are Released from Left and Part of Upper Boundary at x's

Constant Head = 50'
and Particles are caught at right Boundary

Figure 14 - Computer Simulated Landfill Profile
## TABLE 2

### SUMMARY OF RESULTS - LANDFILL EXAMPLE

|                                | Profile 1 | Profile 1A |
|--------------------------------|-----------|------------|
| **Mean Value of Hyd. Conductivity (Ft/Day)** |           |            |
| Arithmetic                      | 5.46      | 5.50       |
| Geometric                       | 4.05      | 5.50       |
| Harmonic                        | 3.01      | 5.50       |
| Effective, Hydraulic (After Applying Shape Factor) | 3.44      | 5.07       |
| Effective, Travel Time (After Applying Shape Factor) | 3.15      | 4.89       |
| **Std. Deviation of Hyd. Conductivity** | 4.87      | 0          |
| **Flow Quantity (Ft³/day)**      | 43.2      | 64.4       |
| **Porosity**                    | 0.3       | 0.3        |
| **Mean Coordinates After 191 Days (x)** | 172.5     | 250.7      |
| (y)                             | 65.6      | 77.2       |
| **Mean y Coordinate at End**    | 27.8      | 27.7       |
| **Mean Travel Time (Days)**     |           |            |
| 50% of Region                   | 392.2     | 240.9      |
| 60% of Region                   | 457.4     | 282.5      |
| 70% of Region                   | 522.6     | 324.2      |
| 80% of Region                   | 584.2     | 365.5      |
| 90% of Region                   | 642.9     | 405.0      |
| 100% of Region                  | 681.9     | 430.6      |
| **Std. Deviation of Travel Time (Days)** |           |            |
| 50% of Region                   | 179.0     | 87.3       |
| 60% of Region                   | 181.5     | 87.4       |
| 70% of Region                   | 182.2     | 87.9       |
| 80% of Region                   | 183.4     | 89.1       |
| 90% of Region                   | 190.1     | 92.9       |
| 100% of Region                  | 199.5     | 97.6       |
simulations indicate that approximately 45% of the water exiting at the river will pass through the landfill and be contaminated.

The mean x and y coordinates after 191 days are 218.8 feet and 54.5 feet, respectively. Figure 15 presents a plot of the x and y coordinates of the flow particles at this time as well as a plot of the starting x coordinate versus the y coordinate at the end of the region. This figure illustrates that the particle swarm separates somewhat with a large number of the particles moving downward into the flow region, the lowest penetration being 120 feet into the 150 foot thick sediment. Generally those particles starting from the end of the landfill closest to the surface water body stay near the surface and exit the highest. Those which start from the upgradient side plunge deeper and exit lower into the stream.

Figure 16 presents the time to traverse the region versus the starting x coordinate. A relationship is suggested similar to that in the dike example that the travel time is increased as the distance away from the river increases. This is expected and is undoubtedly due to the lower velocity, the longer travel distance and the indirect route taken downward into the sediment by those particles farthest from the stream.

The distribution of travel times could not be accepted as normally distributed by the Kolmogorov D statistic because of the several extremely large travel times recorded. Consequently, confidence limits on the travel time could not be developed. However, by inspecting Figure 17 which presents a histogram and breakthrough curve for this
Figure 15 - Particle Location after 191 Days and Starting X Coordinate Versus Ending Y Coordinate
Figure 16 - Total Travel Time Versus Starting X Coordinate
Figure 17 - Statistical Summary on Travel Time
simulation, some confidence may be developed on the range of values of arrival time at the stream.

CONCLUSIONS

The usefulness of the methodology outlined in the companion paper has been demonstrated by two field problems. The following conclusions concerning the results of these examples in steady state groundwater flow may be drawn:

1. The geometric mean is the best predictor of the effective hydraulic conductivity in terms of flow rate and travel time after applying a shape factor.

2. Very few simulations are required to develop a consistent value of the mean flow rate and travel times in the regions considered.

3. The presence of a high hydraulic conductivity stratum at depth may significantly increase the flow through the region even when the flow is generally parallel to the stratum.

4. Estimates of confidence limits may be developed from the results of these analyses when normality is confirmed and assuming that the soil properties adequately characterize the in situ soil.
5. Even when the distribution of travel times and flow rates cannot be accepted as conforming to a normal distribution, confidence may be developed in the predictions of these results by reviewing the histograms and cumulative mean results.

6. More work is needed to develop autoregressive parameters for sediments. It is not likely that these parameters will vary over a large range but more actual field studies are required to develop these parameters.
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APPENDIX A

INTRODUCTION AND REVIEW OF THE PROBLEM

I. Introduction

Groundwater flow problems have always been particularly challenging due to their complexity and the uncertainties involved. Increasingly, predictions of flow quantity, heads, direction and/or travel time are necessary to answer questions on risk and safety. This need for reliable predictions has brought investigators from various disciplines within the sciences into the arena. The result is that considerable progress has been achieved in advancing the state of the art in recent years.

The complexity of these problems is derived from many factors. One factor is the difficulty in scaling up and averaging quantities at the microscopic or particle level to the macroscopic or field scale of the flow region. Another factor is the incomplete knowledge of flow regime caused by the complex conditions during deposition and/or subsequent weathering. Still other factors are the sheer number of variables and the limited resources available for analysis.

Over the years, numerous techniques have been developed to treat these groundwater flow problems. Analytical formulations which lead to exact solutions for the flow conditions, have been developed for many flow situations, (Harr 1962). Analytic techniques suffer from their lack of flexibility and the need to make restrictive simplifying assumptions for...
boundary conditions and media characteristics thereby inhibiting their use with most problems.

Perhaps the most widely used technique today is that of flow nets, see Casagrande (1937), Cedergren (1977). Its greatest advantage is its simplicity and ease in use. This technique is also limited in its ability to vary soil hydraulic conductivity and groundwater free surface.

Scale models in sand tanks have also been utilized to study the flow of groundwater e.g. Bear (1961), Prickett (1975) (Grace 1981). Boundary conditions may be rather flexible but hydraulic conductivity variations cannot be easily simulated, capillarity action and grain size cannot be properly scaled and time is distorted. Other physical models such as the viscous fluid model have been utilized (Rushton and Redshaw, 1979) but they also require considerable expertise and specialized equipment.

A common characteristic of all these techniques is their lack of flexibility in boundary condition treatment and/or soil property characteristics. When these techniques are utilized, the consequences of the required averaging and other approximations are often unknown to the investigator.

With the recent interest in this area from the multitude of scientific disciplines and with the advancements in computer technology in the last decade, major changes in the way these flow problems are treated have occurred. Investigators have developed numerical solutions which allow
much more latitude on boundary conditions and input parameters and therefore allow more realistic characterizations of flow regimes to be economically considered.

Numerical solutions are approximate solutions. However, when properly executed they result in solutions within the desired level of accuracy. The most common types of numerical solutions are the finite element method (FEM) and the finite difference method (FDM). Either of these methods may be used to solve most of the situations encountered, however, one method may have some advantage over the other for particular problems. A review of these methods may be found in Prickett (1975) and Wang and Anderson (1982).

These methods have provided the means to introduce not only more complex boundary conditions and input parameters but have allowed introduction of new considerations. Of these, stochastic generation of a correlated hydraulic conductivity distribution to represent the flow regions, stochastic simulation of microscopic dispersion and the utilization of probability techniques to quantify input and output are major considerations of this work.

II. The State of the Art

The methods outlined herein are intended to provide a tool for solving real problems. It is appropriate to consider the present state of the art for the types of problems for which this method will be appropriate.
Universities and other research institutions have led the way in the development of numerical methods. Here finite element and finite difference methods are routinely used to study groundwater flow. Numerous researchers have investigated the significance and usefulness of introducing variability of soil parameters to the problem. Some of these have proven fruitful; others have not.

Workers in government and industry who are faced with real field problems have generally relied on less sophisticated models for most problems. Numerical models have generally been utilized for only the most critical field problem where large amounts of money and data are available.

The advancement of these techniques in research work coupled with the tremendous increase in computing power available provides the potential to expand the use of these new techniques in all the areas of the field. It is to this technology transfer that this work is directed.

III. Numerical Methods

Both finite element and finite difference methods require that the region be represented as a system of blocks or elements. Mathematical expressions are written for each block or element and combined with the boundary conditions to yield a system of simultaneous equations which can then be solved for the unknown values, normally the hydraulic heads.

The finite difference method was chosen for this work for several
reasons. Working computer codes have been available for some time using
the finite difference method. They are fundamentally quite simple and
adequate for most real problems. More practitioners are familiar with
the finite difference method than finite element method and the numeri-
cal method was of secondary importance to the characterization of the
flow region, the dispersion studies, and output analysis.

The basis of these numerical models are Darcy's Law and the continuity
equation. Darcy (1856) conducted a series of experiments to observe
what factors governed the flow of water through a sand column. Darcy
reported a direct relationship between the flow rate, Q, and the cross-
sectional area, A, and head drop, \( h_2 - h_1 \). An inverse relationship was
found between the flow rate and the length over which the head drop
occurred, \( l_2 - l_1 \). The resulting equation is given below with the nega-
tive sign inserted to indicate that the flow occurs in the direction
that head decreases.

\[
Q = -KA \frac{(h_2 - h_1)}{l_2 - l_1}
\]  

(1)

In this expression, \( K \) is the proportionality constant called hydraulic
conductivity.

The term, hydraulic conductivity, is utilized here and elsewhere (i.e.,
Freeze and Cherry, 1979) for this proportionality term rather than the
permeability term most often used in the civil engineering field.
Hydraulic conductivity is a function not only of the flow media but also
of the pore fluid. When the effects of the pore fluid are extracted
from this term, a second proportionality constant is left which is a function of the flow media only. This second term is also at times referred to as the permeability, the specific permeability or the intrinsic permeability. The adoption of the term hydraulic conductivity for the proportionality constant in Darcy's equation is made to avoid confusion with work done in other disciplines as well as a conviction that eventually this convention will be adopted by all workers in the field.

Laplace's Equation has been derived from the continuity equation for groundwater flow and Darcy's Law by others (i.e., Wang and Anderson, 1982) and is presented below:

\[
\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2} + \frac{\partial^2 h}{\partial y^2} = 0
\]  

(2)

This is the governing equation for groundwater flow in an isotropic homogeneous aquifer in three dimensions under steady state conditions. This equation becomes the basis of the solution by the finite difference method.

To understand the basic concepts, a simplified discussion in two dimensions follows. Figure A.1 presents the overall flow problem to be represented for a two dimensional region as well as a close-up of one section of the finite difference mesh. Here the blocks are node centered and the head value is constant in each block. The size of the blocks is \( \Delta x \) by \( \Delta y \). The head at nodal point \( i, j \) is signified as \( h_{ij} \). The forward finite difference approximation of the first
Figure A.1. - Flow Region Representation
derivative, \( \frac{\partial h}{\partial x} \) is \( \frac{\Delta h}{\Delta x} \) which for nodes 0 to 3 is

\[
\frac{\Delta h}{\Delta x} = \frac{h_0 - h_3}{\Delta x}
\]

The second derivative is approximated as the difference between adjacent first derivatives. Thus for the case considered in Figure A.1, the second derivative is:

\[
\frac{\partial^2 h}{\partial x^2} \left( \frac{h_1 - h_0}{\Delta x} - \frac{h_0 - h_3}{\Delta x} \right) = \frac{h_1 - h_3 - 2h_0}{(\Delta x)^2}
\]

and

\[
\frac{\partial^2 h}{\partial y^2} \approx \frac{h_2 - h_4 - 2h_0}{(\Delta y)^2}
\]

Utilizing Laplace's Equation, and if \( \Delta x = \Delta y \), then we get the equation for this node:

\[
h_1 + h_2 + h_3 + h_4 - 4h_0 = 0
\]

Similar expressions may be written in succession for all the nodes in the region, substituting boundary conditions where appropriate. The result is a series of simultaneous equations which, when solved, yield the head values at all the nodes.

Many techniques have been utilized to perform this job. Reiter (1981) adopted the computer code developed by the USGS in their 1976 finite difference model as described in Trescott, et. al (1976). The Iterative Alternating Direct Implicit (IADI) technique described by Reiter (1981) was used to determine the head values at the nodal points
in the flow region for the problem's boundary conditions in this work.

IV. Boundary Conditions

The conditions at the edges of the flow region which must be entered to obtain a solution are the boundary conditions. These conditions define the limits of flow and make the solution of flow within the region unique.

Boundary conditions are of two general types: constant flow, often no flow, and constant hydraulic head. It is quite common to have combinations of both types in each field problem.

The initial boundary condition considered is one of shape or configuration of the no flow boundary. This is really a type of constant flow condition where some nodes have no flow. The simplest example of this is one dimensional flow such as flow in a narrow pipe. Flow conditions are relatively simple here and will get progressively more complicated as flow in two or three dimensions are considered. It is clear that real field problems are three dimensional problems, however, the study of three dimensional flow can require enormous amounts of data and effort to solve when compared to two dimensional problems. Fortunately, flow in two dimensions can often represent field conditions reasonably well and therefore most studies still rely on two dimensional models.

Another restriction is the need to limit the flow regime. In two dimensional flow the simplest region is a square or rectangular region as
presented in Figure A.1. This configuration often adequately models the flow region. However, oftentimes an irregularly shaped region can more accurately describe the flow region and thus the boundary conditions must be modified.

This initial type of boundary condition generally limits flow at the boundary. This may be necessary to simulate no flow through impervious strata as across groundwater divides. At no flow vertical boundaries, the flow in the horizontal or x direction is zero so that \( \frac{\partial h}{\partial x} \) must also equal zero. Figure A.2 presents a typical problem in two dimensional groundwater flow with its corresponding boundary conditions.

The second type of boundary condition was that of hydraulic head regulation. This condition basically maintains a consistent head of known magnitude at the boundary, either constant or otherwise. Irrespective of conditions within the region, the head values are unchanged at these boundaries. The reason for setting these conditions in the problem may be to simulate a surface water body such as a lake or stream.

For real problems, the boundary conditions are usually determined with the use of observation wells and careful study of the region to locate significant water bodies and other indications of the groundwater gradient. No flow boundaries must also be identified and recognized either in very impervious strata or groundwater divides.

V. Characteristics of the Region
Impervious Boundary

Left Boundary has constant Hydraulic head = $H_u$

Right Boundary has constant Hydraulic head = $H_L$

$\frac{\partial h}{\partial y} = 0$

Figure A.2. - General Flow Region
Perhaps the most significant input to the flow problem solution is that of the characterization of hydraulic conductivity. The range of values which this single parameter may realistically have is very broad. Hydraulic conductivities in natural deposits of soil have been found to vary by thirteen orders of magnitude. Freeze and Cherry (1979) indicate that the hydraulic conductivity of some gravels may be as high as 100 centimeters per second and that of some clays as low as $10^{-11}$ centimeters per second. The hydraulic conductivity of some rocks may even be lower than this.

It is not common for an engineering parameter to vary by this much. Figure A.3 from Cedergren (1967) compares the range of possible values for hydraulic conductivity with other common soil parameters: strength and unit weight. It has been found that the same soil type may vary by as much as six orders of magnitude and the same stratum by more than one order of magnitude. This information suggests that simply knowing the order of magnitude of the hydraulic conductivity will be useful and that it is unlikely that we can determine the value at any point to within much closer than an order of magnitude. We also can expect to see a relatively large variation, perhaps an order of magnitude or more, within a "homogeneous" deposit.

Geologists, geotechnical engineers, irrigation engineers, and petroleum engineers, among others, have attempted to develop methods to estimate the value of hydraulic conductivity insitu. Estimates have been attempted by testing "undisturbed" samples in the laboratory, by empirical relationships with grain size and density, and by field testing, includ-
Figure A.3 - Variability of Soil Engineering Properties, after Cedergren (1967)
ing field pumping tests and outflow tests. The results of these many attempts suggest that no method is very accurate and there are advantages and disadvantages for each of the methods adopted.

Estimates utilizing grain size distribution have been tried by many investigators. Perhaps the most commonly used equation is the Hazen formula given below.

\[ K = C \left( d_{10} \right)^2 \]  

(7)

In this equation \( d_{10} \) is the particle grain size which 90 percent of the soil is larger and 10 percent is smaller. The constant, \( C \), has been estimated to be from 1.0 to 1.5 if \( d_{10} \) is in millimeters and \( K \) is in centimeters per second. Although this equation was developed originally for fairly uniform sands, it has been found to be adequate for most sands and gravels. The major advantage of this equation is its relative simplicity.

A similar empirical relationship was developed by The Corps of Engineers. The relationship presented in Figure A.4 from Leonards (1962) was developed on the basis of results of field pumping tests. This relationship was also based on tests of sands and gravels. The range predicted by the Hazen formula was superimposed on this figure for comparison purposes.

Other more complicated formula have been developed which seek to incorporate other factors which have a demonstrated effect on the hydraulic conductivity values. Some of these factors are the sorting or uniform-
Figure A.4 - Empirical Relationship Between Grain Size and Hydraulic Conductivity, after Leonards (1962)
ity of the grain sizes in the soil. A soil which is well sorted contains mostly one particle size and the hydraulic conductivity will tend to be higher. A soil which is not well sorted will be well graded, the smaller particles filling the voids between the larger particles and thus lower hydraulic conductivity. An example of these is one developed by Masch and Denny (1966) given in the form of a semi-log plot in Figure A.5. The grain size curves plotted in Krumbein \( \Phi \) units where \( \Phi = \log_2 d \) and \( d \) is the particle size in millimeters. The sorting aspect takes the form of a factor referred to as \( \sigma_I \) which equals

\[
\sigma_I = \frac{d_{16} - d_{84}}{4} + \frac{d_5 - d_{84}}{6.6}
\] (8)

These relationships were developed for sands and gravels tested under controlled conditions in the laboratory.

Prugh developed a series of curves dependent on the uniformity coefficient for three levels of density, i.e., loose, medium dense and dense (Powers, 1981). These empirical relationships were developed with results of field pumping tests.

Another soil parameter affecting hydraulic conductivity is porosity or void ratio since the two are directly related. The higher the porosity or void ratio, the higher the hydraulic conductivity, all other factors the same. The best known equation which includes this factor is the Kozeny-Carmen equation (Bear 1972) given below:

\[
K = \frac{P \, g \, n^3}{u \, (1 - n)^2} \frac{d^2}{180}
\] (9)
Figure A.5 - Other Empirical Relationship Between Grain Size and Hydraulic Conductivity, after Masch and Denny (1966)
In this formula, \( p \) is the density and \( u \) is the viscosity of the fluid, \( g \) is the acceleration of gravity and \( d_m \) is the representative grain size.

Other less significant factors such as particle shape and packing have also been suggested, Todd (1980), for correlation with hydraulic conductivity. The effects of these other factors are relatively insignificant when compared with those already discussed, and therefore are not generally accounted for.

Laboratory testing of samples of the soil may yield quite reasonable values for some soils. Lambe (1951) presents the procedures most often utilized in an engineering soils laboratory to conduct these tests. Voids along the edge of the permeameter may affect the results, particularly of cohesive soils. Undisturbed samples of granular soils are virtually impossible to collect so that reconstituted samples are generally tested. These modifications of the samples may also severely modify the results.

Field testing of soil inplace consists of generally two techniques. The best is often referred to as slug or outflow tests. Such tests consist of simply introducing or withdrawing water into a piezometer or observation well and observing the quantity of flow for constant head maintenance or the speed of water surface drop or rise. NAVFAC (1982) presents a good summary on how these tests may be performed and analyzed. The major problems with these tests are that some water may be pushed up voids along the casing, or a collection of silt on the bottom of the casing may distort the results. The test generally
represents only a small volume of soil and the hydraulic resistance of the screen, if any, is not accounted for.

The other type of field test is the pumping test. This test generally consists of pumping from a screened well at a known flow rate and observing drawdowns in observation wells around the well. Stallman (1971) presents a good narrative on designing and analyzing a pumping test. This test is perhaps the most realistic of all the tests conducted but suffers from the fact the hydraulic conductivity value determined is some mean of all those insitu so that a sense of variability is not clear. It also is handicapped by the fact it is very expensive and can only be utilized when its high cost can be justified.

In light of the fact that the value of hydraulic conductivity is highly variable, many investigators have chosen to consider this parameter as a random variable. A random variable is a variable whose precise magnitude cannot be determined with certainty, a priori. This is certainly the case for hydraulic conductivity. Probability aspects will be discussed later in this appendix.

Another input parameter has already been mentioned. This is porosity which is defined as the volume of voids divided by the total soil volume, expressed in percent. Porosity is related to hydraulic conductivity but its maximum range of values is only from zero to 100%. Additionally, typical values for soil are only within the range of 15 to 60 percent. Porosity is utilized to calculate the velocity of groundwater flow since the Darcy velocity is not the actual water particle
velocity but really a homogeneized term.

The other remaining input parameters are the microscopic or particle scale longitudinal and transverse dispersivities. The dispersivity is a property of the soil which relates to the spreading of the water particles about a mean direction of movement. This term attempts to incorporate the spreading due to the tortuous path followed as the water particle traverses the flow region. Dispersivity has been found to be an approximate function of the grain size of the porous media, Kelly (1982). Kelly pointed out the difficulty in scaling up sand column dispersivities from the laboratory to a field problem. A discussion on dispersion will follow in a later section.

VI. Stochastic Soil Modeling

Recent work in the study of groundwater flow indicates that engineers and geologists now recognize that it is oftentimes dangerous to characterize soil properties simply with some average value or some other presumably "conservative" estimate. Even the addition of multi-strata flow regions and sensitivity analyses on input parameters are not always satisfactory. Recently investigators have turned to the use of probability and statistics to facilitate their understanding of these complex problems.

Simple statistics have, of course, long been utilized to characterize soil properties, i.e., the average or mean value. However, it has been only recently that the randomness of the data, to some extent quantified
by its standard deviation, has been incorporated into the problem analysis e.g. Harr (1977). Other more powerful concepts are available and are now also being used.

There are many good introductory texts dealing with probability and statistics for engineers and scientists, e.g., Benjamin & Cornell (1970), Miller and Freund (1977) and Walpole & Myers (1978). It is not the purpose of this appendix to introduce these concepts since they are readily available elsewhere, however, some discussion will follow on their usage in the study of groundwater flow.

It is very unlikely that a soil property such as hydraulic conductivity or porosity will be uniform in situ. Variations are inevitable. However, when analyzing groundwater flow, the investigator must, by necessity, recognize similarities and divide the region into like strata to facilitate analysis.

Soil media involves numerous characteristics which may be considered as random rather than deterministic variables. This implies that the exact value of these characteristics or properties at any point is not known and cannot be predicted with certainty, a priori. There is uncertainty in any estimate prior to experimentation.

The principal difference between stochastic and deterministic soil modeling is that the former recognizes variability and attempts to quantify its effects. Since the probability distribution of a random variable describes the limits of its variability in probabilistic terms,
it may be used to generate a significant number of equally probable representations of the soil medium. The ensemble of solutions to the flow problem provides input on the variability of these results. This repetitive simulation of the flow media and analysis of the ensemble of results is commonly referred to as a Monte Carlo simulation.

Most soil characteristics may be considered continuous random variables, i.e., may have non-integer values. The probability distribution relationship is therefore the probability density function (PDF) which simply relates the respective value of the variable with the corresponding probability.

Figure A.6 presents a typical PDF and the equation for this function which has been found to adequately characterize the characteristics of some soil properties. e.g., Lumb (1974) and Harr (1977). This PDF is for the Gaussian, or normal distribution, which is also the most commonly studied distribution. This distribution is completely defined by two parameters, the mean and the standard deviation.

A unique aspect of the normal distribution proven by probability theory is the Central Limit Theorem. The hypothesis of this theorem is that the normal distribution will approximate a random variable which is itself the sum of many other random variables. Benjamin and Cornell (1971) state the theorem as follows:

"Under very general conditions, as the number of variables in the sum becomes large, the distribution of the sum of random variables will approach the normal distribution."
mean $\bar{x} = 0$

$\sigma_x = 1$

$\bar{x} = 1$

$\sigma_x = 2/3$

$\bar{x} = 1$

$\sigma_x = 1$

$\bar{x} = 1$

$\sigma_x = 1.5$

Equation of Curve :

$f_x(x) = 1/(\sigma_x \sqrt{2\pi}) \exp(-z^2)$

where:

$z = x - \bar{x} / \sigma_x$

Figure A.6 - Probability Density Function for the Normal Distribution
A second PDF which is the result of multiplying many other random variables is the log normal distribution. Figure A.7 presents several forms of the PDF for the log normal distribution with different values for the parameters. The equation for this PDF is also presented. Two aspects of the log normal distribution which have encouraged its use for some engineering aspects are that it fits data which is skewed and it precludes negative values for the random variable. Both of these characteristics are common in engineering data.

It should be pointed out that the log normal distribution may be considered a special case of the normal distribution. If a random variable, \( K \), is log normally distributed with a mean of \( \bar{K} \) and a standard deviation of \( \sigma_K \), then a new variable, \( Y = \ln K \), may be defined. This new variable, \( Y \), will have the normal distribution. In Appendix B, this fact is utilized to handle a random variable with a log normal distribution.

A useful technique of statistics which may be used to infer the probability distribution of a random variable is the transformation of variable technique. Freund and Walpole (1980) present a proof of this technique and some examples of its use. This technique uses the known relationship between two variables and the nature of the probability distribution of one of them to determine the probability distribution of the other.

Soil properties which are treated as random variables need not be categorized into a specific probability distribution with its known PDF.
Figure A.7 - Probability Density Function for the Log Normal Distribution, after Benjamin and Cornell (1970)
However, where this is possible, considerably less data is required to develop confidence in the prediction of the soil property at any given point. Of particular concern with the strategy of matching data with a known PDF are problems in the tails of the distribution, i.e., the extreme values of the distribution.

There are several accepted methods to verify that an assumed PDF properly models the data collected. The probability and statistics texts cited earlier treat these methods in detail. These methods may be divided into two main types, graphical and computational. Graphical techniques may be used to roughly determine if the assumed PDF is adequate. Comparison of histograms generated from collected data and from the assumed PDF such as those in Figure A.8 may be used as a qualitative measure of acceptance. Figure A.8 after Benjamin and Cornell (1971) also presents a plot of the same data on normal probability paper. Data from a normal distribution will plot as a straight line on this paper so that a measure of conformity to the distribution is possible. Large deviations from a straight line would cast doubt on the assumption of normality.

Two quantitative techniques which are utilized to test the appropriateness of a PDF to model observed data are the chi-squared and Kolmogarov–Smirnov tests. These techniques quantify the deviation of the observed data from the assumed PDF or cumulative distribution function (CDF) within a specified significance level. The most popular of these is the chi-squared test although it suffers from the fact that for continuous variables it requires dividing the range of values into
Figure A.8 - Example of Use of Histogram, Probability Density Function and Normal Probability Paper, after Benjamin and Cornell (1970)
discrete intervals prior to testing significance.

In spite of these problems fitting data into these known probability distributions, numerous soil properties have been categorized by various investigators. Table A.1 compiles the results of several of these attempts. Although this review should not be considered exhaustive, it does indicate a consensus for some of these soil properties. Of particular interest to this work is that hydraulic conductivity has been found to have a log-normal PDF and porosity a normal PDF.

With the extreme variability possible for input parameters and output, a measure of confidence in the predictions is desirable. Research work in this area has resulted in several methods for estimating confidence limits on the mean values and estimates of the error in these estimates. Miller and Freund (1977) show that for a normal distribution, the maximum error, $E$, in the prediction of the mean value of the population is:

$$E \leq \frac{Z_{\alpha/2}}{s/\sqrt{N}}$$

In this inequality $Z_{\alpha/2}$ is a tabulated value for the normal distribution, such that the area under this distribution to its right is equal to $\alpha/2$. Also $\alpha$ is the significance level, $s$ is the standard deviation of the sample and $N$ is the number of observations in the sample.

Similarly, they also develop estimates of confidence limits for the population mean, $\bar{X}$ as follows:
| Soil Property                  | Reference                        | Log (1968) | Hussey (1968) | Petrović (1967) | Murray and Pereira (1965) | Sugarny et al. (1965) | Naidoo & Izatt (1965) | Nelder & mex (1966) | Loomis & Hoo (1968) | Loomis (1970) | Loomis (1972) | Van Noordt (1976) | Van Noordt (1976) | Van Noordt (1976) | Taylor (1982) |
|-------------------------------|----------------------------------|------------|---------------|-----------------|---------------------------|-----------------------|----------------------|---------------------|-------------------|----------------|----------------|-----------------|-----------------|-----------------|--------------|
| Grain Size                    |                                  | N          | N             |                 |                           |                       |                      |                     |                   |                |                |                  |                  |                  |              |
| . log d50                     |                                  |            |               |                 |                           |                       |                      |                     |                   |                |                |                  |                  |                  |              |
| . deviation                   |                                  | N          | N             |                 |                           |                       |                      |                     |                   |                |                |                  |                  |                  |              |
| . skewness                    |                                  | N          | N             |                 |                           |                       |                      |                     |                   |                |                |                  |                  |                  |              |
| Void Ratio                    |                                  |            | N             |                 |                           |                       |                      |                     |                   |                |                |                  |                  |                  |              |
| Water Content                 |                                  |            | N             |                 |                           |                       |                      |                     |                   |                |                |                  |                  |                  |              |
| Total Unit Wgt.               |                                  |            | N             |                 |                           |                       |                      |                     |                   |                |                |                  |                  |                  |              |
| Atterberg Limits              |                                  |            | N             |                 |                           |                       |                      |                     |                   |                |                |                  |                  |                  |              |
| Compr. Index                  |                                  |            | N             |                 |                           |                       |                      |                     |                   |                |                |                  |                  |                  |              |
| Compr. Ratio                  |                                  |            | N             |                 |                           |                       |                      |                     |                   |                |                |                  |                  |                  |              |
| Log of Consolid. Coeff.       |                                  | N          | N             |                 |                           |                       |                      |                     |                   |                |                |                  |                  |                  |              |
| Compressibility, DL           |                                  |            |               |                 |                           |                       |                      |                     |                   |                |                |                  |                  |                  |              |
| Max Past. c                   |                                  |            |               |                 |                           |                       |                      |                     |                   |                |                |                  |                  |                  |              |
| Unconf. Comp., qu             |                                  | N          | N             | N               | N                         | N                     | N                    | N                   | N                 | N               |                  |                  |                  |                  |              |
| Tan θ                         |                                  | N          | N             | N               | N                         | N                     | N                    | N                   | N                 | N               |                  |                  |                  |                  |              |
| Strength, c + tan θ           |                                  |            |               |                 |                           |                       |                      |                     |                   |                |                |                  |                  |                  |              |
| Permeability, k               |                                  |            | LN            | LN              | LN                         | LN                    | LN                   | LN                  | LN                | LN             |                  |                  |                  |                  |              |
| Soil Water Diffusivity        |                                  |            |               |                 |                           |                       |                      |                     |                   |                |                |                  |                  |                  |              |
| Porosity                      |                                  |            |               |                 |                           |                       |                      |                     |                   |                |                |                  |                  |                  |              |
| Stratification                |                                  |            |               |                 |                           |                       |                      |                     |                   |                |                |                  |                  |                  |              |
| Rock Components               |                                  |            |               |                 |                           |                       |                      |                     |                   |                |                |                  |                  |                  |              |
| Avg. Soil Values              |                                  |            |               |                 |                           |                       |                      |                     |                   |                |                |                  |                  |                  |              |

Note: N = Normal PDF, LN = Lognormal PDF
B = Binomial PDF, B = Beta PDF
P = Poisson PDF
In this inequality, $\bar{x}$ is the sample mean, $\sigma_x$ is the population standard deviation and $Z_{\alpha/2}$ is the value of $(\bar{x} - \bar{X})$ at which the CDF of the normal distribution equals $\alpha/2$. Unfortunately, the value of the population standard deviation is not known and we must utilize the sample standard deviation as an estimate. This may not have a significant effect on these estimates, particularly if the sample is large.

However, if the sample size is not large but the underlying distribution is the normal distribution, then another similar inequality has been developed and is presented below from Miller & Freund (1977).

$$x - t_{\alpha/2} \frac{s}{\sqrt{N}} < \bar{x} < x + t_{\alpha/2} \frac{s}{\sqrt{N}}$$

(12)

Here the variables are the same as indicated earlier. In all of these expressions, the confidence in the prediction is directly proportional to the scatter in the population and/or sample and indirectly proportional to the sample size. Given the population variance, the confidence in the estimates may be increased by increasing the sample size.

Estimates of confidence in the standard deviation of the variable for large samples taken from normal or near normal distributions may be made by using the following in equality from Miller and Freund (1977):
\[ \frac{S}{1 + \frac{Z_{\alpha/2}}{\sqrt{2N}}} < \sigma < \frac{S}{1 - \frac{Z_{\alpha/2}}{\sqrt{2N}}} \] (13)

In deterministic solutions to groundwater flow problems, data from field explorations and laboratory analysis are utilized to identify soil types, stratification and mean or "conservative" values for soil properties. A stochastic representation of these soil units or strata may be developed in accordance with the definitions in Greenkorn and Kessler (1969). Figure A.9 presents frequency distributions for hydraulic conductivity for the four possible combinations of uniformity and homogeneity.

Case a in Figure A.9 represents the typical deterministic representation of a soil medium. It is virtually inconceivable that a single value or even two values of hydraulic conductivity would be representative of a real soil medium although some attempts have been made in this area. We shall discuss these later. Cases a and b cannot be expected to accurately simulate real field media unless a singular value were determined. Case c is an example of a singular modal probability density function such as a normal or log normal distribution which have been found to adequately represent the variability of several soil properties. This case of soil property distribution has also been referred to as statistically homogeneous and this definition will be adopted here.

The nature of the origin of a soil deposit is reflected in its flow characteristics. The number of factors which affect deposition of soil
Figure A.9 - Possible Probability Density Functions for Hydraulic Conductivity, after Greenkorn and Kessler (1969)
is immense and variable. Conditions predominant at one time and place will undoubtedly be somewhat altered elsewhere resulting in changes in flow characteristics. The combinations of these factors are random, but it should not be unexpected to find similarities at adjacent locations when compared to locations separated by some distance.

Lumb (1974) developed an expression for a soil property which is dependent on the value of that property on either side plus a random distortion. This expression written in terms of the random variable, hydraulic conductivity, $k$, where $a$ and $b$ are measures of dependency is given below:

$$ K_i = a K_{i-1} + b K_{i+1} + E_i $$  \hspace{1cm} (14)

This expression indicates a dependency only in one dimension, i.e., the direction of the $i$ axis. The purely random distortion is included in the term $E_i$ which would be a value taken from a distribution with mean of zero and a specified variance.

Lumb suggests that generally soil properties should be expected to display dependency forward and backward along the $i$ axis when this coincides with the horizontal, and some soil properties may also show dependency in one of the vertical directions.

Bartlett (1975) extended the work of Whittle (1954, 1966) on a nearest neighbor stochastic process model. This model essentially relates the value of a random variable at one point to that at adjacent points.
Other work on the development of this model has been done by Brook (1964), Besag (1974) and Martin (1974) on agricultural forecasting. Smith and Freeze (1979a) developed a similar equation where a and b are equal. They refer to this technique as a nearest neighbor stochastic process model. Their terminology has been adopted herein. In their companion paper, Smith and Freeze (1979b) extended this to allow treatment of a dependency in two dimensions. Their expression is similar to that given below:

\[ K_{ij} = \alpha_x (K_{i-1,j} + K_{i+1,j}) + \alpha_y (K_{i,j+1} + K_{i,j+1}) + E_{ij} \]  

(15)

In this expression, the alpha terms quantify the dependency of the hydraulic conductivity values in the x and y directions.

Smith & Freeze utilized this expression to develop a series of simultaneous equations at all grid points within a specified flow region. These equations are solved for each stochastic representation, and the ensemble of equally probable distributions are statistically analyzed for significance. It is this method of Monte Carlo simulation of equally probable representations of the flow media which was selected for further investigation in this work.

A statistical measure of dependency of one random variable upon another is the correlation. The term autocorrelation refers to that dependency of the value of the random variable at adjacent locations. The autocorrelation coefficient \( \rho \) may be defined as:
\[
\rho (l) = \frac{\frac{1}{N-1} \sum_{i=1}^{N-1} (K_i - \bar{K}) (K_{i+1} - \bar{K})}{\frac{1}{N-1} \sum_{i=1}^{N-1} (K_i - \bar{K})^2}
\] (16)

In this expression, \(K_i\) and \(K_{i+1}\) are the value of \(K\) at node \(i\) and \(i+1\) respectively, and \(\bar{K}\) is the mean value of \(K\). It should be noted that because we have assumed a statistically homogeneous media, the mean and variance of the adjacent \(K\) values are equivalent and that the denominator equals the variance of \(K\).

An interesting result of this parameter is that it may vary only within the range of -1 and +1. A value of zero indicates no dependency, that of one indicates complete dependency, and a minus one indicates an inverse relationship.

Whittle (1963) developed expressions for the autocorrelation function assuming singular direction or one dimensional dependency, i.e., a unilateral Markov Process of:

\[
\rho (l) = \exp (- \alpha l)
\] (17)

Figure A.10 presents a plot of an autocorrelation function which would illustrate this relationship of correlation and distance. The correlation decays with distance.

Whittle also presented a similar equation for a bilateral Markov Process where \(K_1 (x)\) is the modified Bessel function of the second kind:
Figure A.10 - Autocorrelation Decay with Distance, after Smith and Freeze (1979)
Agterberg (1970) derived the expression for line sampling of a three-dimensional autocorrelation which is equivalent to the one for a unilateral Markov Process given above. Agterberg indicated that this expression has been found to be in agreement with experimental autocorrelation function for residuals obtained for geologic data. Lumb (1974) compared these theoretical expressions with results of testing on two natural soils. He concluded that for those soils, the autocorrelation function decayed quite rapidly for most soil properties. The strength of the soil with depth displayed the most sustained autocorrelation function.

Lumb (1974) concluded, however, that for a spacing of 1 to 2 meters, there would be no significant error in assuming an uncorrelated pattern. He suggested that for the soils studied, that a treatment of the soil property random variable as the sum of a trend component and a random component would perhaps be the best approach.

This alternative method of treatment of the similarity of soil parameter is referred to as trend analysis or trend surfacing. The development of this technique is generally credited to Krumbein and Whitten at Northwestern University, see e.g. Krumbein (1959) and Whitten (1959). The technique is something similar to the contouring of an area indicating spatial trends of high values compared to other areas with a lower value trend.
A form of regression equation is typically utilized to relate the unknown value of the parameter, e.g. \( w \), at each location within the region. The value of \( w \) is expressed as a function of one or more independent variables, \( x_i \), representing coordinates, corresponding constant coefficient, and a random component, \( e \). The random component is usually assumed to be normally distributed with a mean of zero and a standard deviation characteristic of the scatter within the soil determined in the field. Koch and Link (1970) present an excellent introduction to this technique with examples of its practical use. The simplest example of this technique is a linear one in one dimension. An equation may be written for the dependent variable \( w \) as follows:

\[
 w = C + Bx + e 
\]  

(19)

Here \( B \) and \( C \) are undetermined constants depending on the data. If we plot the data with the dependent variable as the ordinate and the coordinate \( x \) as the abcissa, then \( C \) will equal the intercept and \( B \) the slope of the line. The "best fit" for this line is characteristically determined by the method of least squares.

The \( e \) term may now be evaluated from the residuals, i.e., the variation of the data points from the fitted line. It is generally assumed to have a normal distribution with a mean of zero and a variance equal to the mean value of the squared distance for the "best fit" line.

This method may get far more intricate as the parameter to be modeled requires it. Two and three dimensional models are possible. The coordinate terms may include not only the first power of these coordinates,
but also higher powers and cross products in order that the trends be adequately mapped.

Tabba and Yong (1981a) have developed a working model for a quasi homogeneous soil utilizing the trend analysis technique. They combine the bias in the parameter measurement method with the random variation component so that the mean of the random variation will no longer always be zero.

Tabba and Yong (1981b) demonstrate how this technique may be utilized to assist the solution of real problems. This technique will essentially provide a complete representation of a flow medium's parameter given the value of flow medium's characteristic at certain locations.

An alternative method most frequently discussed in the literature is the spectral density treatment of the soil property random variable. Bakr (1976), Gelhar (1977), Gutjahr, et. al. (1978) and Gelhar, et. al., have demonstrated its use in groundwater flow problems. This approach recognizes the Fourier Transform pair consisting of the spectral density function for the random variable, \( S(f) \), and the autocorrelation function, \( R(x) \). A brief description of these concepts are presented here. A thorough presentation of this complex subject may be found in random vibration texts such as Newland (1975) and Bendat and Piersol (1971).

The soil medium is considered the result of a random process. The autocorrelation function, \( R(x) \), relates the influence of the value of the random variable at one point to that at some other point. The power
spectral density function, \( S(f) \), describes the general frequency information of the underlying random process. The form of the Fourier transform pair between \( S(f) \) and \( R(x) \) is:

\[
R(x) = \int S(f) \cos 2\pi f x \, df \tag{20}
\]

\[
S(f) = \int_{-\infty}^{\infty} R(x) \cos 2\pi f x \, dx \tag{21}
\]

In these expressions, \( f \) is the frequency defined as the inverse of the distance, \( x \), the distance between data points or the lag distance.

A random process which is large in the space domain will be small in the frequency domain. This is illustrated in Figure A.11 which presents the probability density function, autocorrelation function and power spectral density plot for a wide band random noise process.

The autocorrelation functions for the random variables discussed earlier as being characteristic of soil properties have been positive exponential functions similar to that shown on Figure A.11. Its power spectrum would therefore have a peak at low frequencies and decay fairly rapidly. Conversely, if the autocorrelation function decays rapidly, the power spectral density will shift to higher frequencies. The term white noise is referred to a random process with all frequencies of equal power and no correlation in the space domain.

This approach to the treatment of the media characteristics has a distinct advantage. Variations in soil properties may be treated in the continuum sense and therefore more exact representations of the medium are possible. The method suffers however from difficulties for the
Figure A. 11 - Wide Band Random Noise Process, after Bendat and Piersol (1971)
average practitioner in understanding the concept, as well as the large amount of real data required to make the procedures produce significantly more realistic result. The large amount of data required casts doubt on its use for most real problems due to the difficulty in verifying the parameters.

Van Marke (1977, 1978) describes the benefits of a probabilistic modeling of soil profiles. Van Marke proposed an alternate method for simulation of soil profile modeling which recognizes the variability in the soil and considers one or more of the soil properties as random variables which are functions of location. Figure A.12 presents this concept for a multi-strata representation of a soil profile in two and three dimensions.

Van Marke proposed that the soil parameter could be completely described by three statistical parameters: the mean, the standard deviation and the scale of the fluctuation. The scale of the fluctuation quantifies the distance over which the value of the soil property has strong correlation. He indicates that this scale of fluctuation is close to the mean distance between intersections of the value of the random variable and the mean. This is illustrated in Figure A.12. In fact, Van Marke demonstrated that this technique may be used to estimate the scale of the fluctuation.

Van Marke points out that this representation of the soil parameter random variable is quite similar to the approaches mentioned earlier. The scale of fluctuation is a different but related measure of correla-
Variation of Soil Property with Depth

Variation of Depth to rock in x-y Plane

Figure A.12 - Van Marke's Stochastic Representation of Soil Profile
tion of soil property. The concept of developing a large number of random variables in the problem solution, e.g., numbers and thicknesses of strata and soil properties such as hydraulic conductivity, porosity and dispersivity have great potential but it seems that this diversity will be very difficult to achieve due to the computational effort required.

As indicated earlier, several researchers have attempted to determine if a single "average" value of hydraulic conductivity in a homogeneous soil could satisfactorily represent the conditions in a more realistic heterogeneous soil. Warren and Price (1961) determined that the geometric mean would be the best estimate of this "average" value. The geometric mean, $K_g$, is defined as:

$$K_g = N \sqrt[1]{K_1 \cdot K_2 \cdots K_n}$$

(22)

Bouwer (1969) demonstrated this finding for a heterogeneous soil by numerical and analog methods calling this value the effective hydraulic conductivity.

Smith and Freeze (1979) summarized the results of several other researchers indicating that the geometric mean should be equal to this "effective conductivity" for steady state uniform flow. However, the geometric mean could not accurately estimate the effective hydraulic conductivity for non-uniform and/or transient flow.

Bouwer (1969) points out that the arithmetic mean is the normal average value, $K_a$ where
Willardson and Hurst (1965) indicate that this mean would be the best estimate if the soil were truly homogeneous and all variations were due to measurement error. Bouwer (1969) demonstrates that the arithmetic mean should be the best estimate for a highly stratified flow parallel to the layering and the harmonic mean should be the best estimate for flow perpendicular to the layering. The harmonic mean, $K_h$, is defined as:

$$K_h = \frac{N}{\frac{1}{K_1} + \frac{1}{K_2} + \ldots + \frac{1}{K_N}}$$  \hspace{1cm} (24)$$

Warren and Price (1961) suggested that a shape factor should be utilized to "normalize" the calculation of the effective hydraulic conductivity $K_q'$ for non-uniform and/or transient flow. This may be achieved by calculating $K_q$ for the flow through a homogeneous soil with the same geometry using this result to calculate a shape factor, $\hat{s}'$, where:

$$\hat{s}' = \frac{K_c}{K_q}$$  \hspace{1cm} (25)$$

In this equation $K_c$ is the value of the constant hydraulic conductivity and the $K_q$ is the effective hydraulic conductivity for this homogeneous soil.

VII. MASS TRANSPORT SIMULATION

Mass transport in groundwater through a stochastically generated flow
medium has been studied by various investigators, e.g., Smith and Schwartz (1980) and Gelhar, et. al. (1979). The classical development for mass transport in groundwater in a porous medium is given in the literature by various researchers. Freeze and Cherry (1979) indicate that mass transport may involve as many as six mechanisms: advection, dispersion, adsorption, chemical reaction, biological transformation and radioactive decay. The first two are present in virtually all cases while the remaining four may or may not be significant factors in the groundwater transport.

Advection is the movement of the water caused by hydraulic gradients. Dispersion is the movement of the water resulting from the spreading of the water particles due to diffusion and the natural heterogeneity at the pore scale of the flow medium.

Freeze and Cherry (1979) developed the one dimensional transport equation which includes only these first two mechanisms and it is presented below:

\[
D_L \frac{\partial ^2 C}{\partial l^2} - v_L \frac{\partial C}{\partial l} = \frac{\partial C}{\partial t}
\]  

(26)

In this equation \(D_L\) is the dispersion coefficient and equals the sum of the diffusion coefficient and dispersivity times the mean pore fluid velocity. \(C\) is the concentration, \(l\) is the length dimension, \(v_L\) is the mean tracer velocity, and \(t\) is the time.

Figure A.13 presents the setup and results of a common laboratory test
Continuous supply containing tracer concentration $c_0$ after time $t_0$

Overflow

Column of Sand

Screen

Outflow containing tracer concentration $c$

Sand Column

Schematic View of Water Transport Illustrating Dispersion

Tracer Curve without Dispersion

Tracer Curve with Dispersion

Figure A.13 - Tracer Experiment Layout, after Todd (1980)
which may be used to demonstrate this concept. Initially, a wave front is released from the upper portal and movement and distortion is traced. Ogata (1970) presented the solution to this differential equation in terms of the complementary error function, erfc,

\[
\frac{C}{C_0} = \frac{1}{2} \left[ \text{erfc} \left( \frac{1 - vt}{\sqrt{D_L t}} \right) + \exp \left( vL \right) \text{erfc} \left( \frac{1 + vt}{\sqrt{D_L t}} \right) \right]
\]

(27)

For all practical purposes the second term in the brackets is negligible and may be neglected.

The Central Limit theorem has been utilized to justify the assumption that the breakthrough curve illustrated in Figure A.13 should be normally distributed, e.g., Bear (1972), Fried (1975). This had been suggested for the displacement relationship provided the water particle is allowed to undergo a significant number of uncorrelated displacements. Fried (1975) presents a method to calculate the macroscopic or field scale dispersion coefficients given the results of a tracer transport experiment and utilizing the assumption of a normal distribution.

Smith and Schwartz (1980) utilized a nearest neighbor stochastic process model of hydraulic conductivity to characterize a uniform flow field. Water particles were released on one side and recovered along the down-gradient boundary. The particles were allowed to move by hydraulically driven advection and a stochastic simulation of microscopic dispersion. Their results indicated that normality for the breakthrough curve and a constant macroscopic dispersivity could not be confirmed.
Gelhar, et. al. (1979) studied the mass transport problem and found that for large distances the macroscopic dispersivity did appear to reach a constant value and appeared to be a function of the properties of the medium. They developed an equation for the effective macroscopic dispersivity for large times,

\[
a_{LT} = a_L + A_\infty
\]  

(28)

Where

\[
A_\infty = \frac{1}{3} \frac{\sigma_K^2}{\bar{K}^2} \left( \frac{1}{a_T} \right)^2
\]  

(29)

In this equation \( \bar{K} \) and \( \sigma_K \) are the mean and standard deviation of the hydraulic conductivity, \( a_T \) is the traverse dispersivity and \( l \) is the length scale.

Gelhar, et. al. (1979), concluded that the distance required to reach a constant dispersivity is large, perhaps exceeding 1 km to reach 90% of this value. This could explain the inability to measure a constant dispersivity on most field investigations.

A great deal of work has already been done in this area and yet we do not feel confident with the answers received by the current state-of-the-art procedure. This work will build on the earlier work and perhaps provide some additional measure of confidence in the results computed.
APPENDIX B
Details of Method Used

B.1 Introduction

It has been an objective of this work to develop a procedure to more realistically characterize the medium of groundwater flow for a field problem and to arrange the output so that definitive conclusions may be drawn utilizing statistical models. It is hoped that this will result in an improvement in the confidence that an engineer may have in the predictions of flow quantity and travel times.

B.2 General Technique

In this work, a two dimensional characterization has been chosen because it is the more common and simpler representation. A three dimensional model could have been adopted, but it would have been very difficult to implement to solve any real problems because of the tremendous amount of computation required. Although the computer has made the numerical methods possible, in practice, three-dimensional solutions are still not commonly done.

A rectangular flow region was chosen for study so that a general problem might be solved. Figure B.1 presents the layout of the idealized flow region with boundary conditions. Hydraulic conductivity is presumed to be statistically homogeneous with correlation in accordance with a
Impervious Boundary

Left Boundary has constant Hydraulic head = \( H_u \)

Right Boundary has constant Hydraulic head = \( H_L \)

\( \frac{\partial h}{\partial y} = 0 \)

Figure B.1 - General Plan of Region
stochastic nearest neighbor model. Variations in the soil media characterization, region shape and boundary conditions were also studied and will be discussed later.

The problem considered was one of a steady state flow situation. This condition was chosen because many real problems may be considered to be approximated by steady state conditions. The autocorrelation and dispersion techniques may be adapted to transient solutions as well.

The general procedure adopted to study this groundwater flow problem is detailed below:

1. Select a region size and shape, develop boundary conditions and soil media parameters which approximate the real situation.

2. Generate a stochastic representation of the flow media.

3. Utilizing a finite difference program with the Iterative Alternating Direct Implicit Procedure (IADI), solve for the heads and flow quantity for the steady state condition.

4. Release water particles from the upgradient side of the flow region to traverse the region under the action of advection and a stochastic simulation of dispersion. Record their respective travel times and locations upon reaching the downgradient side of the flow region.
5. Repeat the above process until a sufficient number of Monte Carlo simulations of the region and water transport has been completed.

6. Tabularize the data and perform statistical checks of significance on output so that definitive conclusions may be drawn.

B.3 Problem Definition

The initial step requires a definition of the region size and the soil properties. This step is required in any modeling of groundwater flow whether analytical, numerical or otherwise.

An idealized representation of the region in terms of finite blocks of homogeneous soil media is required. The hydraulic conductivity, porosity and head are assumed to be constant everywhere within each finite block.

As is often the case, a good deal of experience is required to make the selection of the number of blocks to represent the region. A trade-off of accuracy against computation time is necessary for numerical modeling. Often two representations at different grid spacings are made and compared to observe the effect of the variation in grid size to aid in this decision.

B.4 Hydraulic Conductivity
of constant hydraulic conductivity, the so-called block centered approach. Figure B.2.a. presents this diagramatically including the numbering system used. The nearest neighbor model uses the following equation to relate the conductivity at one point to all adjacent points.

\[
K_{ij} = \frac{\alpha_x}{4} (K_{i,j-1} + K_{i,j+1}) + \frac{\alpha_y}{4} (K_{i-1,j} + K_{i+1,j})
\]  

(1)

Where

- \(K_{ij}\) = Hydraulic conductivity at nodal point, \(i, j\).
- \(i\) = Row number with range from 1 to \(N_{ROW}\)
- \(j\) = Column Number with range from 1 to \(N_{COL}\)
- \(\alpha_x, \alpha_y\) = Autoregressive parameters which indicate the degree of correlation of hydraulic conductivity in the \(x\) and \(y\) directions. Range is from 0 to 1.

This relationship may be put in matrix form and a stochastic element introduced as follows:

\[
\{ K \} = [W] \{ K \} + \{ E \}
\]  

(2)

In this equation \([W]\) is a weighting matrix consisting of \(NP\) rows and columns where \(NP\) is the total number of nodal points within the flow region, i.e., \(NP = N_{ROW} \times N_{COL}\). The \([W]\) matrix is square while \(\{ K \}\) and \(\{ E \}\) are column matrices.

The \(\{ E \}\) matrix is a column matrix of random numbers with a preselected mean and standard deviation. The basis for selecting the mean and standard deviation will be discussed later.
\[ K_{ij} = \frac{a_x}{4} (K_{i-1,j} + K_{i+1,j} + K_{i,j-1} + K_{i,j+1}) + \frac{a_y}{4} (K_{i-1,j} + K_{i+1,j}) \]

- Interior Node -

\[ K_{i,j} = \frac{a_x}{3} (K_{i-1,j} + K_{i+1,j} + K_{i,j-1} + K_{i,j+1}) + \frac{a_y}{3} (K_{i+1,j}) \]

- Boundary Node -

Figure B.2 - Finite Difference Representation
Since the \( \{K\} \) matrix is the unknown result, we can rearrange this equation by bringing both \( \{K\} \) matrices to the left side as below.

\[
\{ K \} - \{ W \} \{ K \} = \{ E \}
\]  

(3)

We may then utilize the properties of an identity matrix and write

\[(\{I\} - \{W\})\{K\} = \{ E \}
\]

(4)

Finally, we may solve for \( \{K\} \) by multiplying by the inverse of \((\{I\} - \{W\})\) resulting in

\[
\{ K \} = (I - W)^{-1} \{ E \}
\]

(5)

We now have the necessary matrix equation for this method. We need only develop the Weighting matrix \( \{W\} \), subtract it from the identity matrix, \( \{I\} \), compute an inverse, which we will call the Filter matrix, and multiply by the \( \{E\} \) matrix.

It should be noted that the Filter matrix contains all the information concerning the autocorrelation of hydraulic conductivities with each of the blocks in the flow region. The \( \{E\} \) matrix contains the randomness component which is incorporated into the system of hydraulic conductivity values.

The nearest neighbor model is easily adapted for developing the \( \{W\} \) matrix for interior nodes. However, boundary nodes are another matter. Smith (1978) assumed that the \( \alpha \) term is divided by the number of adjacent nodes. Figure B.2.b. presents the situation along the upper boundary. Here this approach results in the following equation:
An alternative treatment of these boundary nodes was considered. This alternative approach treats these areas in the same way as finite difference grid manipulations at the boundaries resulting in the following equation.

\[ K_{ij} = \frac{a_x}{3} (K_{i,j-1} + K_{i,j+1}) + \frac{a_y}{3} (K_{i+1,j}) \]  

This approach results in greater weight being assigned to the K value horizontally along a soil layer for the end boundaries and less along the upper and lower boundaries. There would be no difference in the equations written at the corners of the flow region. Comparison of results computed by each treatment will be discussed later.

Figure B.3 presents a 7 by 7 flow region and the numbering system adopted. Since there is a maximum of 4 nearest neighbors, there is a maximum of 4 non-zero entries in each row of the matrix. The \([W]\) matrix which results with this numbering system is banded. A band width equal to two times the number of columns plus one is centered on the diagonal. The matrix is, however, not symmetrical. Figure B.4 presents the W matrix for the 7 by 7 flow region shown utilizing Smith's boundary conditions.

A log normal distribution of hydraulic conductivity is adopted here. Appendix A discusses the background for this assumption. As a consequence of this assumption, the \([E]\) matrix generated for each simula-
Figure B.3 - 7 By 7 Example of Region Representation

NP = NROW * NCOL = 7 * 7 = 49
Note: All spaces in matrix not occupied by a letter or zero should contain a zero.

See the Legend below for explanation of letter designation.

| m = 1 | 5 | 10 | 15 | 20 | 25 | 30 | 35 | 40 | 45 | 49 |
|-------|---|----|----|----|----|----|----|----|----|----|
| k = 1 | 0 | A | 0 | 0 | 0 | D | 0 | 0 | 0 | 0 | 0 |

LEGEND:

A = \alpha_x / 2       D = \alpha_y / 2
B = \alpha_x / 3       E = \alpha_y / 3
C = \alpha_x / 4       F = \alpha_y / 4

Figure B.4 - Weighting Matrix for 7 By 7 Region
tion will have a mean value of 0, a standard deviation of 1 and will follow a normal distribution. A log transformation will later be made so that the hydraulic conductivity values will be log normally distributed.

Smith (1978) demonstrated that if the \{ \mathbf{E} \} matrix is multiplied by a constant term, \( n \), the desired variance in the hydraulic conductivity values results. He showed that this constant term, \( n \), is a function of the desired variance of the conductivity distribution and the square root of a quantity \( G \) defined as:

\[
G = \frac{\alpha_y \rho_y (2)}{8} + \frac{\alpha_x \alpha_y \rho (1,1)}{2} + \frac{\alpha_y \rho (1)}{2} - \frac{\alpha_x \rho (1)}{2} + \frac{\alpha^2}{8}
\]

\[
+ \frac{\alpha^2}{8} + 1 + \frac{\alpha^2 \rho (2)}{8}
\]

where \( \rho_x (1) \) and \( \rho_y (1) \) are the lag 1 correlation coefficients of \( K \) in the \( x \) and \( y \) directions respectively. \( \rho_x (2) \) and \( \rho_y (2) \) are the lag 2 correlation coefficients of \( K \) in the \( x \) and \( y \) directions. \( \rho (1,1) \) is the lag 1 in the \( x \) direction and lag 1 in the \( y \) direction correlation coefficients of \( K \).

Because of the assumption of a log normal distribution of hydraulic conductivity, a transformation of the mean and standard deviation is required. It should be pointed out that the mean of the distribution of \( \ln K \) does not equal the natural log of the mean of \( K \). Benjamin and Cornell (1970) among others, present this transformation.
\[
\begin{align*}
\sigma_y^2 &= \ln \left( \frac{(\sigma_K/E)^2}{1} \right) \\
\bar{Y} &= \ln (\bar{K}) - \frac{\sigma_y^2}{2}
\end{align*}
\]

In these equations
\[
\begin{align*}
\sigma_y^2 &= \text{variance of } Y \\
\bar{Y} &= \text{mean of } Y \\
\sigma_K^2 &= \text{variance of } K \\
\bar{K} &= \text{mean of } K \\
Y &= \ln K
\end{align*}
\]

This transformation is performed and the values \(\sigma_y\) and \(\bar{Y}\) used with the \(\{E\}\) matrix. Following the multiplication by the filter matrix and addition of the mean of the \(\ln K\), a transformation back to \(K\) is made. This transformation erodes some of the correlation although this has not been found to be significant (Smith (1978)).

This method does not produce a distribution of hydraulic conductivity which fits exactly the desired correlation structure. This is due to the randomness inserted by the random number generator, the exponential transformation and boundary effects. However each generated distribution is correlated and approximates the desired correlation structure. When the ensemble of all Monte Carlo simulations is studied, a closer approximation to the desired correlation is obtained.

The computer code developed to perform these operations referred to as Inverse is included in Appendix D. A step-by-step description of the procedure is given below.
1. All data on the flow region characteristics are read into the computer and problem setup. (Lines 340 to 2320)

2. The transformation of statistical parameters for K to ln K is performed. (Lines 2330 to 2370)

3. The \( n \) term, (ETAN), is set equal to the required percentage of the standard deviation of ln K. (Lines 2372 to 2373)

4. A column matrix (EPSILN) of random numbers which are normally distributed with a mean of 0 and standard deviation of \( \sigma_y \) is generated, \( N(O,\sigma_y) \). (Lines 2375 to 2410)

5. The square ([I] - [W]) matrix is generated directly by inserting a 1 on the diagonal and making all other non-zero coefficients of the [W] matrix negative. (Lines 2420 to 3300)

6. The ([I] - [W]) matrix is then inverted and the new matrix, FILTR, stored on permanent disk file. (Lines 3310 to 3370)

7. The FILTR matrix is then multiplied by the EPSILN column matrix yielding the LNK matrix having \( N(O,\sigma_y) \). (Lines 3380 to 3440)

8. The desired mean value of ln K is then added to each term resulting in the XLNK matrix with \( N(\bar{Y},\sigma_y) \). (Lines 3450 to 3510)
9. The transformation is then made back to \( \{ K \} \) by taking the exponential of each term in the XLRK matrix and assigning the resulting \( K \) value to its respective position in the flow region. The resulting \( \{ K \} \) matrix has a log normal distribution with the desired statistical parameters within allowable tolerances. (Lines 3520 to 3530)

10. A check is then made for these statistical parameters, i.e., mean, standard deviation and auto correlation by rows, columns and the entire distribution and writes out results. (Lines 3540 to 6020)

This hydraulic conductivity matrix, \( \{ K \} \), is then the input matrix used to solve the flow problem. For subsequent simulations the steps, 1 through 3 and 5 and 6 need not be completed again. Only steps 4 and 7 through 10 are needed for independent values of stochastically generated hydraulic conductivity values for subsequent Monte Carlo simulations.

It should be noted that this computer code utilizes selected subroutines from the International Mathematics and Statistical Libraries (IMSL). These subroutines perform necessary tasks for which new subroutines could have been developed. It is considered unnecessary to do that, however, when efficient, documented routines are available.

An example of the use of such a routine may be found in Step 4. The EPSILN matrix is generated by invoking the GGNQF command. This step generates a random number from a normal distribution with a mean of zero
and a standard deviation of one. This procedure is done within a DO loop as many times as necessary to assign a value at each node.

A second example of the use of the IMSL library may be found in Step 6. The subroutine LGINF is called to invert the (I-W) matrix and thereby determine the FILTR Matrix.

The IMSL library has several routines which may be utilized to invert matrices. LGINF was selected because it is a generalized solution which could easily handle the problem. Other more efficient and/or accurate inversion routines could have been utilized to reduce required computer time or increase the accuracy of the solution. The reduction of required computer time to invert the matrix was not a major objective of this study although some efficiency might be desirable for subsequent work. The results cited later will demonstrate that the accuracy of the solution is sufficient.

Considering the difficulty at the boundary of maintaining the autocorrelation structure, it was decided to "shave off" the outer boundary nodes all around the block region. A 7 x 7 region would have the outer nodes deleted and thereby be reduced to a 5 x 5 region. This technique reduces the boundary effects but also reduces the size of the region which may be considered by this technique in light of the matrix inversion limitations.

To alleviate this limitation, the flow region can be considered a composite of two or more "blocks" that contain statistically homogeneous and
internally correlated hydraulic conductivity meshes. The shaved 5 x 5 region may be systematically added to 3 other statistically equivalent regions to develop in a 10 x 20 region. We will see that the computer time to add these regions together is much less than that required for inverting a larger matrix. Indeed there are real limits to the size of the matrix that may realistically be inverted.

B.5 Numerical Solution of Finite Difference Technique

The finite difference solution utilized to solve the flow problem was that computer code developed by Reiter (1981). This code was adapted from other available work, e.g. Trescott, et. al. (1976) for the two dimensional cross-sectional model.

The initial task to complete in the numerical solution is to write the finite difference equation at each nodal point as described in Appendix A. Several techniques may then be utilized to find the solution, e.g., iterative and simultaneous solution of the equations. Prickett and Lonniquest (1971) and Wang and Anderson (1982) describe some of these techniques. Iterative solutions include Jacobi and Gauss-Seidel iteration, successive overrelaxation and the iterative alternating direction implicit. This work utilized the iterative alternating direction implicit because it was a code which was readily available and earlier work revealed that solutions could be achieved somewhat faster than for example successive over relaxation.

An explicit finite difference solution technique is a forward difference
approximation since the head value which is being calculated is assumed a function of the previous estimate at adjacent nodes. An implicit solution involves a backward difference approximation where the head value is assumed a function of previous estimates at the node being calculated as well as at adjacent nodes. These methods were developed for transient problems but are equally applicable to steady state problems.

The IADI technique processes the equations row by row initially holding head values in adjacent rows constant. Upon completion of one pass, the same equations are processed column by column holding head values in adjacent columns constant. This completes an iteration and iterations continue until the maximum error at any point in the region is less than the requested allowable value.

B.6 Mass Transport

A major objective of this study was to analyze the effects of hydraulic conductivity variations on dispersion. A computer code was developed to simulate transport across the hydraulic field resulting from a steady state solution. Transport occurs due to hydraulic advection and a stochastic simulation of microscopic dispersion.

B.6.1 Advective Transport

The methodology utilized to determine the hydraulic head distribution has been described earlier. The results of each solution of a stoch-
astically generated realization of hydraulic conductivity is a steady state flow field. These results provide all the necessary input data to simulate advective transport.

As cited in Appendix A, the variation in porosity is much less than the variation in hydraulic conductivity. Porosity has been assumed constant throughout the region similar to the assumption in Gelhar, et al. (1979) and Smith & Schwartz (1980).

The solution assumes that hydraulic head, hydraulic conductivity, porosity and therefore the resulting velocity is constant throughout each individual block in the flow region. Velocities are calculated initially for each conductivity simulation and for each block within the region by the method suggested by Sauty (1976). Figure B.5 presents a representation of a portion of the flow region and the finite difference expression utilized to solve for the velocities in the X and Y directions. The method is basically a central difference approximation over the three neighboring nodes.

In these finite difference equations and in the figure, $V_x$ and $V_y$ are the velocities in the X and Y directions, respectively. The subscripts on K indicate the two nodes included in the calculation of harmonic mean, e.g., $K_{10}$ is the harmonic mean of K values at nodes 1 and 0. The value H is the hydraulic head at the node, n is the porosity and DELTAX and DELTAY are the node spacing in the X and Y directions, respectively.

This equation for the velocities has to be modified for boundary blocks
\[ V_x = -\frac{1}{2n}(K_{01}(H_1 - H_0)/\Delta x) + K_{03}(H_0 - H_3)/\Delta x) \]

\[ V_y = -\frac{1}{2n}(K_{02}(H_2 - H_0)/\Delta y) + K_{04}(H_0 - H_4)/\Delta y) \]

Figure B.5 - Schematic View of Interior Node of Finite Difference Mesh
since the velocity orthogonal to the boundary is zero. In these boundary blocks, the gradient is averaged over only one block length. An example is the upper boundary block where $\frac{dh}{dy} = 0$ as in Figure B.5, which is simulated by setting $H_0 = H_2$. The velocity in the X direction is calculated as before but in the Y direction, the equation reduces to the following:

$$V_y = -\frac{K_{04}}{n} \left(\frac{H_0 - H_4}{\Delta Y}\right)$$  \hfill (11)

Similar equations are written for other boundary blocks.

The advective transport $S_X$ and $S_Y$, is then calculated for a given time interval, $\Delta T$, by the equations below:

$$S_X = V_X \times \Delta T$$  \hfill (12)

$$S_Y = V_Y \times \Delta T$$  \hfill (13)

B.6.2 Microscopic Dispersion

Microscopic dispersion is included in the model in a manner first described by Ahlstrom, et al (1977) and then modified in part by Smith and Schwartz (1980). In this method, dispersion is treated as a stochastic phenomenon. The water particle is assumed to undergo a random displacement in the direction of flow and another random displacement perpendicular to flow. These displacements are calculated from the following two equations from Ahlstrom, et al (1977).

$$DL = \left(24 \times DLC \times \Delta T\right)^{\frac{1}{2}} \left(0.5 - RANOL\right)$$  \hfill (14)

$$DT = \left(24 \times DTC \times \Delta T\right)^{\frac{1}{2}} \left(0.5 - RANOT\right)$$  \hfill (15)
In these equations, DL and DT are the displacements in the longitudinal and transverse directions, respectively relative to the direction of advective transport. DLC and DTC are the longitudinal and transverse dispersion coefficients respectively. Anisotropy, if any, is presumed in the advective transport so no anisotropy is assumed in dispersivity. RANOL and RANOT are random numbers normally distributed with a mean of zero and a standard deviation of one then divided by six to keep the range of values in the -0.5 to +0.5 area.

Kelly (1982) developed a relationship which has been adopted for this study and assumes a direct relationship between grain size and microscopic dispersivity. This relationship may be expressed as:

$$\delta = 0.08 D_{50}$$

(16)

Where $\delta$ = dispersivity, in meters

$D_{50}$ = mean particle size in millimeters

The longitudinal dispersion coefficient, DLC, is taken equal to the dispersivity times the velocity, $V_L$, in the direction of flow. The transverse dispersion coefficient, DTC, is taken equal to a percentage of the dispersivity, DSPRAT, times the dispersivity and velocity, $V_L$.

The expressions from Ahlstrom, et al (1977) for microscopic dispersion are then modified by these assumptions to result in the following:

$$DL = (6.3* D_{50} * V_L * DELT) * RANOL$$

(17)

$$DT = (6.3* D_{50} * V_L * DELT) * DSPRAT * RANOT$$

(18)

Prickett and Lonnquest (1981) developed a similar approach which pre-
sumes a constant value for DELT, the time interval.

Since the advective transport direction will not always coincide with the X and Y axes the displacements in the X and Y directions are obtained by a transformation, ie,

\[ \text{THETA} = \arctan \left( \frac{SY}{SX} \right) \]  

(19)

The transformation is computed such that DSX and DSY are the dispersive displacements in the X and Y directions, respectively. Figure B.6 presents the vector diagram illustrating this transformation:

\[ \text{DSX} = DL \times \cos(\text{THETA}) - DT \times \sin(\text{THETA}) \]  

(20)

\[ \text{DSY} = DL \times \sin(\text{THETA}) + DT \times \cos(\text{THETA}) \]  

(21)

B.6.3 Particle Transport

The computer code simulates water movement from the upgradient side of the block or region to the downgradient side. Figure B.7 presents a typical problem flow region with flow from left to right. The manner in which displacements are included in the particle movement simulation within the region can now be detailed. Initially, a particle is released from the upgradient boundary. It moves a distance equal to the advective displacements, SX and SY. The random dispersive displacements, DSX and DSY are then added and the total displacements determined. A check is then made to see if the particle has moved out of the block. If is has not, a new time interval begins, new displace-
Figure B.6 - Velocity Vector Diagram
Figure B.7 - General Flow Region
ments are calculated and added to those previously summed.

Eventually the water particle moves out of the block, either laterally, vertically, or both simultaneously. The code checks for lateral movement out of the block initially. If this has occurred, the code checks to verify that the movement was only into the next block. If movement was beyond the next block, this fact is recorded and printed out so that the time interval can be reduced in a later simulation.

The code then calculates the portion of the time interval spent in each block for this time interval. An adjustment of the displacements in the new block is made to account for the change in velocity in the new block. This adjusted displacement is recorded and a new time interval is begun. If the particle reached the end of the region, the portion of the last time interval remaining after the particle reached the boundary is subtracted from the computed total travel time.

A check is made to determine if the particle is displaced vertically out of the block as well. If not, then the next time interval is begun. However, if vertical movement has occurred into the next block, a check is made for block skipping as before. If vertical movement results in contact with a boundary, the particle is reflected back into the flow region. No additional adjustment in displacements is made in the event of horizontal and vertical block changes, a new time interval is simply begun.

In the event that the particle was displaced vertically out of the block
but not horizontally out of the block, checks are made to record any skipping of blocks and reflection by the boundaries. An adjustment for displacements due to movement into the next block is made similar to the technique for lateral movement and a new time cycle begun.

Upon reaching the downgradient boundary, the following results are recorded in an array, tabularized and recorded on a data set file. These are then available for statistical manipulations and checks.

- Particle Number
- Simulation Number
- Starting Y Coordinate
- X and Y Coordinate at the time after starting estimated for travel to the region midpoint.
- Y Coordinate at Completion
- Time to Travel 50, 60, 70, 80 and 90% of the Region
- Total Travel Time

**B.7 Procedures for the Analysis of Results**

Monte Carlo simulations necessarily result in a great deal of output. It was necessary to develop a data collection and analysis system to properly deal with this. Data from this study is stored in disk data files as it's produced and saved for use and analysis later. Use has been made of a sophisticated data analysis system called the Statistical Analysis System (SAS) to assist in the analysis of the data from this study.
A listing of the computer code referred to as STKBLKNP, which was adapted from that developed by Reiter (1981) is included in Appendix D. The code may be subdivided into 11 steps as listed below with the line numbers referring to the listing.

1. Data input and echo check of data on region size and parameters (lines 100 to 2000).

2. Selection of hydraulic conductivity form, autocorrelation development and stochastic generation of values for each Monte Carlo Simulation (lines 2010 to 3330).

3. Calculate actual statistical parameters of the hydraulic conductivity values generated (lines 3340 to 6280).

4. Computation of harmonic means of hydraulic conductivity at adjacent nodes for use in finite difference solution (lines 6290 - 6910).

5. Finite difference solution for steady state heads (lines 6920 to 9170).

6. Compute flow quantity, equivalent hydraulic conductivity and write out results (lines 9180 to 11650).

7. Compute stream function and write out (lines 11660 to 13630).
8. Compute velocities in all sections of the finite difference grid (lines 13640 to 14220).

9. Read in required data on dispersion and initialize parameters (lines 14230 to 14630).

10. Water particles traverse the region (lines 14640 to 17670).

11. Results written out and stored on files (lines 17680 to 19580).

12. Subroutines to calculate means and correlations (lines 19590 to 20860).

The data stored in disk files is varied but consists of information on the hydraulic conductivity means and correlation for each simulation, travel times and dispersion, hydraulic head values both mean values and those for selected rows in each simulation. These data are then available for input to the SAS programs. SAS programs have been written to perform all types of statistical calculations and checks, as well as to plot these results.

B.8 Discussion of the Results

B.8.1 Computer Time

A considerable amount of computer simulation was performed during this
One major limitation immediately encountered was the large amount of computer time required to invert the \((I-W)\) matrix. The size of the matrix increases very rapidly with the region size since a new row and column is added for each new finite difference block in the region.

Figure B.8 presents a plot of the required computer time for matrix inversion versus the number of nodes in the region. The three sizes computed were 49 (7 x 7 region), 144 (12 x 12 region) and 264 (12 x 22 region). These results suggest a non-linear relationship which is linearized by plotting on a semilog scale (log time) as presented in Figure B.8. This plot suggests a relationship defined by the following expression:

\[
\ln T = 0.01075 B + 0.23
\]  

(22)

where \(T\) is the time to complete the inverse and \(B\) is the number of nodes in the mesh. The practical limit on region size based on this time requirement will depend on the computer system available; however, the largest region considered in this study was a 12 x 22 region.

A check of the accuracy of the inversion was performed by rewriting the inverse code to generate the Weighting matrix, retrieve the completed inverse matrix, FILTR, and pre-multiply the \((I-W)\) matrix by the FILTR matrix. For the region considered, these results indicated that the inverse was accurate to five significant figures which is considered adequate.
Figure B.8 - Computer Time Versus Number of Nodes
B.8.2 Effective Hydraulic Conductivity

The arithmetic, geometric and harmonic means of all the simulations of hydraulic conductivity for the numerous Monte Carlo solutions were calculated. These mean values were compared to the effective hydraulic conductivity calculated on the basis of the flow quantity, $K_q$, by the following equation:

$$K_q = \frac{Q}{h_L} \left[ \frac{L \cdot \frac{S'}{H}}{h_L} \right] = \frac{Q \cdot S}{h_L}$$

(23)

where $Q$ is the flow quantity, $h_L$ is the total head loss within the region, $L$ is the total length over which that head loss occurs, $H$ is the height of the flow region, and $S'$ is a shape factor computed in accordance with a technique suggested by Warren and Price (1961) which will be presented later.

The value of $S$ is a shape factor which may be directly compared with the shape factor, $N_D/N_F$, in a flow net solution or the form factor in the method of fragments. $N_D$ and $N_F$, are the number of equipotential drops and flow lines respectively in the flow net solution.

A second measure of the effective hydraulic conductivity in terms of mean travel time was computed for each Monte Carlo simulation. This effective hydraulic conductivity on the basis of travel time, $K_t$, was calculated by making assumptions similar to those used in calculating $K_q$. Figure B.9 presents a typical layout of a flow region with approximately horizontal-uniform flow from left to right. The flow is
Along left boundary where $J=1$, hydraulic head is maintained constant at value of $H$
Along right boundary where $J=NCOL$, hydraulic head is maintained constant at value of $H_L$

Mean head loss in flow region $= h_L = H - H_L$

Figure B.9 - Region of Mass Transport
not precisely uniform due to the dispersion present in the flow simulation.

The velocity of flow, \( v \), may be calculated by the following formula:

\[
\frac{v}{n} = \frac{K}{n} L
\]

The mean velocity of all flow particles traversing the flow region, \( \bar{v} \), may be calculated by dividing the length of the particle travel, \( L_T \), by the mean travel time, \( \bar{t} \), as below:

\[
\bar{v} = \frac{L_T}{\bar{t}}
\]

The effective hydraulic conductivity on the basis of travel time, \( K_t \), has been calculated by setting \( v \) equal to \( \bar{v} \) in the above two equations, introducing the height of the region, \( H \), by inserting in both the numerator and denominator and solving for \( K_t \) resulting in the following:

\[
K_t = \frac{L_T \cdot n \cdot H}{\bar{t} \cdot h_L} \cdot \frac{S_t \cdot L}{H} = \frac{L_T \cdot n \cdot H}{\bar{t} \cdot h_L} \cdot S_t
\]

where \( L_T \) is the total length of particle travel, \( n \) is the porosity, \( \bar{t} \) is the mean travel time and \( L, H \) and \( h_L \) are as defined above. \( S_t \) is a shape factor computed in the same general manner as \( S \) above except that mean travel time rather than flow rate is used. \( S_t \) is a modified shape factor which may be compared to the shape factors from a flow net, the method of fragments or to \( S \) calculated above.

Over thirty variations of flow region size and characteristics were
studied to determine the relationship between these calculated means. Generally for each flow region, 40 Monte Carlo characterizations were done. The means and effective hydraulic conductivities for each of these was computed.

In addition to calculation of mean values for each of the Monte Carlo characterizations, a mean value of all Monte Carlo characterizations was computed. Correlation of the geometric mean and the two effective hydraulic conductivity values (flow quantity and travel time) were visually observed by plotting and also by computation of correlation coefficients. A typical plot of these results is presented in Figure B.10 and the results are summarized in Table B1.

The results of these computations support the observation that the geometric mean is the best measure of the effective hydraulic conductivity both in terms of flow quantity and travel time. The effective hydraulic conductivity calculated both by flow quantity, $K_q$ and travel time, $K_t$, are relatively close with the flow quantity value generally somewhat larger.

Two boundary flow configurations were considered in addition to uniform flow, i.e., flow from the left boundary to the right boundary of a rectangular region. The two flow configurations are presented in Figure B.11. The first flow configuration is described as S flow for the case of flow from the upper three nodes of the left boundary to the lower three nodes of the right boundary. This case could simulate a general two dimensional flow case such as around an obstruction or low hydraulic
Figure B.10 - Correlation of Effective Hydraulic Conductivities with Geometric Mean of Hydraulic Conductivity
### TABLE B.1 - SUMMARY OF FLOW SIMULATIONS

| File | Region Size | Block Size | Auto. Corr. Data x | Auto. Corr. Data y | No. of Sims | No. of Waves | Int., D | Kmcog | Y Coor. | Total Travel Y Days | Means of Hydraulic Conductivity ft/day |
|------|-------------|------------|--------------------|--------------------|-------------|-------------|---------|--------|---------|---------------------|-------------------------------------|
| 1    | 10 X 20     | 10 X 10    | 0.8                | 0.8                | 0.68        | 40          | 1       | 1.6    | 0.032   | 60.6                | 172.5                              |
| 2    | 10 X 20     | 10 X 20    | 0.8                | 0.4                | 0.68        | 40          | 1       | 1.6    | 0.115   | 60.4                | 168.5                              |
| 3    | 10 X 20     | 10 X 20    | 0.6               | 0.6               | 0.68        | 40          | 1       | 1.6    | 0.15    | 59.5                | 171.1                              |
| 4    | 10 X 10     | 10 X 10    | 0.8                | 0.8                | 0.68        | 40          | 1       | 0.8    | 0.01    | 59.7                | 39.8                               |
| 5    | 5 X 5       | 5 X 5      | 0.8                | 0.8                | 0.68        | 40          | 2       | 6.4    | 0.01    | 35.0                | 9.5                                 |
| 6    | 10 X 20     | 10 X 20    | 0.8                | 0.8                | 0.68        | 10          | 4       | 1.6    | 0.024   | 58.4                | 176.6                              |
| 7    | 10 X 20     | 10 X 20    | 0.8                | 0.8                | 0.68        | 44          | 3       | 1.6    | -       | 58.6                | 234.3                              |
| 8    | 10 X 20     | 10 X 20    | 0.8                | 0.4                | 1.0         | 40          | 1       | 1.6    | 0.01    | 60.0                | 173.0                              |
| 9    | 10 X 20     | 10 X 20    | 0.8                | 0.8                | 0.68        | 40          | 1       | 1.6    | 0.01    | 59.9                | 169.7                              |
| 10   | 10 X 40     | 10 X 20    | 0.8                | 0.8                | 0.68        | 40          | 1       | 3.2    | 0.01    | 59.6                | 703.4                              |
| 11   | 10 X 40     | 10 X 20    | 0.8                | 0.8                | 0.68        | 40          | 1       | 0.3    | 0.15    | 60.2                | 694.4                              |
| 12   | 10 X 40     | 10 X 20    | 0.8                | 0.8                | 0.68        | 40          | 1       | 6.4    | 0.014   | 59.2                | 702.2                              |
| 13   | 10 X 40     | 10 X 10    | 0.8                | 0.8                | 0.68        | 40          | 1       | 3.2    | 0.04    | 60.8                | 697.0                              |
| 14   | 20 X 40     | 10 X 10    | 0.8                | 0.8                | 0.68        | 20         | 1       | 3.2    | 0.15    | 111.7               | 700.0                              |
| 15   | 20 X 40     | 10 X 20    | 0.8                | 0.8                | 0.68        | 20         | 1       | 3.2    | 0.15    | 111.2               | 699.7                              |
| 16   | 10 X 60     | 10 X 20    | 0.8                | 0.8                | 0.68        | 40          | 1       | 4.8    | 0.15    | 59.5                | 1576.2                             |
| 17   | 10 X 60     | 10 X 10    | 0.8                | 0.8                | 0.68        | 40          | 1       | 4.8    | 0.052   | 59.5                | 1576.7                             |
| 18   | 10 X 20     | 10 X 20    | 1.0                | 1.0                | -           | 40         | 1       | 1.6    | 0.15    | 60.2                | 151.9                              |

Note: The table entries include various columns such as 'Auto. Corr. Data x', 'Auto. Corr. Data y', 'No. of Sims', 'No. of Waves', 'Int., D', 'Kmcog', 'Y Coor.', 'Total Travel Y Days', 'Means of Hydraulic Conductivity ft/day', with specific values for each entry.
| File | Region Size | Block Size | Auto. Corr. Data | No. of Waves Days | Kolmog Stat End | Total Travel Time, Days | Means of Hydraulic Conductivity ft/day |
|------|-------------|------------|-----------------|-------------------|-----------------|------------------------|---------------------------------------|
|      |             |            | x    | y    |                  |                   |                        | Ka | Kg | Kh | Kq | Kt | S  |
| 19   | 10 X 20     | 10 X 20    | 0.8  | 0.2  | 1.0              | 40                | 1                       | 1.6 | 60.7 | 170.1 | 5.11 | 4.65 | 4.23 | 4.62 | 4.47 | 2.35 |
| 20   | 10 X 20     | 10 X 20    | 0.8  | 0.2  | 0.9              | 40                | 1                       | 1.6 | .15  | 60.2  | 169.8 | 5.005 | 4.64 | 4.3  | 4.6  | 4.7  | 2.04 |
| 21   | 10 X 60     | 10 X 20    | 0.8  | 0.8  | 0.68             | 40                | 1                       | 1.0 | .048 | 60.3  | 314.5 | 4.96  | 4.58 | 4.23 | 4.48 | 4.41 | 2.05 |
| 22   | 10 X 60     | 10 X 20    | 0.8  | 0.8  | 0.68             | 40                | 1                       | .44 | .066 | 60.5  | 143.0 | 5.07  | 4.68 | 4.33 | 4.59 | 4.50 | 2.07 |
| 23   | 10 X 20     | 10 X 20    | 0.8  | 0.8  | 0.68             | 40                | 1                       | 1.6 | -    | 98.4  | 228.0 | 5.12  | 4.72 | 4.36 | 4.62 | 4.50 | 2.12 |
| 24   | 10 X 20     | 10 X 20    | 1.0  | 1.0  | -                | 1                 | 133                     | 1.6 | -    | 88.7  | 211.8 | 5.0   | 5.0  | 5.0  | 5.0  | 5.0  | 0.0  |
| 25   | 10 X 20     | 10 X 20    | 1.0  | 1.0  | -                | 1                 | 40                      | 1.6 | -    | 98.8  | 200.5 | 5.0   | 5.0  | 5.0  | 5.0  | 5.0  | 0.0  |
| 26   | 10 X 20     | 10 X 20    | 0.8  | 0.4  | 0.84             | 40                | 1                       | 1.6 | 60.2 | 173.7 | 4.90  | 4.55  | 4.23 | 4.51 | 4.39 | 1.98 |
| 27   | 10 X 20     | 10 X 20    | 0.8  | 0.8  | 0.68             | 40                | 1                       | 1.6 | .01  | 58.8  | 254.91| 5.01  | 3.54 | 2.51 | 3.32 | 3.06 | 4.786|
| 28   | 10 X 20     | 10 X 20    | 0.8  | 0.8  | 0.68             | 40                | 1                       | 1.6 | 60.0 | 153.11| 4.98  | 4.96  | 4.98 | 4.97 | 0.50 |     |
| 29   | 20 X 40     | 10 X 20    | 0.8  | 0.8  | 0.68             | 20                | 1                       | 3.2 | 109.6| 2058.4| 2.99  | -     | -    | -    | 1.52 | 2.47 |
| 30   | 10 X 20     | 10 X 20    | 0.4  | 0.3  | 0.95             | 40                | 1                       | 1.6 | .15  | 59.8  | 170.5 | 5.01  | 4.66 | 4.34 | 4.58 | 4.47 | 1.97 |

Note: Uniform flow in all files except 7 and 24 which simulate S Flow and 23 and 25 with cutoff. Values listed for $K_q$ and $K_t$ have been adjusted by use of the shape factor $S$. 
Figure B.11 - Alternate Flow Configurations
conductivity occlusion. The second flow configuration is described as cutoff for the case of flow from the left upper boundary to the bottom right boundary. This case is intended to simulate flow beneath a dam by representing one half of the flow region.

Warren and Price (1961) have indicated that the geometric mean of the hydraulic conductivity is a good approximation of the effective hydraulic conductivity even for non-uniform flow provided a shape factor is utilized to adjust the value for the shape of the flow region. They suggest that the magnitude of this shape factor be determined by first calculating the effective hydraulic conductivity of the flow region using a singular known value of hydraulic conductivity. This effective value of hydraulic conductivity should then be divided into the singular known value and the result is the shape factor. The hydraulic conductivity value determined for the non-uniform flow case with the log normal distribution of hydraulic conductivity is multiplied by the shape factor before comparing with the geometric mean. This approach is similar to that technique embodied in a flow net solution or the one incorporated in the method of fragments.

The results of this study support the technique suggested by Warren & Price (1961) for calculation of a shape factor. For the cases considered, the computed values of effective hydraulic conductivity generally fall between the geometric and harmonic means and is closest to the geometric mean as presented in Figure B12.
| File No. | Flow Type   | Arith K | Geom Kg | Harm Kh | Equivalent Hydraulic Kq | Equivalent Travel Time Kt | S | S | S_t | S_t | Flow of Net Nd/Nf | Method of Fragment | φ_m |
|---------|-------------|----------|--------|--------|-------------------------|--------------------------|---|---|-----|-----|------------------|--------------------|-----|
| 9       | Uniform     | 2        | 5.04   | 4.68   | 4.34                    | 4.62                     | 4.50| 4.50         | 1.0 | 1.9 | 1.0 | 1.9 | 1.9 | 1.9 |
| 18      | Uniform     | 0        | 5.0    | 5.0    | 5.0                     | 5.0                      | 5.0 | 5.0          | 5.0 | 5.0 | 5.0 | 5.0 | 5.0 | 5.0 |
| 7       | S-Flow      | 2        | 5.05   | 4.69   | 4.36                    | 3.17                     | 4.63 | 3.26         | 4.54 | 1.46 | 2.78 | 1.39 | 2.66 | 3.0 | 2.91 |
| 24      | S-Flow      | 0        | 5.0    | 5.0    | 5.0                     | 3.42                     | 5.0 | 3.59          | 5.0 | 3.59 | 5.0 | 3.59 | 5.0 | 5.0 |
| 23      | Cutoff      | 2        | 5.12   | 4.72   | 4.36                    | 2.79                     | 4.62 | 3.41         | 4.50 | 1.66 | 3.15 | 1.32 | 2.57 | 3.25 | -    |
| 25      | Cutoff      | 0        | 5.0    | 5.0    | 5.0                     | 3.02                     | 5.0 | 3.79          | 5.0 | 3.79 | 5.0 | 3.79 | 5.0 | 5.0 |

Note: $K_q$ and $K_t$ are the equivalent mean values of $K_q$ and $K_t$ after adjusting by the shape factor.

Figure B.12 - Hydraulic Conductivity Comparisons
B.8.3 Autocorrelation Coefficients and Integral Scale

The stochastic nearest neighbor process model was utilized to generate random ensembles of hydraulic conductivity meshes which are autocorrelated. Each of the individual representations within the ensemble of representations making up each Monte Carlo simulation was analyzed to determine the degree of correlation by row and column. The formulation below utilized to calculate this value may be found in many references, e.g. Smith (1981).

\[
\rho(L) = \frac{1}{n-L} \sum_{i=1}^{n-L} (K_i - \bar{K})(K_{i+L} - \bar{K})
\]

\[
\left( \frac{1}{n-1} \sum_{i=1}^{n-1} (K_i - \bar{K})^2 \right)^{-1}
\]

In this equation \( \rho(L) \) is the autocorrelation coefficient for lag \( L \). \( L \) is a whole number from zero to the number of elements in the row or column minus one. \( K_i \) is the value of hydraulic conductivity at point \( i \), and \( \bar{K} \) is the mean value. The denominator is the variance of the hydraulic conductivity. It may be easily shown that if \( L \) equals zero, then \( \rho(0) \) equals 1.0.

A graph of a typical result of this computation for lags from one to three is presented in Figure B.13. The concept of integral scale as discussed by Smith and Freeze (1979) is utilized herein to conceptualize the degree of dependency of the hydraulic conductivity value at one node with the value at adjacent nodes. The integral scale has been estimated as the summation of the positive autocorrelation coefficients times the
\[ \alpha_x = \alpha_y = 0.8 \]
Block size = 10 Feet

Integral Scale = \( \lambda \)
\[ \lambda = (1.0 + 0.436 + 0.138 + 0.008)10 \]
= 15.8 Feet

Figure B.13 - Correlation Coefficient Versus Lag
block size. As indicated, the integral scale, $\lambda$, equals 15.8 for the data in Figure B.13.

During the course of this work, the nature of the governing equation for autocorrelation of hydraulic conductivity values at the boundaries was raised. An alternative methodology was written and a Monte Carlo simulation investigated. Figure B.14 presents the mean row autocorrelation coefficients by the two techniques. Utilizing the coefficients resulted in integral scales of 14.9 and 12.4 feet for the x and y directions using the original technique and 14.4 and 12.3 feet using the alternate formulation. It would appear that at least for these conditions the alternative technique provided no significant difference and therefore no further investigation of this alternative was conducted.

Irrespective of this finding, there was still concern over the autocorrelation of hydraulic conductivity in the boundary blocks. This problem was mitigated somewhat by deleting the boundary blocks of the region after development. The effects on the autocorrelation coefficients may be seen on Figure B.15 which presents the autocorrelation coefficients by rows of the log of the hydraulic conductivity before and after deleting these boundary blocks. Also presented are the autocorrelation coefficients by rows of this same simulation after the log transformation to hydraulic conductivity. The results are fairly typical of the simulations conducted and indicate a slight loss of correlation when the boundaries blocks were deleted and some additional loss when the log transformation was completed. This total loss was
LEGEND:

× Smith's Boundary Condition

□ Alternative Technique

Figure B.14 - Comparison of Auto Correlation Coefficients
Figure B.15 - Effects of Shaving and Stacking of Blocks on Autocorrelation
rather slight, however. The reduction in the integral scale is considerably less.

The effect of the region size on the integral scale is demonstrated in Figure B.16. It is clear that as the region size increases, the integral scale increases, although at a decreasing rate. This figure also demonstrates the effects of stacking blocks of internally autocorrelated hydraulic conductivity meshes to achieve larger regions without utilizing a larger FILTR matrix. There is a loss in the integral scale although this loss is relatively small even when the region is increased by three times. The figure also demonstrates that as the region size increases, the integral scale continues to increase, even with the same FILTR matrix.

Figure B.17 demonstrates that the integral scale changes with a change in the autocorrelation parameter, \( \alpha \). This plot indicates that the integral scale in both the x and y direction increases with an increase in the \( \alpha_y \) term. The increase in the y integral scale is expected, but the increase in the integral scale in the x direction may not be. This increase in the integral scale in the x direction resulting from the increase in the \( \alpha_y \) term likely results from a general increase in correlation of all terms in the mesh.

B.8.4 Sensitivity of Ensemble Means and Variances to the Number of Simulations

Computer computations are relatively inexpensive. However, the prac-
Figure B.16 - Effects of Region Size on Autocorrelation

Note: Finite Difference Mesh consists of 10 Foot by 10 Foot Sections in all cases.
Note: Region was 100' by 200'

Figure B.17 - Effects of Autoregressive Parameters on Integral Scale
tioner does not want to do more computations than are necessary to obtain reliable estimates. A study of the number of simulations required to compute reliable mean values of various parameters was then conducted.

Initially consider the mean and standard deviation of the hydraulic conductivity formulations. Figure B.18 presents a plot of an accumulating mean of the arithmetic mean and standard deviation of the hydraulic conductivity for one of the Monte Carlo simulations. This plot demonstrates that these cumulative mean values very rapidly approach a constant value, in this case after approximately 8 simulations.

The SAS program written to compute the cumulative mean of the means and standard deviation is an inexact estimate of the actual mean and standard deviation of all preceding observations. The procedure computes the mean and standard deviation of the previous three observations. A running mean value of these two results is then computed as each new mean and standard deviation is computed for the new observation and the two left from the earlier group. The results have been found accurate to approximately 3 to 4 decimal places for the mean value. However the mean of the running standard deviation computation by this technique may only be used as a qualitative measure of the trend and its stability. A true measure of the actual standard deviation can only be computed after the entire ensemble is sampled.

Figure B.19 and B.20 present similar plots for the effective hydraulic conductivity in terms of flow quantity, \( K_q \), and travel time, \( K_t \),
Figure B.18 - Cumulative Mean of the Arithmetic Mean and Lag 3 Standard Deviation of Hydraulic Conductivity Versus Simulation Number
Figure B.19 - Cumulative Mean of the Mean and Lag 3 Standard Deviation of Effective Hydraulic Conductivity (Flux) Versus Simulation Number
Figure B.20 - Cumulative Mean of the Mean and Lag 3 Standard Deviation of Effective Hydraulic Conductivity (Travel Time) Versus Simulation Number
respectively. Both of these indicate that a fairly constant value is rapidly approached, in this case, in only 7 to 10 simulations. However, the cumulative means of the standard deviation for both terms fluctuates considerably. A truly constant value is not achieved even after the 40 simulations in the ensemble although after the first 20, the fluctuations are greatly reduced.

B.8.5 Sensitivity of Ensemble Means and Variances to Number of Particles

The number of particles which need to be simulated to reach a fairly constant value of the mean and standard deviation of the travel time is another important consideration in the amount of computation time required. A SAS program was written to calculate the cumulative mean of the mean and standard deviation of the travel time for particle transit. A typical plot of the results for one run is presented in Figure B.21. This figure illustrates that a mean value of travel time is reached after only approximately 20 water particles.

The cumulative mean of the lag 3 standard deviation of the travel time fluctuates 20 or 40 percent after 20 water particles reaching a fairly consistent, although still slightly decreasing value after approximately 80 water particles.

Fried (1975) gives an expression for the longitudinal dispersion coefficient assuming that the development of particle concentration at some distant point is normally distributed. He illustrates that this
Figure B.21 - Cumulative Mean of the Mean and Lag 3 Standard Deviation of Travel Time Versus Particle Number
Coefficient is directly related to the variance of the travel times. Here concentrations are simulated by the breakthrough curve. The equation developed for a large travel distance relative to the dispersivity is:

$$D_L = \frac{U^2}{8} \frac{(2 \sigma_t)^2}{t_{0.5}}$$

(28)

where $D_L$ is the longitudinal dispersion coefficient, $U$ and $t_{0.5}$ are the mean velocities and travel time respectively, and $\sigma_t$ is the standard deviation of the travel time.

The distance, $x$, over which the dispersion occurs equals the product $Ut_{0.5}$ and may be substituted in this equation resulting in the following equation:

$$D_L = \frac{\sigma_t^2}{2 (t_{0.5})^3}$$

(29)

These equations illustrate the relationship between the standard deviation of the travel time, $\sigma_t$, and the longitudinal dispersion coefficient. Since the dispersion coefficient equals the dispersivity times the mean velocity, the macroscopic dispersivity may be determined by dividing by the mean velocity to arrive at:

$$\delta = \frac{\sigma_t x}{2 (t_{0.5})^2}$$

(30)

These results and others indicate that the 400 water particles simulated is sufficient to compute mean and standard deviation for travel time.
The macroscopic or field scale lateral dispersion coefficient, $D_T$, has been shown by Fried (1975) to be a function of the scatter about the mean ending location after traversing a region. Fried presented the following equation:

$$D_T = \frac{1}{2} \sigma_y^2 \frac{\bar{U}}{x}$$  

(31)

where $\sigma_y$ is the standard deviation of the normalized location perpendicular to the direction of flow and $\bar{U}$ and $x$ are as defined earlier.

A record was maintained of the starting and ending y coordinate of each water particle. A normalized ending y coordinate was then computed along with a cumulative mean and cumulative mean of the standard deviation as each new record of water transport was added. The same was computed for the y coordinate at the estimated time to transport half the region. A typical plot of these results is presented in Figure B.22. These results also indicate that 400 particles are sufficient to reach a consistent mean value for these variables.

B.8.5 Normality Check on Travel Times

The ensemble of travel times was utilized to plot a breakthrough curve. Figure B.23 presents a representative sample of a breakthrough curve. These curves are similar to a concentration versus time curve and their similarity of shape supports the premise of general conformance of normality.
FILE V. 40 SIMULATIONS OF UNIFORM FLOW IN 100 FT BY 200 FT REGION

PLOT OF CUMULATIVE REVISED SYMBOL USED IS *

Cumulative Mean of the Mean and Lag 3 Standard Deviation of Normalized Ending Y Location

Figure B.22 - Cumulative Mean of the Mean and Lag 3 Standard Deviation of Normalized Ending Y Location
Figure B.23 - Simulation Breakthrough Curve
A check for the goodness of fit of the assumption of a normal distribution for the ensemble of travel time records was made. A SAS program was written to test the null hypothesis that the data could be a random sample from a normal distribution. A Kolomogorov D statistic was computed and compared with critical values. A Kolomogorov statistic was utilized rather than the more common chi square check since it is more easily adapted to continuous uncategorized data.

Table B.1 presents the results of this check for several flow ensembles. Several of the normality checks support the assumption of a normal distribution with a general tendency to do so as the transit distance increases. Cases 10, 11 and 12 suggest that as the time interval decreases, there is a greater likelihood of acceptance of a normal distribution. A Kolomogorov D statistic of 0.10 or greater was considered sufficient for acceptance of the assumption of normality for this study.

B.8.6. Hydraulic Head Value Sensitivity

The hydraulic head value along two rows was tabulated for each of the simulations. This tabulation was then available to allow computation of mean values and variations resulting from variations in region size, hydraulic gradient, conductivity and other factors.

Figure B.24 presents typical results from one of the Monte Carlo simulations. The upper plot presents the mean hydraulic head versus the node number. The averaging over the 40 Monte Carlo simulations results in a fairly smooth straight line relationship. The middle curve
Figure B.24 - Mean, Standard Deviation and Variance of Head Versus Node Number
presents the standard deviation and the lower curve the variance of the hydraulic head for the 40 Monte Carlo simulations versus the node number. These figures clearly demonstrates the boundary effects. At the ends of the flow region the head is held constant and therefore the standard deviation is zero there. At nodes further away, there is less influence from the boundary and therefore the standard deviation and variance are greater.

The number of Monte Carlo simulations required to reach a fairly consistent value of the hydraulic head was also investigated. Figure B.25 presents a typical plot of the results of one such investigation at an interior node. This plot indicates that the initial simulation had a value very close to the resulting mean value and after three simulations the mean value was within 3 percent of that value.

The effect of variations in region size is demonstrated in Figure B.26. The maximum value of the normalized standard deviation of hydraulic head for any of the nodes in the region increases as the region size increased. The maximum value of the standard deviation of hydraulic head was normalized by dividing each value by the mean head loss for each node.

The effect of variations in hydraulic gradient is demonstrated in Figure B.27. There appears to be a gradual increase in the maximum value of the standard deviation of hydraulic head as the hydraulic gradient increases. This is probably due to the larger numbers in the calculation however, since when divided by the mean value there is no general trend.
Figure B.25 - Cumulative Mean of the Head Versus Simulation Number
Note: Finite Difference Mesh consists of 10 Foot by 10 Foot sections in all cases.

Figure B.26 - Maximum Value of Normalized Standard Deviation of Head Versus Region Size
Figure B.27 - Maximum Value of Standard Deviation of Head Versus Hydraulic Gradient
The relationship between this quantity and the standard deviation of the hydraulic conductivity is of more significance. Figure B.28 presents this relationship which results in a direct relationship. This is significant since the uncertainty in the hydraulic conductivity value directly affects our uncertainty in the value of the hydraulic head value within the region.

B.8.7. Macroscopic Dispersivity Sensitivity

The macroscopic or field scale longitudinal dispersivity has been shown to be a function of the standard deviation of the travel time. The macroscopic transverse dispersivity has been shown to be a function of the standard deviation about the mean ending location perpendicular to the general flow direction. For the horizontal uniform flow case this may be taken as the standard deviation in the ending y coordinate. The sensitivity of the macroscopic dispersivity to variations in region size, hydraulic gradient, time interval and standard deviation of hydraulic conductivity was investigated.

Figure B.29 presents results of the effect of region size on the microscopic longitudinal and transverse dispersivity. The upper plot indicates a relatively small change in the longitudinal dispersivity with an increase in region size and no consistent trend. The lower plot indicates a steadily decreasing transverse dispersivity with region size. The values plotted for the macroscopic dispersivities was determined by dividing the dispersion coefficients, determined by the equations taken from Fried (1975) given earlier, by the mean particle
Figure B.28 - Maximum Value of Standard Deviation of Head Versus Standard Deviation of Hydraulic Conductivity
Note: Finite Difference Mesh consists of 10 Ft by 10 Ft Sections in all Cases.
velocity in the region. These results suggest that a constant value of dispersivity is not reached during the transit of these particles.

Figure B.30 presents the effects of a change in hydraulic gradient and Figure B.31 the effects of a change in time interval for mass transport on these same parameters. The variation of both macroscopic longitudinal and transverse dispersivity is small and inconsistent due to the change in hydraulic gradient and time interval. The insensitivity of the observed dispersivity due to time interval variation is important since the computer time required to simulate particle transit is dependent on the time interval utilized.

The effect of a variation in the standard deviation of hydraulic conductivity is much more pronounced than these other variables. The results of a variation of this parameter are presented in Figure B.32. A reduction in standard deviation of the hydraulic conductivity from 2.0 to 0.5 resulted in a reduction from 2.5 to 0.3 in the longitudinal dispersivity and from 0.14 to 0.05 in the transverse dispersivity.

B.8.8. Development of Confidence Limits

The confidence which the engineer has in his prediction of flow quantity, travel times and dispersion of flow particles is the major reason for utilizing these more sophisticated and complex solutions for field flow problems. If the engineer were not able to increase his confidence in his predictions there would be little reason to utilize these techniques. The nature of the output from this method lends
Figure B.30 - Macroscopic Dispersivity Versus Hydraulic Gradient
Figure B.31 - Macroscopic Dispersivity Versus Time Interval
itself to the development of confidence limits on the solution.

A methodology to utilize the knowledge of the variability of the flow region characteristics to establish confidence limits on the output utilizing probability and statistics has been formulated. The emphasis of this methodology is in the quantification of the characteristics of the major input parameter, hydraulic conductivity. Other parameters have been shown to be of lesser importance to the problem solution.

The procedure to develop the site specific soil parameters is essentially unchanged. Field programs are utilized to measure insitu soil parameters and to secure samples for laboratory testing. The field and laboratory tests will be analyzed so that a probability density function of the hydraulic conductivity may be formulated. Other parameters such as porosity, and laboratory dispersivity characteristics must also be developed.

These parameters are then the input to a Monte Carlo computer solution for flow quantity and travel time. The results of these Monte Carlo computer simulations may then be analyzed utilizing the knowledge of the underlying distribution of these results to develop confidence in the results.

In general the flow quantity and travel time results should be expected to conform to a normal distribution. This assertion is made on the basis of the Central Limit Theorem. The water particle movement may be considered the result of adding up the effects of many individual
Figure B.32 - Macroscopic Dispersivity Versus the Standard Deviation of Hydraulic Conductivity
factors (hydraulic conductivity values). This assumption of normality has been generally verified in this study.

The mean value of the flow quantity and travel time may then be estimated with confidence by the method described earlier. The results of one Monte Carlo simulation are presented in Figure B.33. The characteristics of the flow region are also presented. The mean and standard deviation of the effective hydraulic conductivity, $K_q$, is 4.57 and 0.230 respectively. Utilizing the equations developed earlier, the 95% confidence limits on the mean value may be estimated. The magnitude of error of the mean with 95% confidence may be estimated by the following:

$$E < t_{\alpha/2} \cdot \frac{s}{\sqrt{N}} = 1.96 \cdot \frac{0.230}{\sqrt{40}} = 0.071$$

(32)

where $t_{\alpha/2}$ is the value of the cumulative distribution function of the student t distribution at the $\alpha/2$ significance level, $s$ is the value of the standard deviation and $N$ is the sample size.

The mean value would then be expected to lie between the limits of the sample mean (4.57) plus or minus the error (0.07) i.e., 4.50 and 4.64. The effective hydraulic conductivity, $K_q$, was calculated by dividing the flow by the mean hydraulic gradient and area. The flow rate may then be estimated with confidence limits of 95% by multiplying by these constants. In so doing the flow limits of 38.1 to 39.9 ft$^3$/day were estimated with 95% confidence limits.
Figure B.33 - Flow Region and Typical Output of Effective Hydraulic Conductivity (Flux) and Travel Time
The same methodology may be utilized to develop confidence limits on the travel times. The mean and standard deviation of the travel time is 1576.2 and 146.9 days. The 95% confidence limits on the magnitude of error may be estimated as:

\[ E < \frac{1.96 (146.9)}{\sqrt{400}} = 14.4 \text{ days} \]  \hspace{1cm} (33)

The mean value of travel time is therefore expected to lie between 1561.8 and 1590.6 days. The standard deviation of the travel time may also be estimated with confidence by the expressions given earlier.

\[ \frac{146.9}{1 + \frac{1.96}{\sqrt{2(400)}}} < \sigma < \frac{146.9}{1 - \frac{1.96}{\sqrt{2(400)}}} \]  \hspace{1cm} (34)

\[ 137.4 < \sigma < 157.8 \]  \hspace{1cm} (35)

The water particles are expected to follow a normal distribution so that a hypothetical breakthrough curve may be developed for the extremes of these parameters. The result of such an exercise is presented in Figure B.34. This allows the engineer to estimate not only the mean arrival time with confidence but also the distribution of travel times.

B.8.9 Macroscopic Dispersivity

The results of the various flow situations was analyzed for characterizations of macroscopic dispersion coefficients and dispersivity. Using the equation developed by Fried (1975), a macroscopic dispersion coefficient was calculated for the record of 400 flow particle traverses of the flow region. The equation developed by Fried assumes that the
Figure B.34 - Hypothetical Breakthrough Curve
particle breakthrough curve will simulate flow concentration. This macroscopic dispersion coefficient and dispersivity was plotted versus the mean region velocity and is presented in the upper two curves of Figure B.35. The upper curve indicates a general increase in the macroscopic dispersion coefficient with velocity as expected. There is no general trend for the middle curve. The value of macroscopic dispersivity appears not to vary greatly with velocity.

The lower curve plots macroscopic dispersivity versus the standard deviation of hydraulic conductivity. This plot suggests that as the variation in hydraulic conductivity increases, the value of macroscopic dispersivity should increase. This trend suggests that particle transport is less direct as the variation of hydraulic conductivity in the region increases.
Figure B.35 - Macroscopic Dispersion Coefficient and Dispersivity Versus Mean Velocity and Dispersivity Versus Standard Deviation of Hydraulic Conductivity
APPENDIX C - BIBLIOGRAPHY

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APPENDIX D - COMPUTER PROGRAMS

1. INVERSE

110 C THIS IS A PROGRAM WHICH WILL ASSIGN CORRELATED HYD. CONDUCTIVITY VALUES
120 C TO A FINITE DIFFERENCE MESH AND WRITE VALUES ON A DISK
130 C FILE NAME IS INVERSE
160 C
170 C SPECIFICATIONS
180 INTEGER CHECK, CONH, CONK, ELEC, MINI, STRF, FLOW, SKIP, UNILU(10), UNIHU
190 $1(10)
200 INTEGER EXLO, EXHI, WARP, PTPT
210 REAL K, KHARM, LENGTH, KHEQFD, KVEQFD, KVEQCS, KHEQCS, HARMK, MEAN, KLOG
220 REAL K, LNK<300>, WI<300,300)
222 INTEGER IA, NN, IDQT , IER
224 REAL WC300.300l.TOL, FILTRC300.300>.SC300,300>.WKC600l.WIDC300.300)
250 DOUBLE PRECISION H
260 DIMENSION KHARMC52, 52.2l.HC52.52>.K<52,52>.XD<52J,YD<52>.AX<52>,
270 $AY<52l,HEADIN<20>.ANIS0(52>.CHECK(10>. X(52,52J,Y(52, 52>.ERR<300>
280 DIMENSION LAYER<10>.LAYLU<10J,LAYHU<10l.CONMN<10>.SD<10l
290 DIMENSION ETA<10l.ALPHAX<10l,ALPHAY<10l ,EPSILN(300>
300 DIMENSION IC<52, 52> ,KY(52,
310 C INPUT PARAMETERS
320 C NOTE**** ALL INPUT PARAMETERS ARE NODAL VALUES****
330 C
340 C READ(5,30) NROW, NCOL, EC, ISO.PERM
350 C READ(5,35) CONH, CONK, ELEC, MINI, STRF, FLOW, SKIP, WARP
360 C READ(5,30) LSTRM, LEGUIV, DHEAD
370 C LSTRM IS THE COLUMN (FOR THE HORIZONTAL FLOW CASE, FLOW=HORI)
380 C OR THE ROW (FOR THE VERTICAL FLOW CASE, FLOW=VERT)
390 C OR THE COLUMN OF THE CONSTANT HEAD POINT ON THE
400 C LEFT SIDE OF THE UPPER BOUNDARY
410 C WHERE THE TOTAL FLOW IS COMPUTED FOR THE USE OF NONDIMENSIONALIZING
420 C THE STREAM FUNCTION *** IT IS USED ONLY WHEN CHECK(5)=STRF
430 C
440 C LEGUIV IS THE COLUMN (FOR THE HORIZONTAL FLOW CASE, FLOW=HORI)
450 C OR THE ROW (FOR THE VERTICAL FLOW CASE, FLOW=VERT)
460 C WHERE THE TOTAL FLOW IS COMPUTED TO BE USED IN SOLVING
470 C FOR THE EQUIVALENT CONDUCTIVITY (RESISTIVITY) OR WHERE THE
480 C WARREN AND PRICE TECHNIQUE IS APPLIED
490 C READ(5,40) WPFACT
500 NROWM1=NROW-1
510 NCOLM1=NCOL-1
520 NROWM2=NROW-2
530 NCOLM2=NCOL-2
540 NROWM3=NROW-3
550 NCOLM3=NCOL-3
560 NROWM3=NROW-3
570 C NOTE **** THE VALUE READ IN FOR HMIN IS THE LOWEST ITERATION
580 C PARAMETER AND IS USED ONLY IF MINI WAS SPECIFIED IN THE OPTIONS
590 C READ(5,32) ITMAX, NUMPAR, HEAD, HMIN
600 C COMPUTE AX AND AY
800 C AX = X-DISTANCE FROM ONE NODE CENTER TO THE NEXT
810 C AY = Y-DISTANCE FROM ONE NODE CENTER TO THE NEXT

820 C
830  DO 42 J=2, NCOL
840  42 AX(J)= (XD(J)+XD(J-1)) / 2.0
850  DO 44 I=2, NROW
860  44 AY(I)= (YD(I)+YD(I-1)) / 2.0

870 C
880 C READ ANISOTROPY AT EACH ROW
890 C VALUE IS THE RATIO OF KH/KV
900 C
910 120 READ(5, 40) (ANISO(I), I=1, NROW)
920 C
930 C SET BOUNDARY CONDITIONS
940 C NOTE *** PERIMETER BOUNDARY POINTS CAN BE EITHER CONSTANT HEAD OR IMPERMEABLE
950 C NOTE *** FLOW SHOULD BE FROM RIGHT TO LEFT OR TOP TO BOTTOM
960 C I.E. HIGH HEADS SHOULD BE LOCATED AT THE TOP OR LEFT SIDE
970 C
980 C SET ALL HEADS EQUAL TO SOME INITIAL VALUE
990 C AND ALL IC(I, J) VALUES TO ZERO
1000 DO 325 I=1, NROW
1010 DO 330 J=1, NCOL
1020 IC(I, J)=0
1030 330 H(I, J)= 50.0
1040 C
1050 C READ LOCATIONS OF CONSTANT HEAD NODES
1060 C ALONG THE PERIMETER
1070 C NOTE: THE PERIMETER IS THE ONLY LOCATION FOR A SOURCE OR A SINK
1080 C THAT IS --- A HIGH CONSTANT HEAD OR A LOW CONSTANT HEAD
1090 C
1100 C READ THE TOP ROW
1110 READ(5,336) (IC(2, J), J=2, NCOLM1)
1120 336 FORMAT(16I5)
1130 C READ THE BOTTOM ROW
1140 READ(5,336) (IC(NROWM1, J), J=2, NCOLM1)
1150 C READ THE LEFT SIDE
1160 READ(5,336) (IC(I, 2), I=3, NROWM2)
1170 C READ THE RIGHT SIDE
1180 READ(5,336) (IC(I, NCOLM1), I=3, NROWM2)
1190 C
1200 C READ HEAD VALUES ALONG THE PERIMETER
1210 C READ TOP ROW
1220 READ(5,350) (H(2, J), J=2, NCOLM1)
1230 C READ THE BOTTOM ROW
1240 READ(5,350) (H(NROWM1, J), J=2, NCOLM1)
1250 C READ THE LEFT SIDE
1260 READ(5,350) (H(I, 2), I=3, NROWM2)
1270 C READ THE RIGHT SIDE
1280 READ(5,350) (H(I, NCOLM1), I=3, NROWM2)
1290 350 FORMAT (8D10.3)
1300 C
1310 C ECHO CHECK OF INPUT PARAMETERS
1320 C
1330 130 WRITE(6,140) NROW, NCOL, EC, ITMAX
1340 140 FORMAT ('0./4X.,# OF ROWS =',T25,I5./,5X.,# OF COLUMNS =',T25,I5./
1350 5X.,'CLOSURE ERROR CRITERIA=',E16.5/5X.,'MAXIMUM ITERATIONS =',I5)
1360 150 WRITE(6,148) CONH, CONK, ELEC, MINI, STRF, FLOW, SKIP, WARP
1370 148 FORMAT ('0./5X.,PROBLEM OPTIONS SPECIFIED: ',2X,10A8/)
1380 150 IF(SKIP.EQ.CHECK(7)) GO TO 215
1390 WRITE(6,150)
1400 WRITE(6,160) (XD(J), J=1, NCOL)
1410 160 FORMAT ('0./4X.,Deltax Nodal Values')
1420 WRITE(6,170)
1430 WRITE(6,160) (YD(I), I=1, NROW)
1460 170 FORMAT ('O', 5X, 'DELTAY NODAL VALUES')
1470 215 WRITE(6, 220)
1480 220 FORMAT ('O', 5X, 'ANISOTROPY RATIO KH/KV')
1490 WRITE(6, 160)(ANISO(I), I=1, NROW)
1500 C
1510 C WRITE AX AND AY
1520 C
1530 IF(SKIP.EQ.CHECK(7)) GO TO 255
1540 WRITE(6, 250)
1550 250 FORMAT ('O', 5X, 'AX VALUES')
1560 WRITE(6, 160)(AX(J), J=2, NCOL)
1570 WRITE(6, 260)
1580 260 FORMAT ('O', 5X, 'AY VALUES')
1590 WRITE(6, 160)(AY(I), I=2, NROW)
1600 255 CONTINUE
1610 C
1620 C READ IN THE NUMBER OF SOIL STRATA AND REQUESTED SIMULATIONS
1630 READ(5, 96) LAYERS, NOSIM
1640 DO 55 L=1, LAYERS
1650 READ(5, 53) LAYLO(L), LAYHI(L), PERM
1660 53 FORMAT (3I10, 2F10.3)
1670 55 CONTINUE
1680 DO 3000 NSIM=1, NOSIM
1690 NOONE=0
1700 NOTWO=0
1710 NOTHRE=0
1720 NOFOR=0
1730 NOFIV=0
1740 NOHIX=0
1750 NOSEV=0
1760 NOGET=0
1770 NONIN=0
1780 NOTEN=0
1790 NOGETN=0
1800 WRITE(6, 97) NSIM, NOSIM
1810 97 FORMAT ('1',//,5X, 'SIMULATION NUMBER', I4, 1X, 'OF', I4)
1820 C
1830 C THE K VALUES ARE ASSUMED TO EACH NODE ON THE BASIS OF THE TYPE
1840 C OF P. D. F. ASSUMED. IF ISO=1, K IS A CONSTANT; IF ISO=2, K IS UNIFORM
1850 C DIST.; IF ISO =3, K IS LOGNORMAL; IF ISO=4, EXPONENTIAL; IF ISO=5,
1860 C K IS READ IN AT EACH NODE; IF ISO=0, WE HAVE VERTICAL STRATA.
1870 C
1880 IF(ISO.EQ.1) GO TO 80
1890 IF(ISO.EQ.2) GO TO 91
1900 IF(ISO.EQ.3) GO TO 50
1910 IF(ISO.EQ.4) GO TO 84
1920 IF(ISO.EQ.5) GO TO 60
1930 C OTHERWISE
1940 C READ VALUES FOR A VERTICALLY LAYERED DETERMINISTIC MODEL
1950 C
1960 73 FORMAT (2I10, F10.2)
1970 C
1980 C THE MODEL IS VERTICALLY LAYERED
1990 78 DO 79 IL=1, LAYERS
2000 READ(5, 73) LAYLO, LAYHI, PERM
2010 DO 79 J=2, NROWM1
2020 DO 79 J=LAYLO, LAYHI
2030 K(I, J)=PERM
2040 79 CONTINUE
2050 70 GO TO 95
2060 C
2070 C HYDRAULIC CONDUCTIVITY VALUES HAVE A LOG NORMAL DISTRIBUTION
2080 C WITHIN UP TO 10 LAYERS IF REQUESTED
2090 50 CONTINUE
2100 57 N=1, LAYERS
2110 IF(NSIM.NE.1)GO TO 58
2120 READ(5,23)LAYER(N),CONMN(N),SD(N),ETA(N),ALPHAX(N),ALPHAY(N)
2130 IF(N.NE.1)GO TO 76
2140 WRITE(6,31)LAYERS
2150 76 WRITE(6,65)LAYER(N),LAYLU(N),LAYHU(N),CONMN(N),SD(N),ETA(N),
2160 *ALPHAX(N),ALPHAY(N)
2170 58 LAYLO=LAYLU(N)
2180 LAYHI=LAYHU(N)
2190 MEAN=CONMN(N)
2195 SDEV=SD(N)
2200 ETA=ETA(N)
2205 ALFAX=-ALPHAX(N)
2210 ALFAY=-ALPHAY(N)
2220 NORDROWS=LAYHI-LAYLO+1
2225 NP=NORDROWS*NCOLM2
2226 NLASR=(NORDROWS-1)*NCOLM2+1
2230 SUMK=0.0
2240 RECIPK=0.0
2250 PRODK=0.0
2260 SUMDF=0.0
2265 IAINV=300
2270 IA=300
2275 MN=300
2280 TOL=0.0
2285 51 FORMAT('0',/,'5X,'HYDRAULIC CONDUCTIVITY IS LOG-NORMALLY DISTRIBUTED.'
2290 "ED IN'/'4,'LAYERS')'
2295 55 FORMAT('0',/,'5X,'LAYER',/'4,2X,'INITIAL ROW IS',/'4,2X,'LAST ROW IS'
2297 '/,'4,2X,'EXPECTED MEAN=',/,'F10.4',/,'STD. DEV.=',/,'F10.4',
2300 '/,'4,2X,'WITH ETA=',/,'F10.4',/,'7X,'AUTOREGRESSIVE PARAMETERS ARE ',/,'F10.4',
2303 '/,'4,2X,'IN X DIRECTION AND ',/,'F10.4,'IN Y DIRECTION')
2305 C NOW CONVERT SDEV AND MEAN TO LOGARITHMIC VALUES:SDVLNK & AMNLNK
2306 COVKSQ=(SDEV/MEAN)**2
2307 VARLNK=ALOG(COVKSQ+1.0)
2308 SDVLNK=SQRT(VARLNK)
2310 AMNLNK=ALOG(MEAN)-0.5*(VARLNK)
2315 C INITIALLY SET ETA=SDVLNK
2317 ETAN=SDVLNK
2319 C GENERATE THE EPSILON MATRIX, <E>, AND PREMULTIPLY BY ETA
2320 DO 152 I=1,NP
2325 YFL=GGNGF(DSEED)
2330 EPSILN(I)=ETAN*YFL
2335 WRITE(6,194)I,EPSILN(I)
2340 194 FORMAT(/,'7X',10.2F10.5)
2345 152 CONTINUE
2350 C GENERATE A WEIGHTING MATRIX <WT> AND AN IDENTITY MATRIX <I>
2355 DO 54 L=1,NP
2356 DO 54 M=1,NP
2361 IF(L.EQ.M)GO TO 176
2365 W(L,M)=0.0
2370 GO TO 154
2375 176 W(L,M)=1.0
2380 154 CONTINUE
2385 DO 155 L=1,NP
2390 DO 155 M=1,NP
2395 IF(L.EQ.M)GO TO 176
2400 W(L,M)=0.0
2405 GO TO 154
2410 176 W(L,M)=1.0
2415 154 CONTINUE
2420 C GENERATE A WEIGHTING MATRIX <WT> AND AN IDENTITY MATRIX <I>
2430 DO 54 L=1,NP
2435 DO 54 M=1,NP
2441 IF(L.EQ.M)GO TO 176
2445 W(L,M)=0.0
2450 GO TO 154
2455 176 W(L,M)=1.0
2460 154 CONTINUE
2465 DO 155 L=1,NP
2470 DO 155 M=1,NP
2475 IF(L.EQ.M)GO TO 176
2480 W(L,M)=0.0
2485 GO TO 154
2490 176 W(L,M)=1.0
2495 154 CONTINUE
2500 155 CONTINUE
2505 NCOLML=NCOLM2+L
NCLMP2 = NCOLM2 * 2
NRUP = L - NCOLM2
NRDN = L + NCOLM2
NCOLR = L + 1
NCOLL = L - 1

2600 C DETERMINE IF IN THE UPPER ROW
2610 IF (L .EQ. 1) GO TO 158
2620 C DETERMINE IF IN THE MIDDLE OF THE UPPER ROW
2630 IF (L .LT. NCOLM2) GO TO 157
2640 C DETERMINE IF WE'RE IN THE UPPER LEFT HAND CORNER
2650 IF (L .EQ. NCOLM2) GO TO 156
2660 C WE'RE NOT IN THE UPPER ROW, CHECK FIRST COLUMN
2670 NICOL = (L-1)/NCOLM2
2680 CHK1CL = (FLOAT(L) - 1.0) / (FLOAT(NCOLM2))
2690 CHKMTH = CHK1CL - FLOAT(NCOL)
2700 IF (CHKMTH .EQ. 0.0) GO TO 161
2710 C WE'RE NOT IN THE LEFT HAND COLUMN, CHECK RIGHT HAND COLUMN
2720 NLASCL = L/NCOLM2
2730 CHKLC = FLOAT(L)/FLOAT(NCOLM2)
2740 CHKMLS = CHKLC - FLOAT(NLASCL)
2750 IF (CHKMLS .EQ. 0.0) GO TO 163
2760 C WE'RE NOT IN THE RIGHT COLUMN, CHECK LAST ROW
2770 IF (L .GT. NRASR) GO TO 165
2780 C WE'RE NOT IN THE LAST ROW SO WE MUST BE AT AN INTERIOR POINT
2790 W(L,NCOLL) = ALFAX/4.0
2800 W(L,NCOLR) = ALFAX/4.0
2810 W(L,NRUP) = ALFAY/4.0
2820 W(L,NRDN) = ALFAY/4.0
2830 GO TO 155
2840 C
2850 C WE'RE AT THE UPPER LEFT HAND CORNER
2860 158 W(L,2) = ALFAX/2.0
2870 W(L,NCOLM1) = ALFAY/2.0
2880 GO TO 155
2890 C WE'RE IN THE MIDDLE OF THE UPPER ROW
2900 157 W(L,NCOLL) = ALFAX/3.0
2910 W(L,NCOLR) = ALFAX/3.0
2920 W(L,NRDN) = ALFAY/3.0
2930 GO TO 155
2940 C WE'RE IN THE UPPER RIGHT HAND CORNER
2950 156 W(L,NCOLL) = ALFAX/2.0
2960 W(L,NCOLR) = ALFAY/2.0
2970 GO TO 155
2980 C WE'RE IN THE LEFT HAND COLUMN
2990 161 IF (NCOL .EQ. NRW3M) GO TO 162
3000 C WE'RE NOT IN THE LOWER LEFT CORNER
3010 W(L,NRUP) = ALFAY/3.0
3020 W(L,NRDN) = ALFAY/3.0
3030 W(L,NCOLR) = ALFAX/3.0
3040 GO TO 155
3050 C WE'RE IN THE LOWER LEFT COLUMN
3060 162 W(L,NRUP) = ALFAY/2.0
3070 W(L,NCOLR) = ALFAY/2.0
3080 GO TO 155
3090 C WE'RE IN THE RIGHT HAND COLUMN, CHECK IF AT LOWER CORNER
3100 163 IF (NLASCL .EQ. NRW2M) GO TO 164
3110 C WE'RE NOT IN THE LOWER RIGHT CORNER
3120 W(L,NRUP) = ALFAY/3.0
3130 W(L,NRDN) = ALFAY/3.0
3140 W(L,NCOLR) = ALFAX/3.0
3150 GO TO 155
3160 C WE'RE IN THE LOWER RIGHT CORNER
3170 164 W(L,NRUP) = ALFAY/2.0
3180 W(L,NCOLR) = ALFAY/2.0
3190 GO TO 155
C WE'RE IN THE INTERIOR OF THE LOWER ROW

W(L, NCOL) = ALFAX/3.0

W(L, NCOLR) = ALFAX/3.0

W(L, NRUP) = ALFAX/3.0

CONTINUE

C PRINT OUT THE MATRIX THAT IS TO BE INVERTED

WRITE (6, 179) LAY(N)

WRITE (6, 178) '(1)', '5X', 'THE MODIFIED WEIGHTING MATRIX, ((I)-(W)), FOR LAY

$ER', '14.2X', 'AS GENERATED IS')

DO 179 I = 1, NP

WRITE (6, 200) L, (W(L, M), M = 1, NP)

C NOW INVERT THE MATRIX TO DEVELOP THE FILTER MATRIX

CALL LGINF (W, IA, MN, NN, TOL, FILTR, IAINV, S, WK, IER)

C NOW WRITE OUT THE FILTER MATRIX AND STORE ON DISK

WRITE (6, 173) LAY(N)

WRITE (6, 172) 'THE FILTER MATRIX FOR LAYER', '14,

$2X, 'AS GENERATED IS')

DO 181 L = 1, NP

WRITE (6, 201) L, (FILTR(L, M), M = 1, NP)

DO 98 L = 1, NP

98 WRITE (6, 192) IER

C NOW MULTIPLY FILTER MATRIX BY EPSILON AND THESE ARE LOG OF K

M = 0

DO 54 J = 2, NCOLM1

M = M + 1

WRITE (6, 23) L, YEGLK

DISPER = (K(I, J) - ARITHK)**2

SUMDIF = SUMDIF + DISPER

VARK = SUMDIF / (XLAYHI - XLAYLO + 1.0)*XCOLM2

STDEV = SQRT(VARK)

COV = STDEV/ARITHK
CONVERT CONDUCTIVITIES FROM FT/D TO CM/SEC

CARITH=ARITHK* .0003528
CHARH=HARHK* .0003528
CGEOH=GEOMK* .0003528

IF(I.LT.LAYHI) GO TO 57
IF(J.LT.NCOLM1) GO TO 57

WRITE(6,56) ARITHK,CARITH,GEOMK,CGEOM,HARMK,CHARM

56 FORMAT (//, 16X, 'ARITHMETIC MEAN=' , F10.6 , 1X , 'FT/D' , 1X , '=' , 1X , F10.6 , $ , 1X , 'CM/SEC')

WRITE(6,1111) STDEV,COV

57 CONTINUE

GO TO 95

CONDUCTIVITIES ARE READ IN AT EACH NODE

60 READ(5,40) ((K(I,J), J=1, NCOL), I=1, NROW)

GO TO 95

HYDRAULIC CONDUCTIVITY VALUES ARE ALL THE SAME

80 DO 82 I=1, NROW
82 DO 82 J=1, NCOL
82 KCI,J>= PERM
88 CONTINUE

THE HYDRAULIC CONDUCTIVITY VALUES ARE UNIFORMLY DISTRIBUTED WITH A DIFFERENT DISTRIBUTION WITHIN EACH OF THE LAYERS

84 CONTINUE

DO 88 L=1, LAYERS
86 DO 88 L=1, LAYERS
88 DO 88 I=LAYLO,LAYHI
88 DO 88 J=1,NCOLM1
82 YFL=GGEXN(SEDSEED, MEAN)
81 XER=1000 . IF(UNIHU<=100) XER=100
82 DO 88 I=LAYLO,LAYHI
82 DO 88 J=1,NCOLM1
82 YFL=GGEXN(SEDSEED, MEAN)
82 K(I,J)=YFL
88 CONTINUE

THE HYDRAULIC CONDUCTIVITY VALUES ARE UNIFORMLY DISTRIBUTED WITH A DIFFERENT DISTRIBUTION WITHIN EACH OF THE LAYERS

91 CONTINUE

DO 93 L=1, LAYERS
92 DO 93 L=1, LAYERS
93 DO 93 I=LAYLO,LAYHI
93 DO 93 J=2,NCOLM1
93 YFL=GGUBF(SEDSEED, MEAN)
92 K(I,J)=YFL
93 CONTINUE
C SET VALUE OF K IN THE LEFT COLUMN EQUAL TO 0
DO 100 I=1,NROW
K(I,1)=0.0

C SET VALUE OF K IN THE RIGHT COLUMN EQUAL TO 0
DO 110 J=1,NCOL
K(1,J)=0.0

C SET VALUE OF K IN THE UPPER ROW EQUAL TO 0
DO 150 K(I,NCOL)=0.0

C SET VALUE OF K IN THE LOWER ROW EQUAL TO 0
DO 190 K(NROW,J)=0.0

C COMPUTE KY(I,J) VALUES
DO 120 I=2,NROWM1
DO 120 J=2,NCOLM1
KY(I,J)=K(I,J)/ANISO(I)

C CONVERT HYDRAULIC CONDUCTIVITIES TO ELECTRICAL CONDUCTIVITIES IF SPECIFIED
IF(ELEC. NE .CHECK(3))GO TO 117

C THESE ARE THE NODAL VALUES TO BE USED IN COMPUTING
C KHYD(I,J) --THE CONNECTION VALUE IN THE Y-DIRECTION
DO 113 I=2,NROWM1
DO 113 J=2,NCOLM1
KHYD(I,J)=K(I,J)**2

C NOW CALCULATE THE ACTUAL STANDARD DEVIATION AND COEF. OF VARIATION
SUMDIF=0.0
PRODISPER=0.0
SUMIF=SUMDIF
DO 121 I=2,NROWM1
DO 121 J=2,NCOLM1
DISPER=KHYD(I,J)-ARITHK**2
SUMIF=SUMIF+DISPER
CONTINUE
SUMDIF=SUMIF/NROWM2*NCOLM2
STDEV=SQRT<SUMDIF>
COEF=STDEV/ARITHK

C COMPUTE THE ARITHMETIC, HARMONIC AND GEOMETRIC MEANS OF THE
C HYDRAULIC CONDUCTIVITY DISTRIBUTION
SUM=0.0
RECIP=0.0
SUMK=SUMK+K(I,J)
RECIPK=RECIPK+1.0/K(I,J)
CONTINUE
ARITHK=SUMK/NROWM2*NCOLM2
HARMK=SUMK/RECIPK
GEOMK=10.0**(LOG10<K(I,J)>)/RECIPK

C NOW CALCULATE THE Y-DIRECTION VALUE
K(1,J)=1.0/(KHYD(I,J)**2)

C COMPUTE THE ARITHMETIC, HARMONIC AND GEOMETRIC MEANS OF THE
C HYDRAULIC CONDUCTIVITY DISTRIBUTION
SUM=0.0
RECIP=0.0
SUMK=SUMK+K(I,J)
SUMIF=SUMIF+DISPER
CONTINUE
SUMDIF=SUMIF/NROWM2*NCOLM2
STDEV=SQRT<SUMDIF>
COEF=STDEV/ARITHK

C HYDRAULIC CONDUCTIVITY VALUES ARE WRITTEN ONTO A DISK DATA SET
IF(CONK .NE .CHECK(1))GO TO 105
DO 105 I=2,NROWM1
DO 105 J=2,NCOLM1
2. STKBLKNP

C THIS IS FIRST PART OF A PROGRAM WHICH SOLVES
2-D STEADY, HETEROGENEOUS, ANISOTROPIC FLOW THROUGH POROUS MEDIA
USING FINITE DIFFERENCE WITH VARIABLE GRID SPACINGS
AND THE ITERATIVE ALTERNATING DIRECTION IMPLICIT PROCEDURE
FILE NAME IS STKBLKNP AND PROGRAM CONTINUES IN FILE QWCOR2NP
SAME AS STKBLK EXCEPT PRINTOUT IS SEVERELY LIMITED
SIMILAR TO QWCOR1 EXCEPT THE OUTER ROWS AND COLUMNS ARE DELETED
AFTER SHAVING, THE BLOCKS ARE STACKED END TO END AND OR ON TOP OF
ONE ANOTHER. THIS PROGRAM TAKES FILTR MATRIX FROM DSN FILE.

C SPECIFICATIONS

INTEGER CHECK, CONH, CONK, ELEC, MINI, STRF, FLOW, SKIP, UNILU, UNIHU
INTEGER EXLO, EXHI, WARP, PTPT, UPDISC
INTEGER NTREB, NWAV, NBSIM
REAL K, KHARM, LENGTH, KHEQFO, KVEQFO, KVEQCS, KHEQCS, HARMK, MEAN, KLOG
REAL KY, LNK, XLNK, AMEAN, ASOVC
REAL TTHWC, TT60C, TT70, TT80, TT90, RH01C, ARHOAC
REAL TOTM, XLOCHT, YLOCHTC, XLOCEN, XISCALC, CSTA TC, HCSTATC
REAL RH03, ARH05, AMEANAC, ASOVAC
DOUBLE PRECISION H, HNEW, A, B, C, D, E, F, G, QPARM, QKNOWN, DABS, DSEED

DIMENSION KHARMC, KC, XDC, YDC, AX, AY, HEADIN, ANIS0, CHECK(10), X(52,62), Y(52,62)
DIMENSION LAYER, CONMN, SDC
DIMENSION ETA, ALPHAX, ALPHAY, EPSILN
DIMENSION G, F, IC, HSTRAT, KY
DIMENSION V, VALK, RH0, XISCAL
DATA CHEK / 'CONK ', 'CONH ', 'ELEC ', 'MINI', 'STRF', 'FLOW', 'SKIP', 'VERT', 'SKIP', 'WARP', 'PTPT'/
WRITE(6,20) HEADIN

WRITE(10,2110) K(1,J)
10 CONTINUE
IF(NSIM.GT.1) GO TO 3000
WRITE(6,180) I, K(I,J), J=1, NCOL
WRITE(6,201) I, CONMN, STRF, UNILU, UNIHU
WRITE(6,200) I, XR, X(1,10), X(10,10), X(10,52)
WRITE(6,200) I, YR, Y(1,10), Y(10,10), Y(10,52)
WRITE(6,200) I, ZR, Z(1,10), Z(10,10), Z(10,52)
WRITE(6,200) I, VR, V(1,10), V(10,10), V(10,52)
WRITE(6,200) I, HR, H(1,10), H(10,10), H(10,52)
WRITE(6,200) I, SR, S(1,10), S(10,10), S(10,52)
WRITE(6,200) I, HR, H(1,10), H(10,10), H(10,52)
WRITE(6,25) DSEED
380 20 FORMAT ('1',20X,20A4)
390 21 FORMAT (10F12.5)
400 22 FORMAT (1F5.0,16F8.5)
410 23 FORMAT (11I0,6F10.5)
420 24 FORMAT (3I6,2X,6F10.5)
430 25 FORMAT ('0',/,'DSEED=','F12.0')
440 26 FORMAT (F5.0,3F5.3,10F6.3)
450 27 FORMAT (F5.0,6F9.5)
460 28 FORMAT (214,9F8.2)
470 29 FORMAT (3I6,2X,10F10.4,19)

500 C INPUT PARAMETERS
550 C NOTE **** ALL INPUT PARAMETERS ARE NODAL VALUES ****
520 READ(5,30) NROW, NCOL, EC, ISO, PERM
530 READ(5,35) CONK, CONH, ELEC, MINI, STRF, FLOW, SKIP, WARP
540 READ(5,30) LSTRM, LEQUIV, DHEAD
550 C LSTRM IS THE COLUMN (FOR THE HORIZONTAL FLOW CASE, FLOW=HORI)
560 C OR THE ROW (FOR THE VERTICAL FLOW CASE, FLOW=VERT)
570 C OR THE COLUMN OF THE CONSTANT HEAD POINT ON THE
580 C LEFT SIDE OF THE UPPER BOUNDARY
590 C WHERE THE TOTAL FLOW IS COMPUTED FOR THE USE OF NONDIMENSIONALIZING
600 C THE STREAM FUNCTION *** IT IS USED ONLY WHEN CHECK(5)=STRF
610 C
620 C LEQUIV IS THE COLUMN (FOR THE HORIZONTAL FLOW CASE, FLOW=HORI)
630 C OR THE ROW (FOR THE VERTICAL FLOW CASE, FLOW=VERT)
640 C WHERE THE TOTAL FLOW IS COMPUTED TO BE USED IN SOLVING
650 C FOR THE EQUIVALENT CONDUCTIVITY (RESISTIVITY) OR WHERE THE
660 C WARREN AND PRICE TECHNIQUE IS APPLIED
670 READ(5,40) WPFACT
690 NROWM1=NROW-1
700 NCOLM1=NCOL-1
710 NROWM2=NROW-2
720 NCOLM2=NCOL-2
730 NROWM3=NROW-3
740 NROWP2=NROW+2
750 NCOLP1=NCOL+1
760 NCOLP2=NCOL+2
770 C NOTE **** THE VALUE READ IN FOR HMIN IS THE LOWEST ITERATION
780 C PARAMETER AND IS USED ONLY IF MINI WAS SPECIFIED IN THE OPTIONS
790 READ(5,32) ITMAX, NUMPAR, HMAX, HMIN
800 30 FORMAT (2I10.1F10.5,110.1F10.5)
810 32 FORMAT (2I10.6F10.5)
820 33 FORMAT (3I10.3F10.5)
830 34 FORMAT (4I10.4F10.5)
840 35 FORMAT (16(A4,1X))
850 READ(5,40) (XD(J), J=1, NCOL)
860 40 FORMAT (9F10.1)
870 C READ(5,40) (YD(I), I=1, NROW)
880 C COMPUTE AX AND AY
890 C AX= X-DISTANCE FROM ONE NODE CENTER TO THE NEXT
900 C AY= Y-DISTANCE FROM ONE NODE CENTER TO THE NEXT
910 C
920 DO 47 J=2, NCOL
930 42 AX(J)= (XD(J)+XD(J-1))/2.0
940 DO 44 I=2, NROW
950 44 AY(I)= (YD(I)+YD(I-1))/2.0
960 C
970 C READ ANISOTROPY AT EACH ROW
980 C VALUE IS THE RATIO OF KH/KV
1000 120 READ(5,40) (ANISO(I), I=1, NROW)
1010 C SET BOUNDARY CONDITIONS
1020 C NOTE *** PERIMETER BOUNDARY POINTS CAN BE EITHER CONSTANT HEAD OR IMPERMEABLE
1040 C NOTE *** FLOW SHOULD BE FROM LEFT TO RIGHT OR TOP TO BOTTOM
1050 C I.E. HIGH HEADS SHOULD BE LOCATED AT THE TOP OR LEFT SIDE
1070 C SET ALL HEADS EQUAL TO SOME INITIAL VALUE
1080 C AND ALL IC(I,J) VALUES TO ZERO
1090 DO 330 I=1,NROW
1100 DO 330 J=1,NCOL
1110 IC(I,J)=0
1120 HDSMN(I,J)=0.0
1130 330 H(I,J)= 50.0
1140 C
1150 C READ LOCATIONS OF CONSTANT HEAD NODES
1160 C ALONG THE PERIMETER
1170 C NOTE: THE PERIMETER IS THE ONLY LOCATION FOR A SOURCE OR A SINK
1180 C THAT IS -- A HIGH CONSTANT HEAD OR A LOW CONSTANT HEAD
1190 C
1200 C READ THE TOP ROW
1210 DO 336 (IC(2, J), J=2, NCOLM1)
1220 336 FORMAT (16I3)
1230 C READ THE BOTTOM ROW
1240 DO 336 (IC(NROWM1, J), J=2, NCOLM1)
1250 C READ THE LEFT SIDE
1260 DO 336 (IC(I,2), I=3,NROWM2)
1270 C READ THE RIGHT SIDE
1280 DO 336 (IC(1, NCOLM1), I=3,NROWM2)
1290 C
1300 C READ HEAD VALUES ALONG THE PERIMETER
1310 C READ TOP ROW
1320 DO 335 (H(2, J), J=2, NCOLM1)
1330 C READ THE BOTTOM ROW
1340 DO 335 (H(NROWM1, J), J=2, NCOLM1)
1350 C READ THE LEFT SIDE
1360 DO 335 (H(I,2), I=3,NROWM2)
1370 C READ THE RIGHT SIDE
1380 DO 335 (H(I, NCOLM1), I=3,NROWM2)
1390 350 FORMAT (BD10.3)
1400 C
1410 C ECHO CHECK OF INPUT PARAMETERS
1420 C
1440 140 FORMAT ('0', 4X, '# OF ROWS = ', T25.15, '/ 5X, '# OF COLUMNS = ', T25.15, /
1450 #/4X, 'TOTAL DISSIPATED HEAD IS ', F10.5, ' FEET IN ', F10.5, ' FEET', /
1460 #/3X, 'WITH AN AREA OF ', 3X,F10.5, ' SQUARE FEET INTO SECTION', /
1470 #/5X, 'CLOSEURE ERROR CRITERIA=', E16.5 , 5X, 'MAXIMUM ITERATIONS', /
1480 $=', '15)
1490 WRITE(6,148) CONH, CONK, ELEC, MINI, STRF, FLOW, SKIP, WARP
1480 148 FORMAT ('0', 5X, 'PROBLEM OPTIONS SPECIFIED: ', 2X,10A8)
1490 IF(SKIP.EQ.CHECK(7)) GO TO 215
1500 WRITE(6,150)
1510 WRITE(6,160) (XD(J), J=1,NCOL)
1520 150 FORMAT ('0', 5X, 'DELTA X NODAL VALUES')
1530 160 FORMAT ('0', 4X,10F12.1/(5X,10F12.1))
1540 WRITE(6,170)
1550 WRITE(6,160) (YD(I), I=1, NROW)
1560 170 FORMAT ('0', 5X, 'DELTA Y NODAL VALUES')
1570 215 WRITE(6,220)
1580 220 FORMAT ('0', 5X, 'ANISOTROPY RATIO KH/KV')
1590 WRITE(6,160) (ANISO(I), I=1, NROW)
1600 C
1610 C WRITE AX AND AY
1620 C
1630 IF(SKIP.EQ.CHECK(7)) GO TO 255
READ IN THE NUMBER OF SOIL STRATA AND REQUESTED SIMULATIONS
USE A VALUE FOR NCFLO ONLY IF FLOW IS FROM THE UPPER BOUNDARY.
AND THEN USE THE LAST COLUMN FROM THE LEFT WHERE FLOW IS POSSIBLE.
READ(5,96) LAYERS, NOSIM, NRBLK, NCBLK, NCFLO, UPDISC, NCBAR, NRBAR
DO 55 L=1, LAYERS
READ(5,53) LAYERL(1), LAYHL(1), LAYHL(1)
DO 53 CONTINUE
READ(5,23) LAYERN(1), CONMN(1), SDCN(1), ETACN(1), ALPHAX(1), ALPHAY(1)
DO 50 CONTINUE
DO 57 N=1, LAYERS
IF (NSIM .NE. 1) GO TO 58
READ(5,72) LAYLO, LAYHI, PERM
DO 79 I=2, NROWM1
DO 79 J=LAYLO, LAYHI
K(I, J)=PERM
79 CONTINUE
GO TO 95
2120 C OTHERWISE
2130 C READ VALUES FOR A VERTICALLY LAYERED DETERMINISTIC MODEL
2140 C
2150 73 FORMAT(2110, F10.2)
2160 C
2170 C THE MODEL IS VERTICALLY LAYERED
2180 78 DO 79 IL=1, LAYERS
2190 READ(5,72) LAYLO, LAYHI, PERM
2200 DO 79 I=2, NROWM1
2210 DO 79 J=LAYLO, LAYHI
2220 K(I, J)=PERM
2230 79 CONTINUE
2240 GO TO 95
2250 C
2260 C HYDRAULIC CONDUCTIVITY VALUES HAVE A LOG NORMAL DISTRIBUTION
2270 C WITHIN UP TO 10 LAYERS IF REQUESTED
2280 50 CONTINUE
2290 DO 57 N=1, LAYERS
2300 IF (NSIM .NE. 1) GO TO 58
2310 READ(5,23) LAYER(N), CONMN(N), SD(N), ETA(N), ALPHAX(N), ALPHAY(N)
2320 IF (N .NE. 1) GO TO 76
WRITE(6,51) LAYERS
WRITE(6,65) LAYER(N),LAYLU(N),LAYHU(N),CONMN(N),SD(N),ETA(N),
*ALPHAX(N),ALPHAY(N)
58 LAYLD=LAYLU(N)
LAYHI=LAYHU(N)
LALOM=LAYLD-1
LAHPI=LAYHI+1
MEAN=CONMN(N)
SDEV=SD(N)
ETA=ETA(N)
ALFAX=ALPHAX(N)
ALFAY=ALPHAY(N)
NORD=LAYHI-LAYLD+1
NP=NRBLK*NCBLK
NCJM1=NCBLK-1
NCBM2=NCBLK-2
NRBK1=NRBLK-1
NRBM2=NRBLK-2
SUMK=0.0
RECPK=0.0
PRODK=0.0
SUMDIF=0.0
CSTATS(NSIM,2)=0.0
CSTATS(NSIM,3)=0.0
CSTATS(NSIM,4)=0.0
CSTATS(NSIM,15)=0.0
CSTATS(NSIM,17)=0.0
XISCAL(NSIM)=XD(N)
YISCAL(NSIM)=YD(N)
51 FORMAT(0,/,5X,'HYDRAULIC CONDUCTIVITY IS LOG-NORMALLY DISTRIBUTED'
,2X,14,'LAYER(S):')
65 FORMAT(//,5X,'INITIAL ROW IS',14,2X,'LAST ROW IS'
,14,5X,'INITIAL ROW IS',14,5X,'LAST ROW IS'
,14,5X,'EXPECTED MEAN=',F10.4,5X,'STD. DEV.=',F10.4,
,7X,'AUTOREGRESSIVE PARAMETERS ARE',F10.4,
,10X,'IN X DIRECTION AND',F10.4,'IN Y DIRECTION')
C NOW CONVERT SDEV AND MEAN TO LOGARITHMIC VALUES, SDEVLNK & AMNLNK
CDVKSO=SDEV/MEAN**2
VARLNK=ALOG(CDVKSO+1.0)
SDVLNK=SQRT(VARLNK)
AMNLNK=ALOG(MEAN)-0.5*VARLNK
INITIALLY SET ETAN=SDVLNK
ETAN=0.95*SDVLNK
IF(NSIM.NE.1) GO TO 143
WRITE(6,161) AMNLNK,SDVLNK,ETAN
161 FORMAT(0,7X,'REGULAR MEAN OF LOG OF K=',F10.5,' AND STD. DEV. = ',
10X,'THE VALUE OF ETAN IS SET AT ',F10.6)
163 CONTINUE
NBKSL=(NCOL/NCBLK-2)
NBKST=(LAYHI-LAYLD+1)/NRBLK-2
NBKTOT=NBKSL*NBKST
IF(NSIM.NE.1) GO TO 158
WRITE(6,70) N, NBKTOT,NBLKST,NBLKSL
70 FORMAT(0,/,10X,'LAYER',I3,' CONSISTS OF',I4,' BLOCKS.',
10X,'AND',I4,' BLOCKS WILL BE STACKED END TO END, STARTING FROM THE UPER LEFT WORKING DOWN AND THEN TO THE RIGHT')
158 CONTINUE
2880 C GENERATE THE EPSILON MATRIX, (E), AND PREMULTIPLY BY ETA
2890 DO 152 I=1,NP
2900   YFL=QGNQF(DSEEED)
2910 EPSILON(I)=ETAN*YFL
2920 194 FORMAT(//,7X,I10,2F10.5)
2930 152 CONTINUE
2940 CALL MUNSD EPSILON,NP,AMN,SDV,COEVAR
2950 162 FORMAT(C'0',5X,I10,2F10.5,' AND STD . DEV .',' F10.5,' AND COV .='F10.6)
2960 IF(NBLKT.NE.1) GO TO 178
2970 IF(NBLK.NE.1) GO TO 178
2991 IF(NSIM.NE.1) GO TO 178
3000 IF(N.NE.1) GO TO 178
3010 C C RETRIEVE THE FILTR MATRIX FROM THE DIS
3020 C DO 179 L=1,NP
3030 179 READ(14,202) (FILTR(L,M),M=1,NP)
3040 178 CONTINUE
3050 C NOW MULTIPLY FILTER MATRIX BY EPSILON AND THESE ARE LOG OF K
3060 DO 183 L=1,NP
3070 YEGLK=0.0
3080 DO 683 M=1,NP
3090 YEGLK=YEGLK+FILTR(L,M)*EPSILON(M)
3100 683 LNKCL=LNLK+AMNLNK
3110 CALL MUNSD LNK,NP,AMN,SDV,COEVAR
3120 NLCOL=(NBLK-1)*(NCBLK-2)+1
3130 NRCOL=NLCOL+NCBLK-1
3140 M=0
3150 DO 320 I=NTROW,NBROW
3160 MM=I
3170 DO 321 J=NLCOL,NRCOL
3180 MM=MM+1
3190 CALL AUGAR LNK,NCBLK,AMN,SDV,LAGS,RHO
3200 AMEAN(I)=AMN
3210 ASDV(I)=SDV
3220 C THEN CONVERT N(O,SDEV) DEVIATE TO N(MEAN,SDEV) DEVIATE
3230 KLOG=LNK(M)+AMNLNK
3240 IF(I.EQ.NTROW) GO TO 159
3250 IF(I.EQ.NBROW) GO TO 159
3260 IF(J.EQ.NLCOL) GO TO 159
3270 IF(J.EQ.NRCOL) GO TO 159
3280 KLOG=LNK(M)+AMNLNK
3290 C VALUE KLOG = LN OF K
3300 K(I,J)=EXP(KLOG)
3310 SUMK=SUMK+K(I,J)
3320 RECIPK=RECIPK+1./K(I,J)
3330 PRODK=PRODK+ALOG1(K(I,J))
3340 159 CONTINUE
3350 C CHECK THE STATISTICAL PARAMETERS OF LOG K, BY ROWS
3360 159 XLNK(MM)=KLOG
3370 MM=MM+1
3380 IF(MM.LE.NCBLK) GO TO 54
3390 CALL MUNSD XLNK,NCBLK,AMN,SDV,COEVAR
3400 LAGS=5
3410 CALL AUGAR XLNK,NCBLK,AMN,SDV,LAGS,RHO
3420 AMEAN(I)=AMN
3430 ASDV(I)=SDV
3440 C NOW REFIGURE W/O THE EDGES
3450 DO 48 MMM=2,NCBKMK1
3460 MMMREV=MMM-1
3470 XLNK(MM)=XLNK(MM)
3480 48 CONTINUE
3490 CALL MUNSD XLNK,NCBKMK2,AMN,SDV,COVA
3500 CALL AUGAR XLNK,NCBKMK2,AMN,SDV,LAGS,RHDA
3510 AMEANA(I)=AMNA
3520 ASDVA(I)=SDVA
DO 54 IN=1,LAGS
ARHO(I, IN)=RHO(IN)
ARHOA(I, IN)=RHOA(IN)
54 CONTINUE
CORRELATION COEFFICIENTS FOR ALL ROWS OF THIS SEGMENT HAVE BEEN CALCULATED
DO 52 I=NTROW, NROW
IREV=I-NTROW+1
RHO1(IREV)=ARHO(I, 1)
RHO2(IREV)=ARHO(I, 2)
RHO3(IREV)=ARHO(I, 3)
52 CONTINUE
64 FORMAT(’O’, 10X, ’MEAN, STD. DEV. AND AUTOCORRELATION COEFFICIENTS FOR EACH ROW AND LAGS FROM 1 TO 4’, 11, 7X, ’ROW’, 4X, ’MEAN’, SX, 6X, ’STD. DEV.’, 2X, ’RHO1’, 4X, ’RHO2’, 4X, ’RHO3’, 4X, ’RHO4’)
CALL MUNSD(ARHO1, NRBKM2, AMN, SDV, COEVAR)
ARHO1YM=ARHO1YM+AMN*(FLOATINOSIM+FLOATINBKTOT)
CALL MUNSD(ARHO2, NRBKM2, AMN, SDV, COEVAR)
ARHO2YM=ARHO2YM+AMN*(FLOATINOSIM+FLOATINBKTOT)
CALL MUNSD(ARHO3, NRBKM2, AMN, SDV, COEVAR)
ARHO3YM=ARHO3YM+AMN*(FLOATINOSIM+FLOATINBKTOT)
71 FORMAT(’O’, 10X, ’AFTER REMOVING THE OUTSIDE LAYERS OF THE CONDUCTIVITY FIELD, WE ARE LEFT WITH A FIELD WITH THESE STATS’)
DO 153 I=NTRWP1, NBRWM1
JREV=J-NTRWP1+1
RHO1(JREV)=ARHO1(I, 1)
RHO2(JREV)=ARHO1(I, 2)
RHO3(JREV)=ARHO1(I, 3)
153 CONTINUE
DO 72 J=NTRWP1, NBRWM1
IREV=I-NTRWP1+1
72 CONTINUE
NORM2 = NROWS-2
CALL MUNSD(ARHO1, NRBKM2, AMN, SDV, COEVAR)
ARHO1YM=ARHO1YM+AMN*(FLOATINOSIM+FLOATINBKTOT)
CALL MUNSD(ARHO2, NRBKM2, AMN, SDV, COEVAR)
ARHO2YM=ARHO2YM+AMN*(FLOATINOSIM+FLOATINBKTOT)
CALL MUNSD(ARHO3, NRBKM2, AMN, SDV, COEVAR)
ARHO3YM=ARHO3YM+AMN*(FLOATINOSIM+FLOATINBKTOT)
75 CONTINUE
C NOW CALCULATE MEAN CORRELATION COEFFICIENTS AFTER DELETING OUTER NODES
150 FORMAT(’O’, 7X, ’AFTER REMOVING THE OUTSIDE LAYERS OF THE CONDUCTIVITY FIELD, WE ARE LEFT WITH A FIELD WITH THESE STATS’)
DO 153 I=NTRWP1, NBRWM1
IREV=I-NTRWP1+1
153 CONTINUE
72 CONTINUE
NORDM=2*NROWS-2
CALL MUNSD(ARHO1, NRBKM2, AMN, SDV, COEVAR)
ARHO1YM=ARHO1YM+AMN*(FLOATINOSIM+FLOATINBKTOT)
CALL MUNSD(ARHO2, NRBKM2, AMN, SDV, COEVAR)
ARHO2YM=ARHO2YM+AMN*(FLOATINOSIM+FLOATINBKTOT)
CALL MUNSD(ARHO3, NRBKM2, AMN, SDV, COEVAR)
ARHO3YM=ARHO3YM+AMN*(FLOATINOSIM+FLOATINBKTOT)
75 CONTINUE
C COMPUTE THIS SIMULATIONS STATS ON K
   DO 275 I=LAYLO,LAYHI
       IREV=I-LAYLO+1
   DO 275 J=2,NCOLM1
       JREV=J-1
   PARTK(IREV,JREV)=LOG(K(I,J))
   CALL MUNSD2 (PARTK,NOROWS,NCOLM2,AMN,SDV,COEVAR)
   HSTAT(NSIM,8)=AMN
   HSTAT(NSIM,9)=SDV
C CHECK SUBROUTINE MUNSD2 & AUGAR2 BY RECALCULATING INFO ON K
   DO 66 I=LAYLO,LAYHI
       IREV=I-LAYLO+1
   DO 66 J=2,NCOLM1
       JREV=J-1
   PARTK(I,JREV)=K(I,J)
   CALL MUNSD2 (PARTK,NOROWS,NCOLM2,AMN,SDV,COEVAR)
   NINK=NOROWS*NCOLM2
   DO 167 I=LAYLO,LAYHI
       DO 167 J=2,NCOLM1
   DISPER=K(I,J)-ARITHK)**2
   SUMDIF=SUMDIF+DISPER
   VARK=SUMDIF/(XLAYHI-XLAYLO+1.0*NCOLM2)
   STDEV=SGRT(VARK)
   COV=STDEV/ARITHK
   IF (I.LT.LAYHI) GO TO 57
   IF (J.LT.NCOLM2) GO TO 57
   56 FORMAT (/,'ARITHMATIC MEAN=',F10.4,'FT/D',1X,'=',1X,F10.6)
   57 CONTINUE
   GO TO 95
C NOW CALCULATE THE ACTUAL STANDARD DEVIATION AND COEF OF VARIATION
   DISPER=(K(I,J)-ARITHK)**2
   SUMDIF=SUMDIF+DISPER
   VARK=SUMDIF/(XLAYHI-XLAYLO+1.0)*NCOLM2
   STDEV=SGRT(VARK)
   COV=STDEV/ARITHK
C CONVERT CONDUCTIVITIES FROM FT/D TO CM/SEC
   CARITH=ARITHK* .0003528
   CHARM=HARMK* .0003528
   CGEOM=GEOMK* .0003528
   IF (I.LT.LAYHI) GO TO 57
   IF (J.LT.NCOLM2) GO TO 57
   56 FORMAT (/,'ARITHMATIC MEAN=',F10.4,'FT/D',1X,'=',1X,F10.6)
   57 CONTINUE
   GO TO 95
C CONDUCTIVITIES ARE READ IN AT EACH NODE
   READ(5,40)((K(I,J),J=1,NCOL),I=1,NROW)
   GO TO 95
C HYDRAULIC CONDUCTIVITY VALUES ARE ALL THE SAME
HYDRAULIC CONDUCTIVITY VALUES HAVE AN EXPONENTIAL DISTRIBUTION OVER THE ENTIRE REGION

CONMN=L>•MEAN OF THE EXPONENTIAL DISTRIBUTION

CONTINUE

DO 88 I=LAYLO,LAYHI

CONTINUE

THE HYDRAULIC CONDUCTIVITY VALUES ARE UNIFORMLY DISTRIBUTED WITH A DIFFERENT DISTRIBUTION WITHIN EACH OF THE LAYERS

CONTINUE

DO 93 J=2,NCOLM1

CONTINUE

100 5.14,5X, 'EXPECTED MEAN=' ,F10.4)

101 87 LAYLO=LAYLU(L)

85 FORMAT (’0’,/,5X, ’HYDRAULIC CONDUCTIVITIES FOLLOW AN EXPONENTIAL DISTRIBUTION IN ’,I4,2X, ’LAYER(S)’)

86 YFL = GGEXN (DSEED,MEAN)

93 CONTINUE

94 FORMAT (5110,6I5)

95 C SET VALUE OF K IN THE LEFT COLUMN EQUAL TO 0

96 FORMAT (5110,6I5)

97 DO 100 I=1,NROW

98 DO 100 J=1,NCOL

99 C SET VALUE OF K IN THE RIGHT COLUMN EQUAL TO 0

100 C SET VALUE OF K IN THE UPPER ROW EQUAL TO 0

101 C SET VALUE OF K IN THE LOWER ROW EQUAL TO 0

102 C
C CHECK IF A INTERIOR BARRIER IS PRESENT
IF(NCBAR.EQ.0) GO TO 113
DO 113 I=2,NRBARB
K(I,NCBAR)=0.0
113 CONTINUE
C
C COMPUTE KY(I,J) VALUES
IF A INTERIOR BARRIER IS PRESENT
C
COMPUTE KY(I,J) VALUES TO BE USED IN COMPUTING
KHYD(I,J) --THE CONNECTION VALUE IN THE Y-DIRECTION
DO 112 I=2,NROWM1
DO 112 J=2,NCOLM1
KY(I,J)=K(I,J)/ANISO(I)
IF(ELEC.NE.CHECK) GO TO 117
112 CONTINUE
C CONVERT HYDRAULIC CONDUCTIVITIES TO ELECTRICAL CONDUCTIVITIES IF SPECIFIED
DO 115 I=2,NROWM1
DO 115 J=2,NCOLM1
KY(I,J)=KY(I,J)*.0003528/5.13E-06**7
115 CONTINUE
THESE ARE THE NODAL VALUES TO BE USED IN COMPUTING
KHYD(I,J) --THE CONNECTION VALUE IN THE Y-DIRECTION
C COMPUTE THE ARITHMETIC, HARMONIC AND GEOMETRIC MEANS OF THE HYDRAULIC CONDUCTIVITY DISTRIBUTION
SUMK=0.0
RECIPK=0.0
PRODK=0.0
DO 119 I=2,NROWM1
DO 119 J=2,NCOLM1
SUMK=SUMK+K(I,J)
RECIPK=RECIPK+1/K(I,J)
PRODK=PRODK+ALOG10(K(I,J))
119 CONTINUE
XROWM2=FLOAT(NROWM2)
XCOLM2=FLOAT(NCOLM2)
ARITHK=SUMK/XROWM2/XCOLM2
HARMK=10**((XROWM2*XCOLM2)/RECIPK)
GEOMK=10**((XROWM2*XCOLM2)/RECIPK)
NOW CALCULATE THE ACTUAL STANDARD DEVIATION AND COEF OF VARIATION
SUMDIF=0.0
DISPER=(K(I,J)-ARITHK)**2
SUMDIF=SUMDIF+DISPER
121 CONTINUE
VARK=SUMDIF/(XROWM2*XCOLM2)
STDDEV=SQRT(VARK)
COV=STDDEV/ARITHK
AVGAMK=AVGAMK+ARITHK/(FLOAT(NSIM))
AVGSDK=AVGSDK+STDDEV/(FLOAT(NSIM))
HCSTAT(NSIM,1)=FLOAT(NSIM)
HCSTAT(NSIM,2)=ARITHK
HCSTAT(NSIM,3)=GEOMK
HCSTAT(NSIM,4)=HARMK
HCSTAT(NSIM,5)=STDDEV
HYDRAULIC CONDUCTIVITY VALUES ARE WRITTEN ONTO A DISK DATA SET
IF(CONK.NE.CHECK) GO TO 105
DO 105 I=2,NROWM1
DO 105 J=2,NCOLM1
WRITE(10,2110) K(I,J)
105 CONTINUE
TO BE USED WITH PLOTTING
IF(CONK.NE.CHECK) GO TO 105
DO 105 I=2,NROWM1
DO 105 J=2,NCOLM1
WRITE(10,2110) K(I,J)
105 CONTINUE
C
C IF(NSIM.GT.1) GO TO 262
WRITE(6,180)
180 FORMAT ('1',5X,'HORIZONTAL CONDUCTIVITY VALUES AT NODE CENTER')
DO 190 I=1,NROW
190 WRITE(6,200) I, (K(I,J), J=1, NCOL)
200 FORMAT (‘X ’, I3, 2X, 10F12.4/(6X, 10F12.4))
201 FORMAT (I3, 2X, 6F12.10/(5X, 6F12.10))
202 FORMAT (5X, 6F12.10)
203 FORMAT (‘X ’, I3, 2X, 10F12.9/(6X, 10F12.9))
204 FORMAT (8X, 6F12.7)
205 FORMAT (I3, 2X, 6F12.6/(5X, 6F12.6))
210 FORMAT (‘X ’, I3, 2X, 10F12.10/(5X, 10F12.10))

COMPUTE KHARM(I,J, 1) AND KHARM(I,J,2)
KHARM(I,J,1) = HARMONIC MEAN OF THE CONDUCTIVITIES AT ADJACENT NODES IN THE X DIRECTION
KHARM(I,J,2) = HARMONIC MEAN OF THE CONDUCTIVITIES AT ADJACENT NODES IN THE Y DIRECTION

WRITE VALUES OF KHARM
IF(CSIP. EG. CHECK(7)) GO TO 392
WRITE(6,290)
290 FORMAT (‘1’, //, 5X, ‘VALUES OF KHARM I,J’)
300 DO 300 I=2,NROWM1
300 FORMAT (I3, 2X, 10F12.4)
310 WRITE(6,310) I, (KHARM(I,J,1), J=1, NCOL)
310 FORMAT (I3, 2X, 10F12.4)
320 WRITE(6,320) I, (KHARM(I,J,2), J=1, NCOLM1)
320 FORMAT (I3, 2X, 10F12.4)

WRITE STARTING HEAD MATRIX
IF(CSKIP. EG. CHECK(7)) GO TO 392
WRITE(6,360)
360 FORMAT (‘1’, //, 5X, ‘STARTING HEAD MATRIX’)
370 DO 370 I=1,NROW
370 FORMAT (I3, 2X, 10F12.4)
380 WRITE(6,380) I, (HC(I,J), J=1, NCOL)
380 FORMAT (I3, 2X, 10F12.4)
390 WRITE(6,390) I, (IC(I,J), J=1, NCOL)
390 FORMAT (I3, 2X, 10F12.4)

HMIN=2.
XVAL=3. 1415**2/(2. * NCOL**2)
YVAL=3. 1415**2/(2. * NROW**2)
DO 395 J=2, NCOL
395 CONTINUE

IF(K(I,J) > 0.0) GO TO 395
XPART=XVAL*(1/(1+XD(J)**2/YPART**2))
YPART=YVAL*(1/(1+YPART**2/XPART**2))
HMIN=MIN(HMIN, XPART, YPART)

MIN=395 CONTINUE
AFLPHA=EXP(ALOG(HMAX/HMIN)/(NUMPAR-1))
ITPARM(1)=HMIN
DO 397 NTIME=2, NUMPAR
397 ITAPRM(NTIME)=ITPARM(NTIME-1)*ALPHA
IF(NSIM .NE. 1) GO TO 401
WRITE(6,398) NUMPAR, (ITPARM(J), J=1,NUMPAR)
398 FORMAT ('0',3X,15.2X, 'ITERATION PARAMETERS: ',6D12.3, //, 6X,10D12.3)
IF(MINI.EQ.CHECK(4)) WRITE(6,399)
399 FORMAT ('0',2X, 'NOTE--MINIMUM ITERATION PARAMETER WAS SET')
400 CONTINUE
SOLUTION ALGORITHM USING THE ITERATIVE ALTERNATING DIRECTION IMPLICIT PROC.
DO 500 I=1,NROW
DO 500 J=1,NCOL
500 HOLD(I,J)=H(I,J)
DO 510 L=2,NCOLM1
510 HNEW(L)=H(I,L)
IF (MOD(ICTR,NUMPAR)) 520, 520, 530
520 NTH=0
530 NTH=NTH+1
ITPARM=ITPARM(NTH)
ICTR=ICTR+1
ERR(ICTR)=0.0
ROW CALCULATIONS
DO 700 KK=2,NROW
I=KK
DO 620 J=2,NCOLM1
605 A=KHARM(I,J,1)*YD(I)/AX(J)
610 B=(KHARM(I,J+1,1)*YD(I))/AX(J+1)
615 C=(KHARM(I,J,2)*XD(J))/AY(I)
620 D=(KHARM(I+1,J,2)*XD(J))/AY(I+1)
625 GPARM=(A+B+C+D)*ITPARM
630 E=A+B+GPARM
635 GKNOWN=C*H(I-1,J)+D*H(I+1,J)-(C+D-GPARM)*H(I,J)
640 IF(J.EQ.2) GO TO 615
645 IF(IC(I,J-1).EQ.-1) GO TO 610
700 G(J)=(A*G(J-1)+GKNOWN)/(E-A*F(J-1))
650 F(J)=B/E
660 GO TO 620
665 G(J)+=(A*H(I,J-1)+GKNOWN)/E
700 F(J)=B/E
GO TO 620
COLUMN CALCULATIONS
DO 703 L=2,NROWM1
703 HNEW(L)=H(I,L)
DO 800 KK=2, NCOL
J=KK
DO 720 I=2, NROWM1
IF(K(I,J)) 705, 720, 705

A=(KHARM(I, J, 1)*YD(I))/AX(J)
B=(KHARM(I, J+1, 1)*YD(I))/AX(J+1)
C=(KHARM(I, J, 2)*XD(J))/AY(I)
D=(KHARM(I+1, J, 2)*XD(J))/AY(I+1)
QPARM=(A+B+C+D)*PARM
E=(C+D+QPARM)

705 GKNOWN=A*H(J, J-1)+B*H(J, J+1)-(A+B-QPARM)*H(I, J)
770 IF(I.EQ.2) GO TO 715
771 IF(C(1,J).EQ.-1) GO TO 710
772 G(I)=(C*G(I-1)+QKNOWN)/(E-C*F(I-1))
773 F(I)=D/(E-C*F(I-1))
774 GO TO 720
775 G(I)=(C*H(I-1, J)+QKNOWN)/E
776 F(I)=D/E
777 GO TO 720
778 G(I)=C*G(I-1)+GKNOWN/E
779 F(I)=D/E
780 720 CONTINUE
7910 C CALCULATE HEADS BY BACK SUBSTITUTION
7920 N=NROWM1
7930 H(N, J-1)=HNEW(N)
7940 IF(C(N, J).EQ.-1) GO TO 740
7950 HNEW(N)=G(N)
7960 GO TO 755
7970 HNEW(N)=H(N, J)
7980 GO TO 755
7990 HNEW(N)=G(N)+F(N)*HNEW(N+1)
8000 755 N=N-1
8010 IF(N.EQ.1) GO TO 757
8020 H(N, J-1)=HNEW(N)
8030 IF(C(N, J).NE.-1) GO TO 750
8040 GO TO 740
8050 757 IF(J.EQ. NCOL) GO TO 800
8060 DO 770 I=2, NROWM1
8070 ET=DABS(HNEW(I)-HOLD(I, J))
8080 IF(ET.GT.ERR(ICTR)) GO TO 760
8090 GO TO 770
8100 760 ICTR=ET
8110 I=I
8120 J=J
8130 770 CONTINUE
8140 800 CONTINUE
8150 C CHECK CLOSURE CRITERIA FOR STEADY STATE
8160 1000 IF(CTR.GE. ITMAX) GO TO 1045
8170 IF(ERR(ICTR).GT.EC) GO TO 400
8180 C OTHERWISE THE STEADY STATE HEADS HAVE BEEN COMPUTED
8190 C COMPUTE HEADS AROUND THE PERIMETER OF THE MODEL
8200 C THIS IS DONE TO GIVE A BETTER PLOT EFFECT
8210 C ALONG TOP ROW
8220 DO 950 J=1, NCOL
8230 950 H(I, J)=H(2, J)
8240 960 H(I, J)=H(1, J)
8250 970 H(I, 1)=H(I, 2)
8260 980 CONTINUE
8270 C ALONG BOTTOM ROW
8280 DO 960 J=1, NCOL
8290 960 H(NROW, J)=H(NROWM1, J)
8300 970 H(NROW, J)=H(NROW, J)
8310 980 CONTINUE
8320 C ALONG LEFT VERTICAL BOUNDARY
8330 DO 970 I=1, NROW
8340 970 H(I, 1)=H(I, 2)
ALONG RIGHT VERTICAL BOUNDARY

DO 980 I=1,NROW

HDSMN(I,NCOLM1)=H(I,NCOLM1)

C STORE THIS SIMULATION'S HEAD VALUES IN THE CUMULATIVE ARRAY,

HDSMN(I,J)=HDSMN(I,J)+H(I,J)/(FLOAT<NOSIM>)

CONTINUE

C STORE THE HEAD VALUES ALONG TWO SELECTED ROWS

IF<NHDSUP . NE . 0> GO TO 983

NHDSUP=NROW/3

NHDSDN2*NHDSUP

CONTINUE

DO 984 J=2,NCOL-1

JREV=J-1

HDSUP<NSIM,JREV>=H(NHDSUP,J)

HDSDNCNSIM,JREV>=H(NHDSDN,J)

IF<NOSIM . NE . 0) GO TO 1041

WRITEC6,1005) CERR<,I>.I=l,ICTR)

1005 FORMATC5X , 'HEAD DIFFERENCE FOR EACH ITERATION' , //, $(/, 3X, 10F12.5)>

1006 WRITEC6,1020> ICTR.ERRICICTR>.IET,JET

1020 FORMATC '1', //, 1ox. , 'STEADY STATE HEAD MATRIX AFTER', I4.2X, 'ITERATION' , //, $(/, 13X, 'LARGEST HEAD DIFFERENCE =', E12.3, 2X, 'AT POINT', 2X, 'ROW $ ', 13, 2X, 'COLUMN' ,I3)

1022 IF CNSIM . NE. 1 GO TO 1041

DO 1040

1040 WRITEC6,200) I, CHCI,Jl,J=l,NCOL>

GO TO 1100

1045 WRITEC6,1055)

WRITEC6, 1005 l CERR (I>.

1055 FORMATC '0', 4X, '***** HEADS WRITTEN ONTO DSN *****')

1070 WRITEC6,200l I, CH(I,J),J=l,NCOL>

GO TO 3000

C OTHERWISE CONVERT CONDUCTIVITIES FROM FT/D TO CM/SEC

CARITH=ARITHK* .0003528

CHARM=HARMK* .0003528

CGEOM=GEOMK* .0003528

C
274

8900 1110 FORMAT ('1',5X,'STATISTICAL MEANS OF THE HYDRAULIC CONDUCTIVITY',
8910 1'DISTRIBUTION',//,8X,'ARITHMETIC MEAN=',F10.4,1X,'FT/D',1X,
8920 2=',1X,F10.6,1X,'CM/SEC',//,8X,'GEOMETRIC MEAN=',F10.4,1X,'FT/D',
8930 3IX=',1X,F10.6,1X,'CM/SEC',//,8X,'HARMONIC MEAN=',F10.4,1X,
8940 4='FT/D',1X=',1X,F10.6,1X,'CM/SEC')
8950 1126 FORMAT (5X,'STATISTICAL MEANS OF THE HYDRAULIC CONDUCTIVITY',
8960 1'DISTRIBUTION',//,8X,'ARITHMETIC MEAN=',F10.4,1X,'FT/D',1X,
8970 2=',1X,F10.6,1X,'CM/SEC',//,8X,'GEOMETRIC MEAN=',F10.4,1X,'FT/D',
8980 3IX=',1X,F10.6,1X,'CM/SEC',//,8X,'HARMONIC MEAN=',F10.4,1X,
8990 4='FT/D',1X=',1X,F10.6,1X,'CM/SEC')
9000 1124 CONTINUE
9010 1111 FORMAT (//,5X,'ACTUAL STANDARD DEVIATION OF HYDRAULIC CONDUCTIVITY',
9020 "$DISTRIBUTION IS=',F10.4,1X,'AND THE COEFFICIENT OF VARIATION I',F10.4,)
9030 1$5,'F10.4)
9040 C
9050 C CHECK THE DOUBLE SUBSCRIPTED ARRAY SUBROUTINE
9060 GO TO 1140
9070 C
9080 C CONVERT CONDUCTIVITIES TO RESISTIVITIES
9090 1120 ARITHK=1./HARMK
9100 GEOMK=1./GEOMK
9110 HARMK=1./ARITHK
9120, WRITE(6,1130) ARITHK,GEOMK,HARMK
9130 1130 FORMAT ('1',5X,'STATISTICAL MEANS OF THE RESISTIVITY',
9140 1'DISTRIBUTION',//,8X,'ARITHMETIC MEAN=',F10.4,1X,'OHM-METERS',
9150 2IX=',8X,'GEOMETRIC MEAN=',F10.4,1X,'OHM-METERS',//,8X,
9160 3IX='HARMONIC MEAN=',F10.4,1X,'OHM-METERS')
9170 C
9180 1140 IF(FLOW .EQ .CHECK<6) GO TO 1300
9190 IF(WARP .EQ .CHECK<9) OR .FLOW.EQ .CHECK<10) GO TO 1293
9200 C
9210 C
9220 C
9230 C OTHERWISE THE PREDOMINANT FLOW MUST BE HORIZONTAL
9240 C COMPUTE THE EQUIVALENT HORIZONTAL HYDRAULIC CONDUCTIVITY
9250 C
9260 C
9270 G=0.0
9280 AREA=0.0
9290 C AREA= TOTAL CROSS SECTIONAL AREA THAT THE FLOW PASSES THROUGH
9300 C
9310 DO 1200 1=2,NROWM1
9320 AREA=AREA+YD<1>
9330 G=G+<KHARM<1.LEQUIV, 1*<H<1,LEQUIV-11-H<1, LEQUIVJJ/AX<LEQUIVJJ
1200 CONTINUE
9340 C LENGTH=MACROSCOPIC LENGTH OVER WHICH THE TOTAL HEAD DIFFERENCE
9350 C <DHEADJ IS DISSIPATED
9360 C LENGTH=MACROSCOPIC LENGTH OVER WHICH THE TOTAL HEAD DIFFERENCE
9370 C <DHEADJ IS DISSIPATED
9380 C
9390 LENGTH=0.0
9400 DO 1250 J=3,NCOLM1
9410 LENGTH=LENGTH+AX(J)
9420 1250 CONTINUE
9430 C
9440 C KHEGF=DISSIMILAR HORIZONTAL HYDR. COND. IN UNITS OF FT./DAY
9450 KHEGF=(G#LENGTH)/(DHEAD#AREA)
9460 HCSTAT<NSIM.61=KHEGF
9470 C KHEGCS=DISSIMILAR HORIZONTAL HYDRAULIC CONDUCTIVITY IN UNITS OF CM./SEC.
9480 KHEGCS=KHEGF*.0003528
9490 IF(ELEC .EQ .CHECK<3)) GO TO 1290
9500 C
9510 C OTHERWISE WE HAVE THE HYDRAULIC CASE
9520 1200 FORMAT (0',//,5X,'MACROSCOPIC PARAMETERS',//,8X,'EQUIVALENT ',
9530 1'HORIZONTAL HYDR. CONDUCTIVITY=',F10.4,1X,'FT/D',1X,'=',F10.6,1X,
9540 2=',1X,F10.6,1X,'CM/SEC',//,8X,'TOTAL=',F10.4,1X,'FT/D',
9550 3IX=',1X,F10.6,1X,'CM/SEC',//,8X,'AREA=',F10.4,1X,'SQ. FT.',//,8X,
9560 4='TOTAL DISSIPATED HEAD=',F10.4,1X,'FT.')
C THE EQUIVALENT ELECTRICAL HORIZONTAL CONDUCTIVITY WAS CONVERTED TO
C AN EQUIVALENT HORIZONTAL ELECTRICAL RESISTIVITY
C CONVERT CURRENT FLOW TO AMPERES
Q = 0.328
WRITE(6, 1292) KHEQFD, Q, LENGTH, AREA, DHEAD
1292 FORMAT ('O', 5X, 'MACROSCOPIC PARAMETERS', //, 5X, 'EQUIVALENT', HORIZONTAL ELECTRICAL RESISTIVITY=', F10.4, 1X, 'OHM-METERS', //, 5X, TOTAL CURRENT FLOW=', F10.6, 1X, 'AMPERES', //, 5X, 'LENGTH=', F10.3, 1X, '3FT.', //, 5X, 'AREA=', F10.3, 'SQ. FT.', //, 5X, 'TOTAL VOLTAGE DROP=', F10.4, 1X, 'VOLTS')
GO TO 1400
C COMPUTE THE AQUIFER HYDRAULIC CONDUCTIVITY FOR POINT TO POINT FLOW USING
C THE METHOD SHOWN BY WARREN AND PRICE
FKI=0.0
DO 1294 I=2, NROWM1
AREA=AREA+XD(I)
Q=Q+KHARM<LEQUIV,J,2+<CH<LEQUIV-1,J+H<LEQUIV,Jll/AY<LEQUIVll
1294 CONTINUE
C COMPUTE THE EQUIVALENT VERTICAL HYDRAULIC CONDUCTIVITY
KVEQFD= EQUIVALENT VERTICAL HYDR. CONDUCTIVITY IN UNITS OF FT./DAY
KVEQFD= Q*LENGTH/(DHEAD*AREA)
KVEQCS= EQUIVALENT VERTICAL HYDR. CONDUCTIVITY IN UNITS OF CM./SEC.
KVEQCS=KVEQFD* .000352e
IF(CELEC.EQ.CHECK(3)) GO TO 1390
WRITE(6, 1390) KVEQFD, KVEQCS, Q, LENGTH, AREA, DHEAD
1390 FORMAT ('O', 5X, 'MACROSCOPIC PARAMETERS', //, 5X, 'EQUIVALENT VERTICAL HYDR. CONDUCTIVITY=', F10.4, 1X, 'FT/D', //, 5X, 'TOTAL FLOW = ', F10.4, 1X, 'VOLTS', //, 5X, 'LENGTH = ', F10.4, 1X, 'SQ. FT.', //, 5X, 'TOTAL DISSIPATED HEAD = ', F10.4, 1X, 'FT')
GO TO 1400
C HERE THE PREDOMINANT FLOW IS VERTICAL
C COMPUTE THE EQUIVALENT VERTICAL HYDRAULIC CONDUCTIVITY
C (DHEAD) IS DISSIPATED
DO 1370 I=3, NROWM1
LENGTH=LENGTH+AYC(I)
1370 CONTINUE
C LENGTH= MACROSCOPIC LENGTH OVER WHICH THE TOTAL HEAD DIFFERENCE
C COMPUTE LENGTH
DO 1390 I=3, NROWM1
LENGTH=LENGTH+AYC(I)
1390 CONTINUE
C KVEQFD= EQUIVALENT VERTICAL HYDR. CONDUCTIVITY IN UNITS OF FT./DAY
KVEQFD= Q*LENGTH/(DHEAD*AREA)
KVEQCS= EQUIVALENT VERTICAL HYDR. CONDUCTIVITY IN UNITS OF CM./SEC.
THE EQUIVALENT VERTICAL ELECTRICAL CONDUCTIVITY IS CONVERTED TO
c
THE EQUIVALENT VERTICAL ELECTRICAL RESISTIVITY

1/KVEQFD = 1/KVEQFD

CONVERT CURRENT FLOW TO AMPERES

Q = Q/3.2e1

WRITE(6,1392) KVEQFD,G.LENGTH,AREA,DHEAD

FORMAT<

MACROSCOPIC PARAMETERS',/,'EQUIVALENT'.

EQUIVALENT VERTICAL ELECTRICAL RESISTIVITY',/,'TOTAL CURRENT FLOW=',/,'LENGTH='.

AQUIFER HYDRAULIC CONDUCTIVITY FOR VERT. FLOW USING

FKI=0.0

DO J=2.NCOLM1

FKI=FKI+KHARM(LEQUIV,J,2)*(H(LEQUIV-1,J)-H(LEQUIV,J))

CONTINUE

KVEQFD=FKI/WPFACT

WRITE(6,1398)

IF(ELEC.EQ.CHECK(3)) GO TO 1396

WRITE(6,1395) FKI,KVEQFD

GO TO 1400

KVEQFD=1./KVEQFD

WRITE(6,1397) FKI,KVEQFD

1' AQUIFER RESISTIVITY=',/,'TOTAL VOLTAGE DROP=',/,

MACROSCOPIC TRANSPORT PROPERTIES',/,'WERE

COMPUTED BY THE WARREN & PRICE TECHNIQUE'

1400 CONTINUE

IF(ISO.EQ.1) GO TO 1450

Determine 1D AUTOCORRELATION COEFFICIENTS OF HYDRAULIC CONDUCTIVITY

CALL MUNSD(CVALK,NCOLM2,AMN,SDV,COEVAR)

CALL AUGHAR(CVALK,NCOLM2,AMN,SDV,LAGS,RHO)

AMEAN(I)=AMN

ASDV(I)=SDV

CALL MUNSD(CVALY,NCOLM2,AMN,SDV,COEVAR)

CALL AUGHAR(CVALY,NCOLM2,AMN,SDV,LAGS,RHOA)

AMEANA(I)=AMN

ASDVA(I)=SDV

DO 1281 IM=1.LAGS

RHO1(IM)=RHO(1)

RHOA1(IM)=RHOA(1)

1281 CONTINUE

DO 1289 I=LAYLO,LAYHI

IREV=I-LAYLO+1

RHO1(IREV)=RHO(1,1)

RHO2(IREV)=RHO(1,2)

RHO3(IREV)=RHO(1,3)

RHO4(IREV)=RHO(1,4)
RH05(IREV) = ARHO(I, 5)

CONTINUE

CALL MUNSD (RH01, NOROWS, AMN, SDV, COEVAR)

CSTATS(NSIM, 9) = AMN

CCSTAT(NSIM, 1) = AMN

R01MKR = R01MKR + AMN / FLOAT(NSIM)

CALL MUNSD (RH02, NOROWS, AMN, SDV, COEVAR)

CSTATS(NSIM, 10) = AMN

CCSTAT(NSIM, 2) = AMN

CALL MUNSD (RH03, NOROWS, AMN, SDV, COEVAR)

CSTATS(NSIM, 11) = AMN

CCSTAT(NSIM, 3) = AMN

CALL MUNSD (RH04, NOROWS, AMN, SDV, COEVAR)

CSTATS(NSIM, 4) = AMN

CALL MUNSD (RH05, NOROWS, AMN, SDV, COEVAR)

CSTATS(NSIM, 5) = AMN

COMPUTE THE MEAN AUTOCORRELATION COEFFICIENTS FOR LOG OF K BY ROWS

DO 1286 I = LAYLO, LAYHI

IREV = I - LAYLO + 1

RH01(IREV) = ARHOA(I, 1)

RH02(IREV) = ARHOA(I, 2)

RH03(IREV) = ARHOA(I, 3)

RH04(IREV) = ARHOA(I, 4)

RH05(IREV) = ARHOA(I, 5)

CONTINUE

CALL MUNSD (RH01, NOROWS, AMN, SDV, COEVAR)

CSTATS(NSIM, 5) = AMN

R01MKR = R01MKR + AMN / FLOAT(NSIM)

CALL MUNSD (RH02, NOROWS, AMN, SDV, COEVAR)

CSTATS(NSIM, 6) = AMN

CALL MUNSD (RH03, NOROWS, AMN, SDV, COEVAR)

CSTATS(NSIM, 7) = AMN

DETERMINE 1D AUTOCORRELATION COEFFICIENTS OF HYDRAULIC CONDUCTIVITY

BY COLUMNS

DO 1283 J = 2, NCOLM1

M = M + 1

DO 1284 I = 2, NROWM1

VALK(M) = K(I, J)

CONTINUE

CALL MUNSD (VALK, NROWM2, AMN, SDV, COEVAR)

CSTATS(NSIM, 6) = AMN

AMEANCJ = AMN

ASDVCJ = SDV

DO 1283 IM = 1, LAGS

ARHOCJ, IM = ARHO(IM)

CONTINUE

DO 1284 J = 2, NCOLM1

JREV = J - 1

RH01(JREV) = ARHO(J, 1)

RH02(JREV) = ARHO(J, 2)

RH03(JREV) = ARHO(J, 3)

RH04(JREV) = ARHO(J, 4)

RH05(JREV) = ARHO(J, 5)

CONTINUE

DO 1291 J = 2, NCOLM1

JREV = J - 1

CALL MUNSD (RH01, NCOLM2, AMN, SDV, COEVAR)

R01MKC = R01MKC + AMN / FLOAT(NSIM)

CSTATS(NSIM, 12) = AMN

CSTATS(NSIM, 6) = AMN

CALL MUNSD (RH02, NCOLM2, AMN, SDV, COEVAR)

CSTATS(NSIM, 13) = AMN

CSTATS(NSIM, 7) = AMN

CALL MUNSD (RH03, NCOLM2, AMN, SDV, COEVAR)

CSTATS(NSIM, 14) = AMN

CSTATS(NSIM, 8) = AMN
CALL MUNSD (RHO4, NOROWS, AMN, SDV, COEVAR)
CCSTAT (NSIM, 9) = AMN
CALL MUNSD (RHO5, NOROWS, AMN, SDV, COEVAR)
CCSTAT (NSIM, 10) = AMN
CONTINUE

IF (STRF .NE. CHECK (5)) GO TO 3000
OTHERWISE COMPUTE THE STREAM FUNCTION FROM THE
STEADY STATE HEADS
BRANCH TO THE APPROPRIATE LOCATION TO COMPUTE THE STREAM FUNCTION
DEPENDING ON THE FLOW TYPE (HORIZONTAL, VERTICAL OR POINT TO POINT).

IF (FLOW .NE. CHECK (6)) GO TO 2500
IF (FLOW .NE. CHECK (10)) GO TO 2560
OTHERWISE THE FLOW IS PREDOMINATELY HORIZONTAL
SET BOTTOM ROW STREAM FUNCTION VALUES TO ZERO
DO 1500 J = 1, NCOLM1
STRFUN (NROWM1, J) = 0.0
1500 CONTINUE

DO 1800 J = 2, NCOLM2
DO 1800 I = 2, NROWM1
II = NROW - I
STRFUN (I, J) = STRFUN (I + 1, J) + (KHARM (I + 1, J + 1) * (H (I + 1, J) -
H (I + 1, J + 1)) / (AX (J + 1) * YD (I + 1))
1800 CONTINUE

DO 1900 I = 1, NROWM1
DO 1900 J = 1, NCOLM1
STRNOR = STRFUN (I, NROW)
STRFUN (I, J) = STRFUN (I, J) / STRNOR * 100.0
1900 CONTINUE

IF (NSIM .NE. 1) GO TO 3000
A WRITE STATEMENT SHOULD BE PUT HERE IF STRFUN IS DESIRED
WRITE STREAM FUNCTION VALUES ONTO DSN
DO 2200 I = 1, NROWM1
DO 2200 J = 1, NCOLM1
WRITE (6, 2300) STRFUN (I, J)
2200 FORMAT (30X, F10.5)
WRITE (6, 2300) STRFUN (I, J)
2300 FORMAT ('0', '*** STREAM FUNCTION VALUES WRITTEN ONTO DSN ***')

EXECUTION OF THIS PROGRAM TERMINATES.
GO TO 3000

COMPUTE STREAM FUNCTION FOR VERTICAL FLOW

SET RIGHT SIDE STREAM FUNCTION VALUES TO ZERO

2500 DO 2510 I=1,NROWM1

2510 STRFUN(I, NCOLM1) = 0.0

COMPUTE INTERIOR VALUES OF THE STREAM FUNCTION MOVING ALONG SUCCESSIVE ROWS FROM THE RIGHT SIDE STREAM LINE WHERE THE STREAM FUNCTION IS EQUAL TO ZERO

DO 2520 I=2,NROWM2

DO 2520 J=2,NCOLM1

JJ = NCOL-J

STRFUN(I, JJ) = STRFUN(I, JJ+1) + (KHARM(I+1, JJ+1, 2)*((H(I, JJ+1) - 1H(I+1, JJ+1))/AY(I+1))*XD(JJ+1))

CONTINUE

SET THE VALUES OF STRFUN(I, J) PRODUCE A BETTER PLOT EFFECT

DO 2530 I=1,NROWM1

DO 2530 J=1,NCOLM1

STRFUN(I, J) = STRFUN(I, J) / STRNOR(I)*100.

WRITE THE VALUES OF THE NONDIMENSIONALIZED STREAM FUNCTION

IF(NSIM.NE.1) GO TO 3000

WRITE(6,2100) I,STRFUN(I,1),J,(STRFUN(I, J), J=1,NCOLM1)

WRITE STREAM FUNCTION VALUES ONTO DATA SET

DO 2550 I=1,NROWM1

DO 2550 J=1,NCOLM1

WRITE(13,2110) STRFUN(I, J)

CONTINUE

GO TO 3000

COMPUTE STREAM FUNCTION FOR POINT TO POINT FLOW

SET RIGHT SIDE STREAM FUNCTION VALUES TO ZERO

2560 DO 2570 I=2,NROWM2

2570 STRFUN(I, 1) = 0.0

2580 STRFUN(I, NCOLM1) = 0.0

COMPUTE INTERIOR VALUES OF THE STREAM FUNCTION MOVING ALONG SUCCESSIVE ROWS FROM THE RIGHT SIDE STREAM LINE
WHERE THE STREAM FUNCTION IS EQUAL TO ZERO

C COMPUTE TOTAL INFLOW AND OUTFLOW AT THE
C CONSTANT HEAD NODES IN ROW 2

GIN=0.0
GOUT=0.0

DO 2606 J=2,NCOLM1
IF(C(2,J) .GE .0) GO TO 2606

C OTHERWISE COMPUTE FLOW THROUGH THE LEFT(GL), RIGHT(GR)
C AND BOTTOM(GB) FACES OF THE CONSTANT HEAD NODE
GL=KHARM(2,J,1)*(H(2,J)-H(2,J-1))/AX(J)*YD(2)
GR=KHARM(2,J+1,1)*(H(2,J+1)-H(2,J))/AX(J+1)*YD(2)
GB=KHARM(3,J,2)*(H(2,J)-H(3,J))/AY(3)*XD(J)
GNODE=GL+GR+GB
IF(GNODE .LT .0.0) GO TO 2604

C OTHERWISE INFLOW OCCURS AT THE NODE
GIN=GIN+GNODE

GO TO 2606

C OUTFLOW OCCURS AT THE NODE
2604 GOUT=GOUT+GNODE

C MAKE THE BOTTOM ROW OF THE STREAM FUNCTION= 0.0
C AS BASED ON THE TOTAL INFLOW
LSTRM=LSTRM-1
DO 2608 J=1,LSTRM1
J1=LSTRM
J2=NCOLM1
DO 2609 STRFUN(J,1)=0.0

C NONDIMENSIONALIZE THE STREAM FUNCTION
C AS BASED ON THE TOTAL INFLOW
DO 2620 I=1,NROWM1
DO 2620 J=1,NCOLM1
STRFUN(I,J)=CSTRFUN(I,J)/GIN)*100.

WRITE(6,2100)
WRITE(6,2640) I,J,STRFUN(I,J)
WRITE(6,1200) I,GIN,GOUT
2600 CONTINUE
13560 IF(NSIM NE.1) GO TO 3000
13570 DO 2660 I=1,NROWM1
13580 DO 2660 J=1,NCOLM1
13590 2660 WRITE(13,2670) STRFUN(I,J)
13600 2670 FORMAT (30X,F10.4)
13610 WRITE(6,2300)
13620 C 3000 CONTINUE
13630 C CALCULATE THE TRAVEL TIME FROM THE LEFT SIDE TO THE RIGHT
13640 C INITIALIZE ALL VELOCITY VALUES=0
13650 DO 213 I=1,NROW
13660 DO 213 J=1,NCOL
13670 VX(I,J)=0.0
13680 VY(I,J)=0.0
13690 C CALCULATE THE VELOCITY IN EACH INTERIOR BLOCK
13700 DO 191 I=3,NROWM2
13710 DO 191 J=3,NCOLM2
13720 POROCT=1.0
13730 VX(I,J)=-0.5*((KHARM(I,J+1,1)*(H(I,J+1)-H(I,J))/AX(J))+(KHARM(I,J+1,1)+1)*H(I,J+1)-H(I,J))/AX(J))/POROCT
13740 VY(I,J)=-0.5*((KHARM(I,J,2)*(H(I-1,J)+H(I,J))/AY(I))+(KHARM(I+1,J,2)+1)*H(I-1,J)-H(I,J))/AY(I))/POROCT
13750 C COMPUTE VELOCITY IN THE UPPER BOUNDARY BLOCK
13760 DO 193 J=3,NCOLM2
13770 VY(2,J)=-CKHARM(3,J,2)*(H(2,J)+H(3,J))/AY(2))/POROCT
13780 VX(2,J)=-0.5*((KHARM(2,J+1,1)*(H(2,J+1)-H(2,J))/AX(J))+(KHARM(2,J+1,1)+1)*H(2,J+1)-H(2,J))/AX(J))/POROCT
13790 C COMPUTE VELOCITY IN THE LOWER BOUNDARY BLOCK
13800 J=NROWM1
13810 VX(I,J)=-0.5*((KHARM(I,J+1,1)*(H(I,J+1)-H(I,J))/AX(J))+(KHARM(I,J+1,1)+1)*H(I,J+1)-H(I,J))/AX(J))/POROCT
13820 VY(NROWM1,J)=-CKHARM(NROWM1,J,2)*(H(NROWM2,J)-H(NROWM1,J))/AY(NROWM1))/POROCT
13830 VX(NROWM1,J)=-0.5*((KHARM(NROWM1,J,1)*(H(NROWM2,J)-H(NROWM1,J))/AX(NROWM1))/POROCT
13840 C REVISE VERTICAL VELOCITIES IN THE FOUR CORNERS OF FLOW REGION
13850 VX(2,2)=-CKHARM(3,2,2)*(H(2,2)-H(3,2))/AY(2))/POROCT
13860 VX(2,NCOLM1)=-CKHARM(3,NCOLM1,2)*(H(2,NCOLM1)-H(3,NCOLM1))/AY(2))/POROCT
13870 VX(NROWM1,2)=-CKHARM(NROWM1,2,2)*(H(NROWM2,2)-H(NROWM1,2))/AY(NROWM1))/POROCT
13880 VX(NROWM1,J)=-CKHARM(NROWM1,J,2)*(H(NROWM2,J)-H(NROWM1,J))/AY(NROWM1))/POROCT
13890 J=NCOLM1
13900 VX(I,J)=0.5*((KHARM(I,J,1)*(H(I-1,J)-H(I,J))/AY(I))+(KHARM(I+1,J,1)+1)*H(I-1,J)-H(I,J))/AY(I))/POROCT
13910 C REVISE RESIDUAL VELOCITIES IN THE LEFT BOUNDARY BLOCKS
13920 VX(2,2)=-CKHARM(3,2,2)*(H(2,2)-H(3,2))/AY(2))/POROCT
13930 VX(2,J)=-0.5*((KHARM(2,J+1,1)*(H(2,J+1)-H(2,J))/AX(J))+(KHARM(2,J+1,1)+1)*H(2,J+1)-H(2,J))/AX(J))/POROCT
13940 VX(NROWM1,2)=-CKHARM(NROWM1,2,2)*(H(NROWM2,2)-H(NROWM1,2))/AY(NROWM1))/POROCT
13950 VX(NROWM1,J)=-CKHARM(NROWM1,J,2)*(H(NROWM2,J)-H(NROWM1,J))/AY(NROWM1))/POROCT
13960 VX(2,2)=VY(1,2)
13970 IF(VEXAMP.EQ.0.0) VX(2,2)=VY(I,3)
13980 VX(I,J)=VX(2,2)
13990 IF(NSIM.NE.1) GO TO 182
14000 C SET CUMULATIVE MEAN VALUES EQUAL TO 0.0
14010 AVGXH=0.0
14020 AVGYH=0.0
14030 AVGTTT=0.0
14040 WRITE(6,140) NROW,NCOL,DHEAD,LENGTH,AREA,EC,ITMAX
READ IN THE VARIABLE INPUT DATA

C USE STFLOC=0.0 FOR FLOW FROM ENTIRE LEFT SIDE, 1.0 FOR ONLY PART
OF THE LEFT SIDE, OR 2.0 FOR FLOW FROM UPPER BOUNDARY.

READ(5,34) NWAVES,NROWT,NROWB,NRCUTO,DELT,D50,DSPRAT,STFLOC

NPTOT=NWAVES*(NROWB-NROWT+1)*(FLOAT(NOSIM))

NPSIM=NWAVES*(NROWB-NROWT+1)

STXLOC=XD(J)*1.0

ENXLOC=FLOAT(NCOLM1)*XD(J)

TDIST=ENXLOC-STXLOC

HALFWY=STXLOC+0.5*(ENXLOC-STXLOC)

REG60P=STXLOC+0.6*(ENXLOC-STXLOC)

REG70P=STXLOC+0.7*(ENXLOC-STXLOC)

REG80P=STXLOC+0.8*(ENXLOC-STXLOC)

REG90P=STXLOC+0.9*(ENXLOC-STXLOC)

ESTTTT=TDIST*LENGTH*POROCT/(CONMN*N*DHEAD)

THT=ESTTTT/2.0

NESHT=INTCTHT/DELT

THT=DELT*FLOAT(NESHT)

MP IS A COUNTER OF THE PARTICLES TRAVERSING THE REGION

CONTINUE

SET HORIZ. VELOCITIES IN UPPER ROW EQUAL TO NEIGHBOR IF CUTOFF PROBLEM

HDCHK1=H(2,2)

HDCHK2=H(2,3)

IF(HDCHK1._NE.HDCHK2) GO TO 197

DO 196 J=1,NCFL0

196 VX(2,J)=VX(3,J)

197 CONTINUE

HDCHK1=H(2,2)

HDCHK2=H(2,3)

IF CHDCHK1 .NE .HDCHK2) GO TO 197

DO 186 J=1,NCFL0

WRITE(6,184)

184 FORMAT(2,5X,'THE VELOCITY MATRIX IN THE X DIRECTION IS TABULATED BELOW, WHERE J=', //, '1','12X','2','12X','3','12X','4','12X','5','/)

DO 188 I=1,NROW

WRITE(6,200) I,

188 FORMAT(2,5X,'THE VELOCITY MATRIX IN THE Y DIRECTION IS TABULATED BELOW, WHERE J=', //, '1','12X','2','12X','3','12X','4','12X','5','/)

DO 161 I=1,NROW

161 CONTINUE

176 CONTINUE

177 CONTINUE

1640 SIMTIM=0.0

1650 DO 45 NT=1,NWAVES

45 Y=Y+DTSX=0.0

460 MP=MP+1

4690 NWAV(MP)=NT

4700 SKIPS=0.0

4710 NTIM=0

4720 TTHW(MP)=0.0

4730 TT60(MP)=0.0

4740 TT70(MP)=0.0

4750 TT80(MP)=0.0

4760 TT90(MP)=0.0

4770 NTREB(MP)=0

4780 IF(STFLOC.EQ.2.0) GO TO 41

4790 I=Y

4800 YLOC=FLOAT(I)*YD(I)+(YD(I)/2.0)

4810 STY(MP)=YLOC

4820 J=1

4830 XLOC=FLOAT(J)*XD(J)

4840 GO TO 1

4850 WRITE(6,62) MP,NTIM

4860 62 FORMAT('MP =',I4,' TIME INTERVAL NO.',I4,' GOT BUMPED BACK BEYOND THE ORIGIN')

CONTINUE
14900 NSKOUT=NSKOUT+1
14910 355 FORMAT ('0',7X, 'THE PARTICLE WAS KICKED BACK OUT OF THE REGION')
14920 IF(NTIM GT 10) GO TO 354
14930 GO TO 357
14940 362 WRITE(6,355)
14950 WRITE(6,356) NTIM, MP
14960 356 FORMAT('0',8X, 'DURING TIME INTERVAL',I4, ' THE PARTICLE WAS ALLOWED')
14970 * TO CONTINUE TRAVERSING ANYWAY',2X, 'PARTICLE NO WAS ',I4)
14980 357 YLOC=YLOC+SY+DSY
14990 NTIM=NTIM-1
15000 GO TO 1
15010 371 CONTINUE
15020 IF(XLOC .GE. REG60Pl GO TO 372
15030 IF(TT60(MP), EQ. 0.0) TT60(MP)=FLOAT(NTIM-1)*DELT-TREM
15040 GO TO 379
15050 372 CONTINUE
15060 IF(XLOC .GE. REG70Pl GO TO 373
15070 IF(TT60(MP), EQ. 0.0) TT60(MP)=FLOAT(NTIM-1)*DELT-TREM
15080 GO TO 379
15090 373 CONTINUE
15100 IF(XLOC .GE. REG80Pl GO TO 374
15110 IF(TT60(MP), EQ. 0.0) TT60(MP)=FLOAT(NTIM-1)*DELT-TREM
15120 GO TO 379
15130 374 CONTINUE
15140 IF(XLOC .GE. REG90Pl GO TO 375
15150 IF(TT60(MP), EQ. 0.0) TT60(MP)=FLOAT(NTIM-1)*DELT-TREM
15160 GO TO 379
15170 375 CONTINUE
15180 IF(TT60(MP), EQ. 0.0) TT60(MP)=FLOAT(NTIM-1)*DELT-TREM
15190 GO TO 379
15200 41 I=1
15210 YLOC=FLOAT(I)*YD(I)
15220 J=I
15230 XLOC=FLOAT(J)*YD(J)+(XD(J+1)/2.0)
15240 STY(MP)=XLOC
15250 TOTSX=XD(J+1)/2.0
15260 IF(MP .NE. 1) GO TO 1
15270 WRITE(6,25) DSEED
15280 WRITE(6,189) MP, NTIM, I, J, NI, SY, DSY, YLOC, SX, DSX, XLOC, TOTSX
15290 1 NTIM=NTIM+1
15300 IF(XLOC .LT. 0.0) GO TO 43
15310 IF(XLOC .GE. HALFWY) GO TO 371
15320 379 CONTINUE
15330 NBLKSX=0
15340 NBLKSY=0
15350 C RESTART THE I&J VALUES AT THE PARTICLE LOCATION
15360 J=INT(XLOC/XD(J+1)+1
15370 I=INT(YLOC/YD(I+1)+1
15380 C PARTICLE CANNOT MOVE BACKWARDS OR UPWARDS OUT OF THE REGION
15390 IF(J, GT. 1) GO TO 352
15400 J=2
15410 TOTSX=0.0
15420 352 CONTINUE
15430 IF(I, GT. 1) GO TO 351
15440 I=2
15450 YLOC=FLOAT(I)*YD(I)
15460 IF(MP .NE. 1) GO TO 351
15470 WRITE(6,25) DSEED
15480 C CALCULATE THE PARTICLE CONVECTIVE MOVEMENT IN THE X * Y DIRECTIONS
15490 351 SX=VX(I,J)*DELT
15500 SY=VY(I,J)*DELT
15500 C CALCULATE THE PARTICLE DISPERSIVE MOVEMENT IN THE X & Y DIRECTIONS
15500 RAND=NGNDF(DSEED)/6.0
15500 RANDT=NGNDF(DSEED)/6.0
15500 THETA=ATAN(SY/SX)
15500 VL=SQR(VX(I,J)**2+VY(I,J)**2)
DL=SGRT(6.3*D50*VL*DELT)*(RANOL)
DT=SGRT(6.3*D50*VL*DSPRAT*DELT)*(RANOT)
DSX=DL*COS(THETA)-DT*SIN(THETA)
DSY=DL*SIN(THETA)+DT*COS(THETA)
YLOC=YLOC-DSY
IF(NI.LE.1) GO TO 353
354 TOTSX=TOT SX+DSX
XLOC=XLOC+DSX
IF(NTIM.EQ.NESHT) GO TO 18
CONTINUE
IF(MP.LT.401) GO TO 15
WRITE(6,189) MP,NTIM,I,J,NI,SY,DSY,YLOC,SX,DSX,XLOC,TOTSX
CONTINUE
189 FORMAT (/I,7X,5I5.8F10.5)
CHECK TO SEE IF THE PARTICLE HAS MOVED LATERALLY TO THE NEXT BLOCK
IF(TOT SX.GE.XRD(J)) GO TO 3
CHECK TO SEE IF THE PARTICLE MOVED VERTICALLY OUT OF THE BLOCK
IF(NI.NE.I) GO TO 4
THE PARTICLE REMAINS IN THE SAME BLOCK SO START A NEW TIME INTERVAL
GO TO 1
PARTICLE HAS MOVED LATERALLY OUT OF THE BLOCK
3 NBLKXS=INT(TOT SX/XD(J))
VERIFY THAT IT HAS MOVED ONLY ONE BLOCK
IF(NBLKXS.GT.1) GO TO 2
PARTICLE HAS ONLY MOVED INTO THE NEXT BLOCK OR A SKIP WAS RECORDED
13 PREVX=TOT SX-SX-DSX
XREMB=XD(J)-PREVX
PRCTXM=XREMB/(SX+DSX)
PARD SX=PRCTXM*DSX
RXREMB=XREMB-PARD SX
TREM=DELT-(RXREMB/VX(I,J))
J=J+NBLKXS
PARTICLE HAS REACHED THE END OF THE REGION
IF(J.GE.NCOL) GO TO 74
PARTICLE HAS NOT REACHED THE END OF THE REGION
IF(J.NE.NCBAR) GO TO 361
PARTICLE HAS ENCOUNTERED THE BARRIER
J=J-NBLK XS
IF(J.GT.NCBAR) GO TO 361
XLOC=FLOAT(NCBAR)*XD(J)-(XLOC-FLOAT(NCBAR)*XD(J))
GO TO 359
361 XLOC=(FLOAT(NCBAR)*XD(J))*2.0-XLOC
358 TOT SX=XLOC-(FLOAT(J-1)*XD(J))
NTREB(MP)=NTREB(MP)+1
GO TO 1
PARTICLE HAS MOVED MORE THAN ONE BLOCK
TREM=(TOT SX-XD(J))/VX(I,J)
J=J+INT(TOT SX/XD(J))
IF(J.GE.NCOL) GO TO 74
31 CONTINUE
IF(NI.NE.I) GO TO 4
PARTICLE HAS NOT MOVED UP OR DOWN OUT OF THE BLOCK, SO NEW TIME INT.
GO TO 1
PARTICLE HAS MOVED MORE THAN ONE BLOCK
2 SKIPS=SKIPS+1.0
GO TO 13
PARTICLE HAS MOVED VERTICALLY AT LEAST ONE BLOCK
4 CONTINUE
CHECK TO VERIFY THAT THE PARTICLE HAS NOT MOVED BEYOND THE BOUNDARIES. CHECK THE UPPER BOUNDARY FIRST
IF(NI.LT.2) GO TO 6
C NOW CHECK THE LOWER BOUNDARY
NBLKSY=NI-1
IF(NI.GT.NROW-1) GO TO 7
C THE PARTICLE REMAINS IN THE REGION
I=NI
11 CONTINUE
C CHECK TO SEE IF THE PARTICLE MOVED MORE THAN ONE BLOCK
NBSY=IABS(NBLKSY)
IF(NBSY.GT.1) GO TO 5
C IT HADN'T, BUT SEE IF THE DISPLACEMENT HAS BEEN ADJUSTED
12 CONTINUE
IF(NBLKSY.NE.0) GO TO 1
C FIRST CHECK IF THE PARTICLE WAS REBOUNDED FROM THE BOUNDARY
IF(NI.LT.1) GO TO 1
IF(NI.GT.NROW-1) GO TO 1
C PARTICLE HADN'T MOVED LATERALLY, SO RECALCULATE DISPLACEMENTS
14 CONTINUE
IF(NBLKSY.LT.0) GO TO 14
PARTICLE MOVED DOWNWARD
YREMB=YD(I)*CIPREV>-YLOC
GO TO 16
PARTICLE MOVED UP
YREMB=YLOC-YD(I)*CIPREV+1
C NOW CALCULATE THE TIME REMAINING AFTER LEAVING BLOCK
C FIRST CHECK IF VY=0 CONTINUE
IF(VY(IPREV,J).EQ.0.0) GO TO 8
IT ISN'T SO CONTINUE
PRCTDY=YREMB/(SY+DSY)
PARDY=YREMB-PARDY
TREM=DELT-(YREMB/ABS(VY(IPREV,J)))
C NOW RECALCULATE DISPLACEMENTS
SX=VX(IPREV,J)*(DELT-TREM)+VX(I,J)*TREM
SY=VY(IPREV,J)*(DELT-TREM)+VY(I,J)*TREM
TOTSX=PREVX+SX+DSX
YLOC=PREVY-SY-DSY
XLOC=FLOAT(J)-1*XDCJ+TOTSX
NJ=INT(CXLOC/XDCJ)+1
IF(NJ.GE.NCOL) GO TO 7
C RECALCULATE DISPLACEMENTS
GO TO 11
16880 C PARTICLE MOVED MORE THAN ONE BLOCK BEYOND THE UPPER BOUNDARY
16890  17 YLOC=ABS(YLOC)+YD(I)*2.0
16900  I=INT(YLOC/YD(I))+1
16910 IF(J.GE.NCOL) GO TO 231
16920 GO TO 11
16930 C PARTICLE HIT THE LOWER BOUNDARY
16940  7 YLOC=FLOAT(NROWM1)*YD(I)*2.0-YLOC
16950  NTREB(MP)=NTREB(MP)+1
16960  I=INT(YLOC/YD(I))+1
16970 GO TO 11
16980 C PARTICLE HAS TRAVELED HALF THE ESTIMATED TIME REQUIRED TO TRAVERSE THE REGION. STORE THE X & Y LOCATIONS AT THIS TIME
16990 C PARTICLE REACHED THE END BEFORE END OF TIME CYCLE
17000  18 AVGYH=AVGYH+YLOC/FLOAT(NPTOT)
17010  AVGXH=AVGXH+XLOC/FLOAT(NPTOT)
17020  XLOCHT(MP)=XLOC
17030  YLOCHT(MP)=YLOC
17040 GO TO 19
17050 C PARTICLE REACHED THE END BEFORE ENDDD OF TIME CYCLE
17060  19 CONTINUE
17070  NCHK=NI
17080 IF(UPDISC.GT.0) NCHK=NROW-NI
17090 IF(NCHK.GT.NRCUTO) GO TO 61
17100 C PARTICLE HAS ENCOUNTERED THE CUTOFF, SO REBOUND IT
17110  XLOC=FLOAT(NCOLM1)*XD(J)-(XLOC-FLOAT(NCOLM1)*XD(J))
17120  NJ=INT(XLOC/XD(J))+1
17130  TOTSX=XLOC-(FLOAT(NJ-1)*XD(J))
17140  NTREB(MP)=NTREB(MP)+1
17150 GO TO 1
17160  61 TOTIM=FLOAT(NTIM)*DELT-TREM
17170  TOTM<MP)=TOTIM
17180  NSIM<MP)=NSIM
17190 CHECK TO SEE IF THE PARTICLE MOVED VERTICALLY OUT OF THE REGION
17200 C CHECK UPPER BOUNDARY
17210 IF(NI.LT.2) GO TO 6
17220 C CHECK LOWER BOUNDARY
17230 IF(NI.GT.NROWM1) GO TO 232
17240 GO TO 231
17250 C PARTICLE WENT BEYOND THE LOWER BOUNDARY
17260  232 YLOC=FLOAT(NROWM1)*YD(I)*2.0-YLOC
17270  I=INT(YLOC/YD(I))+1
17280  231 AVGYL=AVGYL/FLOAT(NPTOT)+AVGYL
17290  YLOCEN(MP)=YLOC
17300 C DETERMINE IF THE PARTICLE SKIPPED ANY BLOCKS DURING TRANSIT
17310 IF(SKIPS.EQ.0.0) GO TO 49
17320 NSKIPS=NSKIPS+INT(SKIPS)
17330 WRITE (6,47) NT,IV,SKIPS,NSIM
17340 IF(SKIPS.EQ.0) GO TO 49
17350 FORMAT ('0','5X,'DURING TRANSIT IN WAVE # ','I3,2X,'AND IY =','I3,2X,'THE PARTICLE SKIPPED AT LEAST ONE BLOCK','IF5.1,'TIMES','I3,2X,'SIM # IS ','I4')
17360  47 CONTINUE
17370 SIMTM=SIMTM+TOTIM/FLOAT(NPSIM)
17380  45 AVGTTT=AVGTTT+TOTIM/FLOAT(NPTOT)
17390  RATIO=FLOAT(NOSIM)/FLOAT(NSIM)
17400  RAVXH=AVGXH/RATIO
17410  RAVYH=AVGYH/RATIO
17420  RAVYL=AVGYL/RATIO
17430  RAVQTY=AVQTTY/RATIO
17440  RR01YM=RH01YM/RATIO
17450  RR02YM=RH02YM/RATIO
17460  RR03YM=RH03YM/RATIO
17500 RAR01Y=ARH01Y*RATIO
17510 RAR02Y=ARH02Y*RATIO
17520 RAR03Y=ARH03Y*RATIO
17530 RR1MKR=RO1MKR*RATIO
17540 RR1MKR=RO1MKR*RATIO
17550 RR1MKC=RO1MKC*RATIO
17560 RMK=AVGAMK*RATIO
17570 RSDK=AVGSDK*RATIO
17580 RTTTK=(TDIST*LENGTH)*(POROCT)/(DHEAD*RAVGGT)
17590 SIMKTT=(TDIST*LENGTH)*(POROCT)/(DHEAD*SIMTMT)
17600 HCSAT=(NSIM,7)*SIMKTT
17610 IF(NSIM,NE,1) GO TO 3500
17620 WRITE(6,32) NSIM,NSIM,RATIO,AVGXH,AVGYH,AVGXYL,AVGTTT
17630 WRITE(6,32) NSIM,MP,H,T,RAVGGY,RAVGGY,RAVGGY,RAVGGY,RTTTK
17640 WRITE(6,32) NSIM,NTIM,RAH,RSMK,RSK
17650 WRITE(6,23) NSIM,RQ01YM,RQ02YM,RQ03YM,RR1MKR,RR1MKC
17660 WRITE(6,23) NSIM,RAR01Y,RAR02Y,RAR03Y
17670 3500 CONTINUE
17680 WRITE(6,321) NSKOUT
17690 321 FORMAT('1','X','Y','THE NUMBER OF PARTICLES WHICH WERE KICKED BACK OUT
17700 [# OF THE REGION DURING INITIAL STAGES OF TRAVELING WERE '1',4)
17710 WRITE(6,46) NPOT,N link,NROWB,DELT,D50,DSRAT
17720 ANROWS=FLOAT(NROWT+NROWB)/2.0
17730 AVGSI=ANROWS*YD(I)+YD(I)/2.0
17740 WRITE(6,226) STXLOC,ENXLOC
17750 WRITE(6,224) AVGSI
17760 224 FORMAT('0',5X,'THE AVERAGE STARTING Y LOCATION WAS '1F10.4)
17770 226 FORMAT('0',5X,'PARTICLE TRAVEL WAS FROM X='1F10.4,
17780 # TO X='1F10.4.
17790 WRITE(6,222) THL,AVGHH,AVGHL,AVGHL,AVGTTT
17800 222 FORMAT('0',5X,'THE AVERAGE X & Y LOCATION AFTER '1F10.4,
17810 # 'DAYS IS '1F10.3,' AND '1F10.3,'7X,' THE AVERAGE Y LOCATION AT THE
17820 # 'DAYS IS '1F10.3,'2X,'AND TRAVEL TIME OF '1F10.5,'2X,'DAYS')
17830 46 FORMAT('0',5X,'A TOTAL OF '1F10.4,'PARTICLES WERE RELEASED UNIFORM
17840 # 'Y FROM THE NODE SPACING BELOW ROW '+1F10.2,9X,'TO HALF THE NODE
17850 $ 'SPACING BELOW ROW '+1F10.2,9X,'TO HALF THE NODE
17860 $ 'SPACING BELOW ROW '+1F10.2,9X,'TIME INTERVAL OF '+1F10.4,2X,
17870 $ 'DAYS'+1F10.2,9X,'AND MEDIAN GRAIN SIZE OF '+1F10.4,2X,
17880 $ 'Y RATIO OF '+7F5.3,' WAs UTILIZED. ')
17890 IF(NSKIPS.EQ.0) GO TO 223
17900 WRITE(6,221) NSKIPS
17910 221 FORMAT('0',5X,'DURING PARTICLE TRANSIT '1F10.4,'PARTICLES SKIPPED A
17920 # COMPLETE BLOCK')
17930 223 CONTINUE
17940 IF(STFLOC.EQ.0) GO TO 223
17950 WRITE(6,234)
17960 234 FORMAT('0',7X,'******** note: references to starting y location sho
17970 #uld really be starting x locations ******')
17980 230 CONTINUE
17990 WRITE(6,223) THL,THL
18000 223 FORMAT('1','25X,'SUMMARY TABLE OF TRAVEL TIME INFORMATION'1,1X,
18010 # 'PARTICLE 1X,'SIM 1X,'WAVE 6X,'Y LOCALIATIONS AT 4X,
18020 # 'LOC AT 2X,'TOTAL TIME (DAYS) FOR TRANSIT OF EACH X REGION
18030 # '9X,'LOC AT 1X,'2X,'TIMES'1,2X,'NUMBER'1,2X,'NO.'1X,'NUMBER'3,X,
18040 # 'START'1,4X,1F4.1,'DAYS'1,1F4.1,'DAYS'1,3X,'50X'1X,'60X'7X,
18050 # '70X'7X,'80X'7X,'90X'6X,'100X'6X,'END'4X,'REBOUNDED')
18060 DO 235 M=1,NPTOT
18070 WRITE(15,24) MP,NBSIM(MP),NNAV(MP),STY(MP),YLOCHT(MP),XLOCHT(MP),
18080 # YLOCHT(MP),TOCM(MP)
18090 235 FORMAT(15,MP,NBSIM(MP),NNAV(MP),STY(MP),YLOCHT(MP),XLOCHT(MP),
18100 # TTHW(MP),TT0(MP),TT70(MP),TT80(MP),TT90(MP),TOCM(MP),YLOCHT(MP),
18110 # NTRBK(MP)
18120 CALL MUNS (TOTH,NPTOT,AMN,SDV,COEVAR)
18130 WRITE(6,236) AMN,SDV,COEVAR
18140 236 FORMAT('0',5X,'MEAN TRAVEL TIME '1F10.5,'DAYS W/ STD DEV '1F10.5,
18150 $'FIO.5,' AND COV '1F10.5)
18160 TTTK=(TDIST*LENGTH)*(POROCT)/(DHEAD*AMN)
WRITE(6,238) TTTK
WRITE(6,239) FORM C 'O ', 5X, 'EFFECTIVE HYDRAULIC CONDUCTIVITY OF THE REGION ON BASIS OF TRAVEL TIME IS ',F10.5, ' FT/DAY')
WRITE(6,237) AMN, SDV, COEVAR
WRITE(6,238) AMN, SDV, COEVAR
WRITE(6,237) AMN, SDV, COEVAR
WRITE(6,238) AMN, SDV, COEVAR
WRITE(6,237) AMN, SDV, COEVAR
WRITE(6,238) AMN, SDV, COEVAR
WRITE(6,239) FORM C 'O •, 5X, 'MEAN Y COORDINATE AT END OF TRANSIT IS',F10.4,' WITH STD DEV. OF ',F10.4)
WRITE(6,237) AMN, SDV, COEVAR
WRITE(6,238) AMN, SDV, COEVAR
WRITE(6,237) AMN, SDV, COEVAR
WRITE(6,238) AMN, SDV, COEVAR
WRITE(6,239) FORM C 'O •, 5X, 'MEAN OF HYDRAULIC CONDUCTIVITY FOR A TOTAL OF '•I4,' WITH A MEAN STD. DEV. OF '•F10.41)
WRITE(6,237) AMN, SDV, COEVAR
WRITE(6,238) AMN, SDV, COEVAR
WRITE(6,237) AMN, SDV, COEVAR
WRITE(6,238) AMN, SDV, COEVAR
WRITE(6,239) FORM C 'O •, 5X, 'MEAN OF THE HEAD MATRIX COMPUTED FOR ALL THE SIMULATIONS IS •, F10.4,' WITH A MEAN STD. DEV. OF •F10.41)
WRITE(6,237) AMN, SDV, COEVAR
WRITE(6,238) AMN, SDV, COEVAR
WRITE(6,237) AMN, SDV, COEVAR
WRITE(6,238) AMN, SDV, COEVAR
WRITE(6,239) FORM C 'O •, 5X, 'MEAN OF THE HEAD MATRIX COMPUTED FOR ALL THE SIMULATIONS IS •, F10.4,' WITH A MEAN STD. DEV. OF •F10.41)
WRITE(6,237) AMN, SDV, COEVAR
WRITE(6,238) AMN, SDV, COEVAR
WRITE(6,237) AMN, SDV, COEVAR
WRITE(6,238) AMN, SDV, COEVAR
WRITE(6,239) FORM C 'O •, 5X, 'MEAN OF THE HEAD MATRIX COMPUTED FOR ALL THE SIMULATIONS IS •, F10.4,' WITH A MEAN STD. DEV. OF •F10.41)
WRITE(6,237) AMN, SDV, COEVAR
WRITE(6,238) AMN, SDV, COEVAR
WRITE(6,237) AMN, SDV, COEVAR
WRITE(6,238) AMN, SDV, COEVAR
WRITE(6,239) FORM C 'O •, 5X, 'MEAN OF THE HEAD MATRIX COMPUTED FOR ALL THE SIMULATIONS IS •, F10.4,' WITH A MEAN STD. DEV. OF •F10.41)
WRITE(6,237) AMN, SDV, COEVAR
WRITE(6,238) AMN, SDV, COEVAR
WRITE(6,237) AMN, SDV, COEVAR
WRITE(6,238) AMN, SDV, COEVAR
WRITE(6,239) FORM C 'O •, 5X, 'MEAN OF THE HEAD MATRIX COMPUTED FOR ALL THE SIMULATIONS IS •, F10.4,' WITH A MEAN STD. DEV. OF •F10.41)
WRITE(6,237) AMN, SDV, COEVAR
WRITE(6,238) AMN, SDV, COEVAR
WRITE(6,237) AMN, SDV, COEVAR
WRITE(6,238) AMN, SDV, COEVAR
WRITE(6,239) FORM C 'O •, 5X, 'MEAN OF THE HEAD MATRIX COMPUTED FOR ALL THE SIMULATIONS IS •, F10.4,' WITH A MEAN STD. DEV. OF •F10.41)
WRITE(6,237) AMN, SDV, COEVAR
WRITE(6,238) AMN, SDV, COEVAR
WRITE(6,237) AMN, SDV, COEVAR
WRITE(6,238) AMN, SDV, COEVAR
WRITE(6,239) FORM C 'O •, 5X, 'MEAN OF THE HEAD MATRIX COMPUTED FOR ALL THE SIMULATIONS IS •, F10.4,' WITH A MEAN STD. DEV. OF •F10.41)
WRITE(6,237) AMN, SDV, COEVAR
WRITE(6,238) AMN, SDV, COEVAR
WRITE(6,237) AMN, SDV, COEVAR
WRITE(6,238) AMN, SDV, COEVAR
WRITE(6,239) FORM C 'O •, 5X, 'MEAN OF THE HEAD MATRIX COMPUTED FOR ALL THE SIMULATIONS IS •, F10.4,' WITH A MEAN STD. DEV. OF •F10.41)
WRITE(6,237) AMN, SDV, COEVAR
WRITE(6,238) AMN, SDV, COEVAR
WRITE(6,237) AMN, SDV, COEVAR
WRITE(6,238) AMN, SDV, COEVAR
WRITE(6,239) FORM C 'O •, 5X, 'MEAN OF THE HEAD MATRIX COMPUTED FOR ALL THE SIMULATIONS IS •, F10.4,' WITH A MEAN STD. DEV. OF •F10.41)
WRITE(6,237) AMN, SDV, COEVAR
WRITE(6,238) AMN, SDV, COEVAR
WRITE(6,237) AMN, SDV, COEVAR
WRITE(6,238) AMN, SDV, COEVAR
WRITE(6,239) FORM C 'O •, 5X, 'MEAN OF THE HEAD MATRIX COMPUTED FOR ALL THE SIMULATIONS IS •, F10.4,' WITH A MEAN STD. DEV. OF •F10.41)
WRITE(6,237) AMN, SDV, COEVAR
WRITE(6,238) AMN, SDV, COEVAR
WRITE(6,237) AMN, SDV, COEVAR
WRITE(6,238) AMN, SDV, COEVAR
WRITE(6,239) FORM C 'O •, 5X, 'MEAN OF THE HEAD MATRIX COMPUTED FOR ALL THE SIMULATIONS IS •, F10.4,' WITH A MEAN STD. DEV. OF •F10.41)
ADD A WRITE STATEMENT HERE TO PRINT THE STREAM FUNCTION

DO 245 I=1,NROWM1
DO 245 J=1,NCOLM1
WRITE(6,204) STRFMN(I,J)

243 FORMAT('1',//,10X,'MEAN STEADY STATE STRFMN MATRIX FOR ',I4,
* SIMULATIONS')

245 CONTINUE
WRITE (6,228)

248 FORMAT('1',7X,'HYDRAULIC CONDUCTIVITY STATISTICS BY SIMULATION NUM
1BER',//,2X,'SIMULATION',//,1X,'STATISTICAL MEANS',//2X,'STANDARD',4X,
1EFF K VALUE ON BASIS OF',//,4X,'NUMBER',5X,'ARITHMETIC',2X,
1*GEOMETRIC',4X,'HARMONIC',4X,'DEVIATION',3X,'FLOW QUANTITY',1X,
*TRAVEL TIME')

WRITE OUT CORR & HYD COND STATS AND STORE ON A DISK DATA FILE

DO 247 I=L NOSIM
WRITE(6,217) (HCSTAT(I,J),J=1,9)
WRITE(6,218) (HCSTAT(I,J),J=1,9)
WRITE(6,219) (HCSTAT(I,J),J=1,9)
WRITE(6,222) (CSTATS(I,J),J=1,17)
WRITE(6,224) (CSTATS(I,J),J=1,17)
WRITE(6,229) (CSTATS(I,J),J=1,17)

DO 249 I=L NOSIM
WRITE(6,220) I,AMEAN(J)> ,ASDV(J)
DO 251 J=2,17
DO 251 I=L NOSIM
M=M+1
VALC(M)=CSTATS(I,J)
CONTINUE
CALL MUNSD(VALC,NOSIM,AMN,SDV,COEVAR)
AMEAN<J>=AMN
ASDV<J>=SDV

WRITE(6,223) J,AMEAN(J),ASDV(J)
WRITE(6,23) I,XISCAL<I>,YISCAL<I>

THE MEAN INTEGRAL SCALES IN THE X FOR THESIM NO $IRECTION$ AND Y DIRECTIONS X DIRECT, Y D
CALL MUNSD (XISCAL, NOSIM, AMN, SDV, COEVAR)
CALL MUNSD (YISCAL, NOSIM, AMNA, SDVA, COVA)
WRITE (6,256) AMN, SDV, AMNA, SDVA
256 FORMAT ('0', 2X, 'THE MEAN INTEGRAL SCALE IS ', F6.2, ' FEET IN THE X DI', F6.2, ' FEET IN THE Y DIRE', 'TION WITH A SD=', F6.2)
DO 257 MP=1, NPTOT
WRITE(19,256) MP, NBSIM(MP), STY(MP), TTHW(MP), TT60(MP), TT70(MP), TT80(MP), TT90(MP)
STOP
END
*******************************************************************
SUBROUTINE FOR COMPUTATION OF MEAN & STD DEV., ETC
OF A SINGLE SUBSCRIPTED VARIABLE ARRAY
*******************************************************************
SUBROUTINE MUNSD (VAL, N, AMN, SD, COEVAR)
REAL VALCN>
5 FORMAT (10,5F10.5)
CALCULATE THE MEAN VALUE OF THE ARRAY
7690 SUMVAL=0.0
7700 DO 10 I=1, N
7710 SUMVAL=SUMVAL+VAL(I)
7720 10 CONTINUE
7730 AMN=SUMVAL/(FLOAT(N))
7740 C
7750 C NOW CALCULATE THE STANDARD DEVIATION, VARIANCE & COEF. OF VARIATION
7760 SUMDIS=0.0
7770 DO 20 I=1, N
7780 SUMDIS=SUMDIS+DISPER
7790 20 CONTINUE
7800 VAR=SUMDIS/(FLOAT(N))-1.0
7802 SD=SQR(T(VAR)
7803 COEVAR=SD/AMN
7804 RETURN
7805 END
7806 C
7807 C
7808 C
7809 C
7810 C
7811 C
7812 C
7813 C
7814 C
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20000 DO 20 J=1, L
20010 SUMVAL=SUMVAL+VAL(I, J)
20020 10 CONTINUE
20030 AMN=SUMVAL/(FLOAT(N*L))
20040 C
20050 C NOW CALCULATE THE STANDARD DEVIATION, VARIANCE & COEF. OF VARIATION
20060 SUMDIS=0.0
20070 DO 20 I=1, N
20080 DO 20 J=1, L
20090 DISPER=(VAL(I, J)-AMN)**2
20100 SUMDIS=SUMDIS+DISPER
20110 20 CONTINUE
20120 VAR=SUMDIS/(FLOAT(N*L))-1.0
20130 SD=SQR(T(VAR)
20140 COEVAR=SD/AMN
20150 RETURN
20160 END
***SUBROUTINE TO CALCULATE THE AUTOCORRELATION OF AN ARRAY OF ORDERED VALUES (SINGLE SUBSCRIPTED ARRAY)***

```fortran
SUBROUTINE AUGAR (VAL, N, AMN, SD, LAGS, RHO)
  REAL VAL(N), RHO(LAGS)
  5 FORMAT (2I10, 6F10.5)
  DO 20 NL=1, LAGS
  COV=0.0
  DO 10 I=1, N
  DISP=VAL(I)-AMN
  RHO(CNL)=COV/SD**2
  CONTINUE
  RETURN
END
```

***SUBROUTINE TO CALCULATE THE AUTOCORRELATION OF AN ARRAY OF ORDERED VALUES FOR A LAG OF ONE AHEAD & BELOW***

```fortran
SUBROUTINE AUGAR2 (VAL, N, L, AMN, SD, RHO)
  REAL VAL(32, 62), RHO(N), AMN(N), SD(N)
  15 FORMAT ('O', I3, 2X, 10F12.4/C6X, 10F12.4)
  CALCULATE THE MEAN VALUE OF EACH ROW OF THE ARRAY
  DO 30 I=1, N
  SUMVALC(I)=0.0
  DO 30 J=1, L
  SUMVAL(I)+VAL(I, J)
  30 CONTINUE
  AMN(I)=SUMVAL(I)/FLOAT(L)
  NOW CALCULATE THE STANDARD DEVIATION OF EACH ROW
  DO 50 I=1, N
  SUMDIS(I)=0.0
  DD 50 J=1, L
  DISPER=(VAL(I, J)-AMN(I))**2
  SUMDIS(I)=SUMDIS(I)+DISPER
  50 CONTINUE
  VAR=SUMDIS(I)/FLOAT(L)-1.0
  SD(I)=DSRT(VAR)
  NM1=N-1
  LM1=L-1
  DO 20 I=1, NM1
  COV=0.0
  DD 10 J=1, LM1
  DISP=VAL(I, J)-AMN(I)
  ACOV=DISP*DISP/FLOAT(LM1)
  10 CONTINUE
  RHO(I)=COV/(SD(I)*SD(I+1))
  RETURN
END
```